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DEVELOPMENT OF A MULTI-MECHANISTIC
TRIPLE-POROSITY, TRIPLE-PERMEABILITY COMPOSITIONAL MODEL
FOR UNCONVENTIONAL RESERVOIRS

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ABSTRACT

Most existing compositional reservoir simulators often model fractures using local grid refinement, unstructured-grid, or fine-grid models. Modeling different scales of fractures requires a large number of grid blocks to capture the heterogeneity of the formation. Using a large number of grid blocks presents computational challenges, even with today’s powerful processors. An enhanced matrix permeability on the grid block that hosts short-scale fractures is commonly used to eliminate natural fractures and simplify the model. Additionally, several existing multi-porosity models may not be able to capture heterogeneity and flow behavior in different porosity domains. Sequential flow assumption is frequently made in their models. Flows between different porosity types are not fully coupled, and in some model, a simplified inter-porosity transmissibility function is used for any porosity pairs.

The oil and gas reserves and flow of reservoir fluids are strongly dependent on phase behavior. Large capillary pressure values are encountered in tight formations such as tight-rocks and shales. The tiny pore throats in these formations result in large capillary pressure. The effect of capillary pressure in tight formations can significantly impact the fluid phase behaviors in the reservoir during production and enhanced oil recovery (EOR) processes. Not incorporating this effect into the simulation can result in an inaccurate estimation of ultimate recovery as well as inefficient design and implementation of EOR techniques. In spite of this, the effect of capillary pressure on phase behavior in tight reservoirs has not been well studied using compositional simulation, especially for hydraulically fractured reservoirs.

In this research, a fully implicit, multi-mechanistic, fully coupled, triple-porosity, triple-permeability compositional model has been developed for unconventional reservoirs. The hydraulically fractured tight rock and shale reservoir is treated as a triple-porosity system
consisting of matrix blocks, natural fractures (micro fractures), and hydraulic fractures (macro fractures). Small-scale fractures are handled by a dual-continuum model. An embedded discrete fracture model is used to effectively and efficiently capture the flow dynamics of hydraulic fractures at any orientations, honoring the complexity and heterogeneity of the fracture networks. The triple-porosity model enables us to assign reservoir properties corresponding to the porosity type. The flows in three porosity types are fully coupled without making the assumption of sequential flow. The inter-porosity fluid transfer honors the geometry of the intersecting porosity pair. The development of the proposed numerical model incorporates the effect of capillary pressure on phase behavior. The transport of hydrocarbon follows a multi-mechanistic flow mechanism that is driven by pressure and concentration fields.

The simulator has been validated with analytical solutions and a commercial reservoir simulator for a single-porosity model and a dual-porosity, dual-permeability model, both with and without grid refinement. With the proposed model, we can accurately capture major physics of transport phenomena that have been done to date and have the most realistic modeling of fluid flow in hydraulically fractured tight rock and shale reservoirs. The simulator is used in parametric studies to investigate the production performance from hydraulically fractured reservoirs under different modeling techniques and the effect of capillary pressure on phase behavior on reserves and ultimate recovery. The simulator is used to study the impact of inter-porosity transport on the recovery and fluid transport and phase behavior in hydraulically fractured tight rocks and shale formations under high capillary pressure. The outcomes of this project are an improved understanding of phase behavior and fluid flow in hydraulically fractured shale and tight rocks and an increased accuracy of the production prediction and ultimate recovery.
Table of Contents

List of Figures .................................................................................................................... ix
List of Tables ....................................................................................................................... xvii
Nomenclature .................................................................................................................... xix
Acknowledgements ........................................................................................................... xxviii

Chapter 1 Introduction ........................................................................................................ 1

Chapter 2 Literature Review ............................................................................................... 4
  2.1 Formulation of Compositional Simulation ............................................................... 4
  2.2 Modeling of Naturally Fractured Reservoirs ............................................................. 5
    2.2.1 Shale Modeling ................................................................................................. 5
    2.2.2 Gas Adsorption / Desorption ......................................................................... 8
  2.3 Effect of Nano-pore Capillary Pressure on Phase Behaviors .................................... 9
  2.4 Embedded Discrete Fracture Model ....................................................................... 14
  2.5 Stimulated Reservoir Volume Model ................................................................... 17
  2.6 Highlights of the Chapter ...................................................................................... 18

Chapter 3 Problem Statement .......................................................................................... 20

Chapter 4 Formulation of the Compositional Model ....................................................... 23
  4.1 Governing Flow Equations ..................................................................................... 23
    4.1.1 Overall Compositional Balance ..................................................................... 24
    4.1.2 Conservation Equations in Cartesian Coordinates ..................................... 24
    4.1.3 Three-phase (Oil, Gas, Water) Nc-component Flow Equations ............... 25
  4.2 Phase Behavior Model ............................................................................................. 26
    4.2.1 Generalized Cubic Equation of State ......................................................... 26
    4.2.2 Rachford-Rice Objective Function .............................................................. 27
    4.2.3 Successive Substitution Method .................................................................. 28
    4.2.4 Minimum-variables Newton-Raphson Algorithm .................................... 29
    4.2.5 Fugacity ........................................................................................................ 31
    4.2.6 Phase Stability ............................................................................................. 32
  4.3 Compressibility of Formation ............................................................................... 34
  4.4 Capillary Pressure .................................................................................................. 36
  4.5 Wettability .............................................................................................................. 36
    4.5.1 Water-wet Reservoir ................................................................................... 37
    4.5.2 Oil-wet Reservoir ...................................................................................... 37
  4.6 Relative Permeability ............................................................................................... 38
  4.7 Diffusion .................................................................................................................. 38
Chapter 7 Model Validation ................................................................. 101

7.1 Validation of Single-porosity, Single-permeability Model ......................... 102
  7.1.1 Primary Depletion ................................................................. 102
  7.1.2 Water Injection ................................................................. 106
  7.1.3 Gas Injection ................................................................. 112

7.2 Validation of Dual-porosity, Single-permeability Model ............................ 121
7.3 Validation of Dual-porosity, Dual-permeability Model .............................. 126
7.4 Validation of Embedded Discrete Fracture Model ................................. 131
7.5 Highlights of the Chapter .................................................................. 134
Chapter 8 Simulation of Multi-mechanistic Triple-porosity Triple-permeability Compositional Model .......................................................... 135

8.1 Comparison with the single-porosity model coupled with EDFM ....................... 135
8.2 Comparison with Dual-porosity Models .......................................................... 140
8.3 Parametric Study of the Triple-porosity Model ............................................... 145
  8.3.1 Multi-mechanistic Flow ............................................................................. 146
  8.3.2 Natural Fracture-Hydraulic Fracture Intersecting Coefficient ...................... 148
  8.3.3 Fully Coupled Triple-porosity Model ...................................................... 151
8.4 Rate Transient Analysis of the Triple-porosity Model ........................................ 159
8.5 Highlights of the Chapter ............................................................................... 162

Chapter 9 Effect of Capillary Pressure on Phase Behavior ........................................ 164

  9.1 Effect of Capillary Pressure on Original Oil and Gas in Place and Cumulative
     Production ......................................................................................................... 167
    9.1.1 Bakken Oil ............................................................................................... 167
    9.1.2 Eagle Ford Oil .......................................................................................... 172
  9.2 Handling of Large Capillary Pressure in the Well Model .................................... 178
    9.2.1 Use of Small Grid Block Size ................................................................. 179
    9.2.2 Ignoring Capillary Pressure in the Well Model ........................................ 182
    9.2.3 Use Wetting Phase Pressure as Reference Phase ...................................... 188
  9.3 Simulation of EDFM Incorporating the Effect of Capillary Pressure ................. 188
    9.3.1 Grid Convergence ..................................................................................... 189
    9.3.2 Three-stage Hydraulically Fractured Reservoir ....................................... 191
    9.3.3 Three-stage Hydraulically Fracture Reservoir with Branch Fractures ......... 194
    9.3.4 Fractured Well with Fracture Network .................................................. 197
  9.4 Simulation of Dual-porosity Model Incorporating the Effect of Capillary
     Pressure ............................................................................................................ 200
  9.5 Simulation of Triple-porosity Model Incorporating the Effect of Capillary
     Pressure ............................................................................................................ 205
    9.5.1 TPTK Model without Enhanced Fracture Permeability Due to Hydraulic
           Fracturing ..................................................................................................... 205
    9.5.2 Simulation of Three-stage Hydraulically Fractured Reservoir with
           Fracture Network using TPTK ................................................................. 208
  9.6 Highlights of the Chapter ............................................................................... 212

Chapter 10 Summary and Conclusions .................................................................... 215

References .............................................................................................................. 220

Appendix A Derivation of Generalized Flow Equation ............................................. 228

  A.1 Conservation Equations for a Component in a Phase ...................................... 228
  A.2 Overall Compositional Balance ................................................................. 231
  A.3 Compositional Conservation Equation in Cartesian Coordinates ................. 233
  A.4 Inventory of Equation and Unknowns ...................................................... 234
  A.5 Three-phase (oil, gas, water) Flow Equations ............................................ 235
Appendix B Thermodynamic Model ................................................................. 239

B.1 Stability Analysis Based on Minimization of Tangent Plane Distance........ 239
B.2 Flash Calculation Based on Minimum-variable Newton-Raphson Protocol .... 242
B.3 Molecular Weight ....................................................................................... 243
B.4 Density ....................................................................................................... 243
   B.4.1 Hydrocarbon ....................................................................................... 243
   B.4.2 Water .................................................................................................. 244
B.5 Viscosity .................................................................................................... 244
B.6 Saturation ................................................................................................. 246
B.7 Formation Volume Factor ......................................................................... 246

Appendix C Analytical Differentiation.............................................................. 247

C.1 Derivatives of Hydrocarbon Conservation Equations ................................. 247
   C.1.1 Transport Terms ............................................................................... 247
   C.1.2 Accumulation Term ......................................................................... 253
   C.1.3 Source/Sink Term ........................................................................... 254
C.2 Derivative of Water Conservation Equation ............................................. 259
   C.2.1 Transport Terms ............................................................................... 259
   C.2.2 Accumulation Term ......................................................................... 261
   C.2.3 Source/Sink Term ........................................................................... 262
C.3 Derivatives of Phase Equilibrium Constraints .......................................... 263
   C.3.1 Derivative with respect to $P_o$ ......................................................... 263
   C.3.2 Derivative with respect to $x_i$ ........................................................ 264
   C.3.3 Derivative with respect to $y_i$ ........................................................ 265
C.4 Derivatives of Effect of Capillary Pressure on Phase Behaviors ............... 266
C.5 Derivatives of Embedded Discrete Fracture Model .................................... 267
   C.5.1 NNC Source Term for Hydrocarbon Components ......................... 267
   C.5.2 NNC Source Term for Water .......................................................... 270
   C.5.3 Fracture-Fracture Intersection ......................................................... 272
C.6 Miscellaneous Derivatives ....................................................................... 272
   C.6.1 Permeability .................................................................................... 272
   C.6.2 Relative Permeability ..................................................................... 272
   C.6.3 Capillary Pressure .......................................................................... 273
   C.6.4 Compressibility of Formation ......................................................... 274
   C.6.5 Phase Equilibrium .......................................................................... 274

Appendix D User Guide................................................................................... 276

D.1 Model Descriptions .................................................................................. 276
D.2 Reservoir Descriptions .......................................................................... 277
D.3 Well Descriptions .................................................................................. 281
D.4 Rock-Fluid Properties ........................................................................... 283
D.5 Component ............................................................................................ 283
D.6 Numerical Control .................................................................................. 286
D.7 Output Control ....................................................................................... 287
List of Figures

Figure 2-1: Flow mechanism of coalbed methane and shale gas (Remner, 1986) .................. 9
Figure 2-2: Stimulated reservoir volume around a horizontal well in a thick formation ....... 17
Figure 4-1: Illustration of wettability distribution in a triangular pore for (a) water-wet case and (b) oil-wet case (Zhou and Blunt, 1998) ............................................................ 37
Figure 4-2: Steps in solving thermodynamic equilibrium for adsorption capacity and adsorbed composition ........................................................................................................ 44
Figure 5-1: Overall flow chart of the simulator ................................................................. 75
Figure 6-1: Calculation of capillary pressure on phase behavior .................................... 81
Figure 6-2: Flow chart for modified negative flash algorithm ........................................ 82
Figure 6-3: Non-neighboring connection ........................................................................ 84
Figure 6-4: Transverse fracture intersects a well ......................................................... 88
Figure 6-5: Flow schematic of the triple-porosity, triple-permeability model .............. 91
Figure 7-1: Relative permeability data for validation tests ............................................ 102
Figure 7-2: Reservoir model for validation of primary depletion .................................. 103
Figure 7-3: Validation of primary depletion in single-porosity model – oil production rate comparison .................................................................................................................. 104
Figure 7-4: Validation of primary depletion in single-porosity model – gas production rate comparison .................................................................................................................. 104
Figure 7-5: Validation of primary depletion in single-porosity model – water production rate comparison .................................................................................................................. 105
Figure 7-6: Validation of primary depletion in single-porosity model – well block pressure comparison .................................................................................................................. 105
Figure 7-7: Reservoir model for validation of water injection ....................................... 106
Figure 7-8: Validation of water injection in single-porosity model – Well-1 oil production rate comparison .................................................................................................................. 107
Figure 7-9: Validation of water injection in single-porosity model – Well-1 gas production rate comparison ................................................................. 108

Figure 7-10: Validation of water injection in single-porosity model – Well-1 water production rate comparison ................................................................. 108

Figure 7-11: Validation of water injection in single-porosity model – Well-1 producer well block pressure comparison ................................................................. 109

Figure 7-12: Validation of water injection in single-porosity model – Well-2 oil production rate comparison ................................................................. 109

Figure 7-13: Validation of water injection in single-porosity model – Well-2 gas production rate comparison ................................................................. 110

Figure 7-14: Validation of water injection in single-porosity model – Well-2 water production rate comparison ................................................................. 110

Figure 7-15: Validation of water injection in single-porosity model – Well-2 producer well block pressure comparison ................................................................. 111

Figure 7-16: Validation of water injection in single-porosity model – Well-3 injector well block pressure comparison ................................................................. 111

Figure 7-17: Validation of water injection in single-porosity model – Well-3 injector well bottom-hole pressure comparison ................................................................. 112

Figure 7-18: Reservoir model for validation of gas injection ............................................. 114

Figure 7-19: Case 1 – validation of gas injection under constant injection rate in single-porosity model – oil production rate comparison ................................................................. 114

Figure 7-20: Case 1 – validation of gas injection under constant injection rate in single-porosity model – gas production rate comparison ................................................................. 115

Figure 7-21: Case 1 – validation of gas injection under constant injection rate in single-porosity model – water production rate comparison ................................................................. 115

Figure 7-22: Case 1 – validation of gas injection under constant injection rate in single-porosity model – producer well block pressure comparison ................................................................. 116

Figure 7-23: Validation of gas injection under constant injection rate in single-porosity model – injector well block pressure comparison ................................................................. 116

Figure 7-24: Validation of gas injection under constant injection rate in single-porosity model – gas injection rate at reservoir condition comparison ................................................................. 117

Figure 7-25: Validation of gas injection under constant injection rate in single-porosity model – injector bottom-hole pressure comparison ................................................................. 117
Figure 7-26: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – oil production rate comparison ........................................... 118

Figure 7-27: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – gas production rate comparison ........................................... 118

Figure 7-28: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – water production rate comparison ................................... 119

Figure 7-29: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – producer well block pressure comparison ...................... 119

Figure 7-30: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – gas injection rate at surface condition comparison .................. 120

Figure 7-31: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – gas injection rate at reservoir condition comparison ............... 120

Figure 7-32: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – injector well block pressure comparison ......................... 121

Figure 7-33: Reservoir model for validation of DPSK model ........................................... 121

Figure 7-34: DPSK validation – Well-1 oil production rate comparison ......................... 122

Figure 7-35: DPSK validation – Well-1 gas production rate comparison ......................... 123

Figure 7-36: DPSK validation – Well-1 water production rate comparison ..................... 123

Figure 7-37: DPSK validation – Well-1 well block pressure comparison ....................... 124

Figure 7-38: DPSK validation – Well-2 oil production rate comparison ......................... 124

Figure 7-39: DPSK validation – Well-2 gas production rate comparison ......................... 125

Figure 7-40: DPSK validation – Well-2 water production rate comparison ..................... 125

Figure 7-41: DPSK validation – Well-2 well block pressure comparison ....................... 126

Figure 7-42: DPDK validation – Well-1 oil production rate comparison ......................... 127

Figure 7-43: DPDK validation – Well-1 gas production rate comparison ......................... 127

Figure 7-44: DPDK validation – Well-1 water production rate comparison ..................... 128

Figure 7-45: DPDK validation – Well-1 well block pressure comparison ....................... 128

Figure 7-46: DPDK validation – Well-2 oil production rate comparison ......................... 129

Figure 7-47: DPDK validation – Well-2 gas production rate comparison ....................... 129
Figure 7-48: DPDK validation – Well-2 water production rate comparison 

Figure 7-49: DPDK validation – Well-2 well block pressure comparison 

Figure 7-50: Reservoir model for EDFM validation run 

Figure 7-51: EDFM validation – oil production rate comparison 

Figure 7-52: EDFM validation – gas production rate comparison 

Figure 7-53: EDFM validation – water production rate comparison 

Figure 8-1: Three-stage hydraulically fractured reservoir model for study of the TPTK model. Each grid block contains matrix and natural fracture 

Figure 8-2: Oil production rate comparison between EDFM and TPTK model 

Figure 8-3: Cumulative oil production comparison between EDFM and TPTK model 

Figure 8-4: Pressure distribution after 365 days for EDFM-AVE and TPTK model 

Figure 8-5: Oil production rate comparison between DPDK and DPSK models 

Figure 8-6: Grid block that hosts a segment of hydraulic fracture. (a) Grid refinement is used to represent discrete fracture in the DPDK model; (b) Discrete fracture is embedded in the grid block 

Figure 8-7: Oil production rate comparison between the DPDK and TPTK models 

Figure 8-8: Pressure distribution after 365 days for the DPDK and TPTK models 

Figure 8-9: Oil production rate comparison between DPDK and TPTK models with coefficient for effective intersecting area coefficient of 1 

Figure 8-10: Three-stage hydraulically fractured reservoir with fracture network 

Figure 8-11: Oil production rate profiles for parametric study on the natural fracture-hydraulic fracture communication coefficient of 0.01, 0.1, and 1 

Figure 8-12: Cumulative oil production profiles for parametric study on the natural fracture-hydraulic fracture communication coefficient of 0.01, 0.1, and 1 

Figure 8-13: Oil production rate comparison between fully coupled and sequential flow models for two-component fluid in three-stage hydraulically fractured reservoir 

Figure 8-14: Cumulative oil production comparison between fully coupled and sequential flow models for two-component fluid in three-stage hydraulically fractured reservoir 

Figure 8-15: Oil production rate comparison between fully coupled and sequential flow models for Bakken oil in three-stage hydraulically fractured reservoir
Figure 8-16: Cumulative oil production comparison between fully coupled and sequential flow models for Bakken oil in three-stage hydraulically fractured reservoir. 155

Figure 8-17: Oil production rate comparison between fully coupled and sequential flow models for Eagle Ford oil in three-stage hydraulically fractured reservoir. 157

Figure 8-18: Cumulative oil production comparison between fully coupled and sequential flow models for Eagle Ford oil in three-stage hydraulically fractured reservoir. 157

Figure 8-19: Oil production rates of fully coupled and sequential flow models for Bakken oil in three-stage hydraulically fractured reservoir with fracture network. 158

Figure 8-21: Log-log plot of oil production rate for natural fracture permeability ranging from 0.001 mD to 1 mD and a fixed matrix permeability of 100 nD. 161

Figure 8-22: Log-log plot of oil production rate for matrix permeability ranging from 10-1,000 nD and a fixed natural fracture permeability of 0.01 mD. 162

Figure 9-1: Relative permeability for Bakken formation. 168

Figure 9-2: Capillary pressure for Bakken formation. 168

Figure 9-3: Phase envelope of Bakken oil. 169

Figure 9-4: Effect of capillary pressure on OOIP estimation for Bakken oil at reservoir temperature of 240 °F. 171

Figure 9-5: Effect of capillary pressure on cumulative oil production after 1 year for Bakken oil at reservoir temperature of 240 °F. 171

Figure 9-6: Cumulative oil production after 10 years of production for initial reservoir pressure of 3,500 psia for Bakken oil. 172

Figure 9-7: Relative permeability for Eagle Ford formation (Agboada and Ahamadi, 2013). 173

Figure 9-8: Capillary pressure for Eagle Ford formation. 173

Figure 9-9: Phase envelope of Eagle Ford oil. 175

Figure 9-10: Effect of capillary pressure on OOIP estimation for Eagle Ford oil at reservoir temperature of 237 °F. 176

Figure 9-11: Effect of capillary pressure on cumulative oil production after 1 year for Eagle Ford oil at reservoir temperature of 237 °F. 177

Figure 9-12: Cumulative oil production after 10 years of production for initial reservoir pressure of 3,000 psia for Eagle Ford oil. 178
Figure 9-13: Half of the reservoir model for study of impact of large capillary pressure near the wellbore ................................................................. 179

Figure 9-14: Water phase pressure in the well grid block for 5-ft, 10-ft, 15-ft, 25-ft, and 5-ft grid block sizes as a function of time ........................................ 180

Figure 9-15: Water phase pressure in the well grid block for 5-ft, 10-ft, 15-ft, 25-ft, and 50-ft grid block sizes after 365 days of production .................................. 181

Figure 9-16: Different phase pressures in the well grid block for 5-ft grid block sizes at the end of the simulation .......................................................... 182

Figure 9-17: Oil phase pressure in the well grid block for different well models after 365 days of production ............................................................. 184

Figure 9-18: Gas phase pressure in the well grid block for different well models after 365 days of production ............................................................. 185

Figure 9-19: Water phase pressure in the well grid block for different well models after 365 days of production ............................................................. 185

Figure 9-20: Oil production comparison with and without consideration of capillary pressure in the wellbore model ......................................................... 186

Figure 9-21: Gas production comparison with and without consideration of capillary pressure in the wellbore model ......................................................... 187

Figure 9-22: Water production comparison with and without consideration of capillary pressure in the wellbore model ......................................................... 187

Figure 9-23: Reservoir model for simulation study of fractured reservoir .................. 190

Figure 9-24: Grid convergence – oil production rate for coarse, base, and 3x refinement ..... 190

Figure 9-25: Grid convergence – cumulative oil production for coarse, base and 3x refinement ......................................................................................... 191

Figure 9-26: Case 1 – Pressure distribution after 30, 90, 180, and 365 days ................ 192

Figure 9-27: Case 1 – oil production rate and cumulative oil production .................... 193

Figure 9-28: Case 1 – gas production rate and cumulative gas production .................... 193

Figure 9-29: Case 2 – Pressure distribution after 30, 90, 180, and 365 days ................ 195

Figure 9-30: Case 2 – oil production rate and cumulative oil production .................... 196

Figure 9-31: Case 2 – gas production rate and cumulative gas production .................... 196

Figure 9-32: Reservoir model for case 3 .................................................................. 197
Figure 9-33: Case 3 – Pressure distribution after 30, 90, 180, and 365 days ................. 198

Figure 9-34: Case 3 – oil production rate and cumulative oil production ...................... 199

Figure 9-35: Case 3 – gas production rate and cumulative gas production ...................... 199

Figure 9-36: Natural fracture permeability of the DPDK model ....................................... 201

Figure 9-37: Oil production rate comparison at initial reservoir pressure of 5,500 psia for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior in both matrix and natural fracture ....................................................... 202

Figure 9-38: Cumulative oil production comparison at initial reservoir pressure of 5,500 psia for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior in both matrix and natural fracture ....................................................... 202

Figure 9-39: Cumulative oil production comparison at initial reservoir pressure of 5,500 psia for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior only in the matrix ................................................................. 203

Figure 9-40: Cumulative oil production comparison at initial reservoir pressure of 3,000 psia for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior only in the matrix ................................................................. 204

Figure 9-41: Oil production rate comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture ...... 207

Figure 9-42: Cumulative oil production comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture ................................................................. 207

Figure 9-43: Cumulative gas production comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture ................................................................................. 208

Figure 9-44: Natural fracture permeability of the TPTK model ....................................... 209

Figure 9-45: Case 1 – Oil production rate comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture ................................................................................. 210

Figure 9-46: Case 1 – Cumulative oil production comparison for simulation of the TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture ................................................................................. 210

Figure 9-47: Case 2 – Oil production rate comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix ...................... 211
Figure 9-48: Case 2 – Cumulative oil production comparison for simulation of the TPTK model incorporating the effect of capillary pressure on phase behavior in matrix. 212

Figure A-1: Arbitrary control volume in flow motion. 228

Figure A-2: Example of arbitrary function showing integrand must be zero. 230

Figure A-3: Elemental Control Volume. 233
List of Tables

Table 4-1: Equation of State constant parameters .......................................................... 27
Table 6-1: Regression coefficients for Fanchi (1990) correlation ..................................... 83
Table 7-1: Compositional data for 6-component fluid for validation tests ...................... 101
Table 7-2: Compositional data for 2-component fluid for validation tests ...................... 101
Table 7-3: Input data for validation test for primary depletion in single-porosity model ...... 103
Table 7-4: Input data for validation test for water injection in single-porosity model......... 106
Table 7-5: Input data for validation test for gas injection in single-porosity model.......... 113
Table 7-6: Input data for validation test for dual-porosity, single-permeability model ....... 122
Table 7-7: Input data for validation test for embedded discrete fracture model............... 131
Table 8-1: Parameters for comparison of EDFM with TPTK model................................ 137
Table 8-2: Parameters for comparison of DPDK model with TPTK model ..................... 142
Table 8-3: Input Data for Study of Multi-mechanistic Flow of the TPTK model ............... 147
Table 8-4: Oil and gas production comparison showing the effect of diffusion on recovery ................................................................................................................. 148
Table 8-5: Input data for study of natural fracture-hydraulic fracture intersecting coefficient of the TPTK model ................................................................................. 149
Table 8-6: Comparison of cumulative oil production from natural fracture-hydraulic fracture communication coefficient ranging from 0.01 to 1 ......................................................... 151
Table 8-7: Input data for production analysis of the TPTK model using the two-component fluid .................................................................................................................. 152
Table 8-8: Input data for production analysis of the TPTK model using Bakken oil ........ 154
Table 8-9: Input data for production analysis of the TPTK model using Eagle Ford oil ...... 156
Table 8-10: Input data for rate transient analysis of the TPTK model............................. 160
Table 9-1: Compositional data for Bakken oil (Nojabaei et al., 2013) .............................. 164
Table 9-2: Binary interaction parameters for Bakken oil (Nojabaei et al., 2013) .................. 165
Table 9-3: Compositional data for Eagle Ford oil (Orangi et al., 2011) .......................... 165
Table 9-4: Binary interaction parameters for Eagle Ford oil (Orangi et al., 2011) ............. 166
Table 9-5: Parameters for study of importance of capillary pressure on original oil-in-place (Bakken) .................................................................................................................. 167
Table 9-6: Parameters for study of importance of capillary pressure on original oil-in-place (Eagle Ford) ................................................................................................................ 173
Table 9-7: Parameters for simulation studies of EDFM incorporating the effect of capillary pressure using Bakken oil .......................................................................................... 189
Table 9-8: Comparison of cumulative oil production at various initial reservoir pressures for Bakken oil and Eagle Ford oil .................................................................................. 194
Table 9-9: Input data for simulation of the DPDK model incorporating the effect of capillary pressure on phase behavior .............................................................................. 200
Table 9-10: Input data for simulation of the TPTK model incorporating the effect of capillary pressure on phase behavior for Bakken oil ...................................................... 205
# Nomenclature

**Roman**

- $A_x, A_y, A_z$: Cross sectional area in $x$, $y$- and $z$- direction
- $A_{mnc}^m$: Area open to flow via NNC for fracture segment $m$
- $B_w$: Formation volume factor of water phase
- $c_{f,k}$: Compressibility of formation on permeability
- $c_{f,\phi}$: Compressibility of formation on porosity
- $c_i$: Composition of fluid (single-phase, oil, or gas)
- $d_{mnc}^m$: Average normal distance of fracture segment $m$ to grid block
- $D_{eff}$: Effective diffusion coefficient of the gas phase
- $f_{i,j}$: Fugacity of component $i$ in phase $j$
- $f_{nj}$: Mole fraction of phase $j$
- $f_{nl,s}$: Liquid mole fraction at separator stage $s$
- $f_{sj}$: Overall mole fraction of phase $j$ from separator at stock tank
- $F_{g}^{inj}$: Total moles being injected into the reservoir
- $g$: Gravitational acceleration
- $g_c$: Gravitational conversion factor, 32.174 $lb$-$ft/lbf$-$s^2$
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G$</td>
<td>Depth from surface to the center of the grid block</td>
<td>ft</td>
</tr>
<tr>
<td>$h$</td>
<td>Thickness of the well block</td>
<td>ft</td>
</tr>
<tr>
<td>$J$</td>
<td>Leverette J-function</td>
<td>-</td>
</tr>
<tr>
<td>$k$</td>
<td>Permeability</td>
<td>mD</td>
</tr>
<tr>
<td>$k_{ave}$</td>
<td>Average permeability</td>
<td>mD</td>
</tr>
<tr>
<td>$k_{m}^{mc}$</td>
<td>Harmonic average of permeability of fracture segment $m$ for transport via NNC</td>
<td>mD</td>
</tr>
<tr>
<td>$k''$</td>
<td>Permeability at initial / reference condition</td>
<td>mD</td>
</tr>
<tr>
<td>$k_{rj}$</td>
<td>Relative permeability of phase $j$</td>
<td>-</td>
</tr>
<tr>
<td>$K_{i}$</td>
<td>Vapor-liquid equilibrium ratio of component $i$ in the hydrocarbon mixture</td>
<td>-</td>
</tr>
<tr>
<td>$L$</td>
<td>Liquid mole fraction</td>
<td>fraction</td>
</tr>
<tr>
<td>$M_{i,p}$</td>
<td>Molar flow rate of component $i$ entering/leaving a well from porosity $p$</td>
<td>lbmol RB day ft$^3$</td>
</tr>
<tr>
<td>$M_{i}^{inj}$</td>
<td>Molar injection rate of component $i$ into the reservoir</td>
<td>lbmol RB day ft$^3$</td>
</tr>
<tr>
<td>$MW_{i}$</td>
<td>Molecular weight of component $i$</td>
<td>lb/lbmol</td>
</tr>
<tr>
<td>$n_{i}^{j}$</td>
<td>Moles of component $i$ in phase $j$</td>
<td>lbmol</td>
</tr>
<tr>
<td>$n_{s}$</td>
<td>Number of stages in the separator</td>
<td>-</td>
</tr>
<tr>
<td>$N_{B}$</td>
<td>Number of grid blocks</td>
<td>-</td>
</tr>
<tr>
<td>$N_{C}$</td>
<td>Number of hydrocarbon component</td>
<td>-</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------------------------------------------------</td>
<td>---------------</td>
</tr>
<tr>
<td>$N_F$</td>
<td>Number of fractures</td>
<td>-</td>
</tr>
<tr>
<td>$N_i$</td>
<td>Molar rate of hydrocarbon component $i$ entering/leaving the reservoir</td>
<td>lb mol RB/ day ft$^3$</td>
</tr>
<tr>
<td>$N_P$</td>
<td>Number of phase</td>
<td>-</td>
</tr>
<tr>
<td>$N_S$</td>
<td>Number of fracture segments</td>
<td>-</td>
</tr>
<tr>
<td>$N_r$</td>
<td>Total molar rate entering/leaving the reservoir</td>
<td>lb mol RB/ day ft$^3$</td>
</tr>
<tr>
<td>$P_{cjk}$</td>
<td>Capillary pressure between phase $j$ and $k$</td>
<td>psi</td>
</tr>
<tr>
<td>$P_{ci}$</td>
<td>Critical pressure of component $i$</td>
<td>psia</td>
</tr>
<tr>
<td>$P_j$</td>
<td>Pressure of phase $j$</td>
<td>psia</td>
</tr>
<tr>
<td>$P_L$</td>
<td>Langmuir pressure</td>
<td>psia</td>
</tr>
<tr>
<td>$P_{ref}$</td>
<td>Reference pressure</td>
<td>psia</td>
</tr>
<tr>
<td>$P_{ri}$</td>
<td>Reduced temperature of component $i$</td>
<td>-</td>
</tr>
<tr>
<td>$P_{sc}$</td>
<td>Pressure at standard condition</td>
<td>psia</td>
</tr>
<tr>
<td>$P_{wf}$</td>
<td>Well flow / sandface / bottom-hole pressure</td>
<td>psia</td>
</tr>
<tr>
<td>$q_{ij}^{ inj}$</td>
<td>Volumetric rate of gas injected to the reservoir at standard condition</td>
<td>Mscf/day</td>
</tr>
<tr>
<td>$q_{ij}^{ sc}$</td>
<td>Molar production/injection of component $i$ in phase $j$</td>
<td>lb mol RB/ day ft$^3$</td>
</tr>
<tr>
<td>$q_{ij}^{ sc}$</td>
<td>Volumetric production rate of phase $j$ at standard condition</td>
<td>scf/day</td>
</tr>
</tbody>
</table>
\( q_{w,p} \) Volumetric production/injection rate of water at standard condition from porosity \( p \) \( \text{STB/day} \)

\( r \) Pore radius \( \text{nm} \)

\( r_e \) Equivalent well block radius \( \text{ft} \)

\( r_w \) Wellbore radius \( \text{ft} \)

\( R \) Universal gas constant, 10.73 \( \frac{\text{psi} \cdot \text{ft}^3}{\text{lbmol} \cdot R} \)

\( R_i \) Residual equation for component \( i \) \( \frac{\text{lbmol} \cdot RB}{\text{day} \cdot \text{ft}^3} \)

\( R_w \) Residual equation of water component \( \text{STB/day} \)

\( S \) Skin factor -

\( S_j \) Saturation of phase \( j \) fraction

\( S_{jc} \) Critical saturation of phase \( j \) fraction

\( t \) Time \( \text{days} \)

\( T \) Reservoir temperature \( \text{°F} \)

\( T_{ci} \) Critical temperature of component \( i \) \( R \)

\( T_{ri} \) Reduced temperature of component \( i \) -

\( T_{jx}, T_{jy}, T_{jz} \) Inter-block transmissibility of phase \( j \) in \( x-, y-, \) and \( z \)-direction -

\( T'_{jx}, T'_{jy}, T'_{jz} \) Gravity inter-block transmissibility of phase \( j \) in \( x-, y-, \) and \( z \)-direction -

\( T_{sc} \) Temperature at standard condition \( \text{°F} \)
\( T_{wx}, T_{wy}, T_{wz} \) \hspace{1cm} \text{Inter-block transmissibility of water phase in } x-, y-, \text{ and } z\text{-direction}

\( T'_{wx}, T'_{wy}, T'_{wz} \) \hspace{1cm} \text{Gravity inter-block transmissibility of water phase in } x-, y-, \text{ and } z\text{-direction}

\( V \) \hspace{1cm} \text{Vapor mole fraction}

\( V_{a,i} \) \hspace{1cm} \text{Amount of adsorbed gas of component } i \text{ scf}

\( V_{c,i} \) \hspace{1cm} \text{Adsorption capacity of component } i \text{ scf/ton}

\( V_b \) \hspace{1cm} \text{Bulk volume ft}^3

\( V_L \) \hspace{1cm} \text{Langmuir volume scf/ton}

\( V_p \) \hspace{1cm} \text{Pore volume ft}^3

\( x_i \) \hspace{1cm} \text{Liquid composition of component } i \text{ fraction}

\( y_i \) \hspace{1cm} \text{Gas composition of component } i \text{ fraction}

\( y_i^{\text{inj}} \) \hspace{1cm} \text{Molar composition of component } i \text{ in the injection gas fraction}

\( z_i \) \hspace{1cm} \text{Overall composition of component } i \text{ fraction}

\( z_i^{\text{ws}} \) \hspace{1cm} \text{Molar composition of component } i \text{ in the wellstream fraction}

\( Z_j \) \hspace{1cm} \text{Compressibility factor of phase } j \text{ -}

\( Z_j^{sc} \) \hspace{1cm} \text{Compressibility factor of phase } j \text{ at standard condition -}

\textbf{Greek}

\( \beta_j \) \hspace{1cm} \text{Total moles in phase } j \text{ lbmol}
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Unit Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \chi_i )</td>
<td>Parachor of component ( i )</td>
<td>( (\text{dyne/cm})^{\frac{1}{4}} ) gmol/cm³</td>
</tr>
<tr>
<td>( \eta_P )</td>
<td>Time-step tuning factor for pressure</td>
<td>-</td>
</tr>
<tr>
<td>( \eta_S )</td>
<td>Time-step tuning factor for saturations</td>
<td>-</td>
</tr>
<tr>
<td>( \eta_X )</td>
<td>Time-step tuning factor for component mole fraction</td>
<td>-</td>
</tr>
<tr>
<td>( \phi )</td>
<td>Porosity</td>
<td>fraction</td>
</tr>
<tr>
<td>( \phi^o )</td>
<td>Porosity at initial / reference condition</td>
<td>fraction</td>
</tr>
<tr>
<td>( \phi_i^j )</td>
<td>Fugacity coefficient of component ( i ) in phase ( j )</td>
<td>-</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>Surface tension</td>
<td>dyne/cm</td>
</tr>
<tr>
<td>( \gamma_j )</td>
<td>Specific weight of phase ( j )</td>
<td>lb/lbf/ft³</td>
</tr>
<tr>
<td>( \lambda_{total} )</td>
<td>Total mobility of the fluid in the well block</td>
<td>( 1/cP )</td>
</tr>
<tr>
<td>( \mu_j )</td>
<td>Viscosity of phase ( j )</td>
<td>cP</td>
</tr>
<tr>
<td>( \rho_j )</td>
<td>Mass density of phase ( j )</td>
<td>lbm/lbf/ft³</td>
</tr>
<tr>
<td>( \tilde{\rho}_j )</td>
<td>Molar density of phase ( j )</td>
<td>lbmol/lbf/ft³</td>
</tr>
<tr>
<td>( \tilde{\rho}_{sc,j} )</td>
<td>Molar density of phase ( j ) at standard condition</td>
<td>lbmol/lbf/ft³</td>
</tr>
<tr>
<td>( \sigma_{jk} )</td>
<td>Interfacial tension between phase ( j ) and ( k )</td>
<td>dyne</td>
</tr>
<tr>
<td>( \omega )</td>
<td>Time-step tuning factor</td>
<td>-</td>
</tr>
<tr>
<td>( \omega_i )</td>
<td>Pitzer’s acentric factor of component ( i )</td>
<td>-</td>
</tr>
</tbody>
</table>
\( \omega_{ij} \) Mole fraction of component \( i \) in phase \( j \) 

\( \tau \) Pseudo-steady state sorption time constant 

\( \Phi_j \) Potential of phase \( j \) 

\( \Gamma_p \) Matrix-natural fracture flow source term in porosity \( p \) 

\( \Lambda_p \) Natural fracture-hydraulic fracture flow source term in porosity \( p \) 

\( M_p \) Matrix-hydraulic fracture flow source term in porosity \( p \) 

\( \Omega^o_{ai} \) EoS attraction parameter constant for component \( i \) in the mixture 

\( \Omega^p_{bi} \) EoS co-volume parameter constant for component \( i \) in the mixture 

\( \Omega \) Productivity or injectivity index 

\( \psi^p_i \) Spreading coefficient of component \( i \) at standard state 

**Acronym**

CMB Cumulative Material Balance 

DPDK Dual-Porosity Dual-Permeability 

DPSK Dual-Porosity Single-Permeability 

EDFM Embedded Discrete Fracture Model 

EOR Enhanced Oil Recovery 

EoS Equation of State
IMB  Incremental Material Balance

IMPES  Implicit Pressure Explicit Saturation

NNC  Non-Neighboring Connection

OGIP  Original Gas In Place $Mscf$

OHIP  Original Hydrocarbon In Place $lbmol$

OOIP  Original Oil In Place $STB$

OSIP  Original Specie In Place $lbmol$

OWIP  Original Water In Place $STB$

PR  Peng-Robinson equation of state

SPSK  Single-Porosity Single-Permeability

SRK  Soave-Redlich-Kwong equation of state

SRVM  Stimulated Reservoir Volume Model

TPTK  Triple-Porosity Triple-Permeability

**Subscripts**

$f$  Index for natural / micro fracture porosity domain

$F$  Index for hydraulic / macro fracture porosity domain

$g$  Index for gas phase

$i$  Index for hydrocarbon component

$j$  Index for phase

$l$ Index for oil phase
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M$</td>
<td>Index for matrix porosity domain</td>
</tr>
<tr>
<td>$o$</td>
<td>Index for oil phase</td>
</tr>
<tr>
<td>$p$</td>
<td>Index for porosity type</td>
</tr>
<tr>
<td>$sc$</td>
<td>Standard condition ($60 ,^\circ F$ and 14.7 psia)</td>
</tr>
<tr>
<td>$u$</td>
<td>$u$-direction spatial coordinate (for hydraulic fracture)</td>
</tr>
<tr>
<td>$v$</td>
<td>$v$-direction spatial coordinate (for hydraulic fracture)</td>
</tr>
<tr>
<td>$w$</td>
<td>Index for water component</td>
</tr>
<tr>
<td>$x$</td>
<td>$x$-direction spatial coordinate</td>
</tr>
<tr>
<td>$y$</td>
<td>$y$-direction spatial coordinate</td>
</tr>
<tr>
<td>$z$</td>
<td>$z$-direction spatial coordinate</td>
</tr>
</tbody>
</table>

**Superscripts**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>Iteration level in Newton iteration</td>
</tr>
<tr>
<td>$L$</td>
<td>Liquid phase</td>
</tr>
<tr>
<td>$n$</td>
<td>Time level in Newton iteration</td>
</tr>
<tr>
<td>$o$</td>
<td>Initial condition</td>
</tr>
<tr>
<td>$t$</td>
<td>Time level in Newton iteration</td>
</tr>
<tr>
<td>$V$</td>
<td>Vapor phase</td>
</tr>
</tbody>
</table>
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Chapter 1

Introduction

Naturally fractured reservoirs contribute to a significant amount of the world oil and gas reserves. These reservoirs exist throughout the world. Increasing demands for oil and gas accelerate the exploration and production from unconventional resources. Oil and gas production from naturally fractured reservoirs is increasing in popularity in the United States. Shale is a type of clay or mud that can split easily into layers. Shale formations function as source rocks and seals for conventional reservoirs. Shale generally contains high organic content, which results in a large amount of gas adsorbed on the surface of shale and extremely low values of permeability. This factor makes production of hydrocarbon from shale more challenging. Studies of flow, transport, and mechanisms have been made for fractured reservoirs (Dean & Lo, 1988; Thararoop et al., 2012; Moinfar, 2013). Investigations of multi-phase flow and transport phenomena in fractured reservoirs are increasing. Recent research shows that this ultra-low permeability affects capillary pressure between phases and consequently the phase behaviors of reservoir fluid (Sigmund et al., 1973; Brusilovsky, 1992; Nojabaei et al., 2012). To economically produce hydrocarbon from shale, hydraulic fracturing is universally implemented. Additionally, a large portion of original oil-in-place remains trapped in the reservoirs after primary and secondary recoveries (e.g., water flood). An opportunity exists to recover the remaining oil through various enhanced oil recovery (EOR) techniques. Through EOR techniques, it may be possible to ultimately produce 20-30% or more of the original oil-in-place. One of the most widely implemented EOR techniques is miscible gas flooding by injection of CO₂. Injected CO₂ forms a single-phase fluid with the remaining oil, causing the oil to swell and reducing irreducible oil
saturation. An indirect benefit from this process is the reduced amount of carbon dioxide emissions to the atmosphere. Miscible gas flooding is a mature technology that is commonly used to enhance oil recovery. According to the U.S. Department of Energy, gas injection accounts for nearly 60% of the EOR production in the United States.

Two types of reservoir simulators are commonly used in the industry: black-oil and compositional. Black-oil simulators operate under the assumption that hydrocarbon components form pseudo oil and gas components. In other words, black-oil simulator assumes limited mass exchange of components. Black-oil simulators are widely used to model systems of simple to moderate complexity due to the robustness and speed of the simulation. However, this assumption is insufficient to accurately model complex fluid behaviors and transport phenomena in more complicated processes such as EOR. In compositional simulation, a differential mass conservation equation is written for each component in the reservoir. A phase behavior calculation is performed in each grid block to determine the fluid equilibrium and property predictions. With compositional simulation, we can track the flow of each component in the reservoir as well as accurately model the fluid behavior. The composition of gas and oil can change over the course of the simulation. Therefore, a compositional reservoir simulator is more suitable in our research. Compared to black-oil simulation, compositional simulation is computationally demanding, especially in the phase equilibrium calculations and component transport calculations. The reservoir simulator must be able to model fluid behavior accurately and efficiently and capture fluid flows and phase behavior of fluid under the effect of pore confinement during production and EOR processes. Therefore, a robust reservoir simulator is required.

In this dissertation, related literature reviews on effect of capillary pressure on phase behavior, the embedded discrete fracture model (EDFM), the stimulated reservoir volume model (SRVM), and gas adsorption on shale surfaces are discussed in Chapter 2. The problem statement
and research objectives are discussed in Chapter 3. Formulation and numerical implementation of the compositional model are presented in Chapter 4 and Chapter 5. Chapter 6 discusses the development of the proposed triple-porosity, triple-permeability model. Validations of the model against existing models are shown in Chapter 7. A parametric study of the proposed model and the effect of capillary pressure on phase behavior are presented in Chapter 8 and Chapter 9, respectively. Finally, Chapter 10 summarizes and concludes the work developed in this project.
Chapter 2

Literature Review

This chapter briefly explains compositional formulations, modeling of naturally fractured reservoirs, dual-porosity and dual-permeability characteristics, effect of capillary pressure on phase behaviors, gas adsorption on shale, the Embedded Discrete Fracture Model, and the Stimulated Reservoir Volume Model.

2.1 Formulation of Compositional Simulation

In the first step of the development of the simulator, various compositional formulations are reviewed. Two of the most common types of formulation are semi-implicit and fully implicit. The semi-implicit formulation solves pressure implicitly and calculates the corresponding compositions or saturations explicitly. This formulation is often known as IMPES (IMplicit Pressure, Explicit Saturation/Compositions). Thus, the stability of this formulation is limited by the time-step size, and it must satisfy the Courant-Friedrichs-Lewy condition (i.e., fluid cannot move from one grid block to an adjacent grid block more than the amount of fluid that can be stored in that grid block). For a shale formation, large variations in flow rates occur near the wellbore and in the natural fractures or hydraulic fractures. In the matrix system, flow rate is relatively low, but storativity is high. Conversely, in the fracture system, flow rate is high but the storativity of hydrocarbon is low. This could result in the small time step in IMPES formulation to maintain stability of the numerical simulation. Therefore, the IMPES-type formulation is not applicable for our study, as the flow in the fracture domain can dominate the time step size in the IMPES formulation. Thus, this simulator is developed based on the fully implicit formulation.
Several fully implicit formulations have been reviewed: Fussell and Fussell (1979), Coats (1980), Young and Stephenson (1983), and Chien, Lee, and Chen (1985). These models are distinguished by the chosen primary equations and variables, and they are briefly described below.

**Fussell and Fussell (1979):** The primary variables are pressure \( P \), hydrocarbon liquid mole fraction \( L \), and either liquid or vapor composition \( x_i \) or \( y_i \) for \( i = 2, \ldots, N_C \). This model uses phase equilibrium relations as primary equations.

**Coats (1980):** The model uses mass balances for hydrocarbon and water and primary equations. The primary variables are pressure, two saturations, and one phase composition.

**Young and Stephenson (1983):** This model uses \( N_C \) mass balance equations, saturation constraint, and the total hydrocarbon mass balance equations.

**Chien, Lee, and Chen (1985):** In this model, the primary equations are \( N_C \) mass balance equations for hydrocarbon components and water. The primary variables are pressure and total moles of component \( i \) for \( i = 1, 2, 3, \ldots, N_C - 1 \) and water in one unit volume of fluid.

Voskov et al. (2009) and Schmall et al. (2013) compared each formulation in terms of the number of Newton iterations for various test scenarios and constraints. Based on their studies, Coats (1980) fully implicit formulation outperforms other formulations based on total number of Newton iterations for various study cases. Therefore, in this work, we follow Coats (1980) fully implicit formulation to develop our simulator.

### 2.2 Modeling of Naturally Fractured Reservoirs

#### 2.2.1 Shale Modeling

Shale reservoirs are naturally fractured systems mainly consisting of two porosity domains. Oil and gas can be stored in both shale matrix and fracture networks, but a significant
amount of hydrocarbons is stored in the matrix. In addition, in the case of a saturated reservoir, gas can adsorb on the shale surface. Occasionally, the adsorbed gas is considered as another porosity domain.

Some commonly used mathematical methods for modeling flow through fractured rocks are the explicit discrete fracture model and the dual-continuum model. The discrete fracture model can accurately represent the fracture and matrix. However, the method is computationally expensive, as many grid blocks are required to capture each individual fracture. Often, an unstructured grid is needed to capture fracture orientation. The dual-continuum model is more widely used in various applications due to its lower computational demand and its ability to handle matrix-fracture interactions under multi-phase flow in fractured reservoirs (Kang et al., 2006). Naturally fractured reservoirs are typically modeled with the dual-porosity model. These porosity domains are fracture and matrix. The mathematical formulation of the dual-porosity system of matrix blocks and fractures was first presented by Barenblatt et al. (1960). These two porosity domains are fracture system and matrix system. Warren and Root (1963) later applied the dual-porosity model, also known as dual-continuum model, in petroleum reservoirs. In the dual-porosity model, fractures form a continuum filled by the discontinuous matrix blocks. The matrix system has high fluid storativity but low fluid transmissibility. Conversely, the fracture system has low storage capacity but serves as high permeability conduits for hydrocarbon to flow to the wellbore. Thus, flow occurs from matrix to fracture and from fracture to well. In this model, fluid neither flows directly from the matrix to the well nor flows between matrix blocks, and convection is the only flow mechanism in the matrix. In the Warren and Root dual-porosity model, mass exchange between matrix and fracture domain is represented by a source/sink term in the governing flow equations.

In an attempt to improve accuracy in modeling naturally fractured reservoirs, researchers have modified the Warren and Root model and added more complexities to the model. Currently,
the dual-porosity, dual-permeability model in which flows occur between matrix blocks has been widely implemented to simulate flow in naturally fractured reservoirs (Blaskovich et al., 1983; Hill and Thomas, 1985; Dean and Lo, 1988; Ayala et al., 2005). Ertekin et al. (1986) proposed a dual-mechanism flow model (also known as multi-mechanistic flow) for gas flow in the coal matrix and fracture network. In the proposed model, flow in naturally fractured reservoirs is driven by two mechanisms: flow under pressure field (Darcian flow) and flow under concentration field (Fickian flow). In dual-porosity models, another set of mass conservation equations has to be simultaneously solved to determine unknowns in the matrix domain at each time step.

Several multi-porosity models have been proposed to capture the flow mechanism in naturally fractured reservoirs. Al-Ahmadi and Wattenbarger (2011) showed that reservoir heterogeneity can be captured by subdividing each medium and assigning different reservoir properties. Their triple-porosity model consists of matrix, micro-fracture, and macro-fracture. Simulation results from the triple-porosity model when reduced to the dual-porosity model are in perfect agreement with the results generated from the conventional dual-porosity model. These multi-porosity models aim to handle the heterogeneity in the matrix and fracture. Kang et al. (2006) studied multi-phase flow in naturally fractured vuggy reservoirs. Their triple-porosity model tackles the heterogeneity in the matrix domain (i.e., they subdivide the matrix rock into low-permeability matrix and void space in the matrix rock, which is typically called a vug). Hinkley et al. (2013a) proposed design of a simulator that is applicable up to N porosity types. In their model, the inter-porosity transmissibility function following Coats (1989) was used for all porosity pairs. Hinkley et al. (2013b) explored the advantages and disadvantages of dual-, triple-, and quad-porosity models for simulation by comparing the multi-porosity models with the fine-scale grid model where micro-fractures, macro-fractures, organic matrix, inorganic matrix, and vugs are explicitly modeled. In this study, the triple-porosity model attempts to capture
heterogeneity in the fracture; i.e., the model subdivides fractures into hydraulic fractures (or macro fractures) and natural fractures (micro fractures). Hinkley et al. (2013b) also stated that no significant impact occurs from increasing the number of porosity beyond three types.

Li and Lee (2008), Hajibeygi et al. (2011), and Moinfar et al. (2013) developed a new discrete fracture modeling technique for naturally fractured reservoirs. In their work, long and large-scale fractures are modeled explicitly. However, short and small-scale fractures are lumped into the matrix block by increasing the effective permeability of the matrix block. Recently, Jiang and Younis (2015) proposed a hybrid-triple porosity model in which the multiple interacting continua (MINC) proposed by Pruess (1985) was coupled with the discrete fracture model proposed by Li and Lee (2008), Hajibeygi et al. (2011), and Moinfar et al. (2013). In the MINC, the matrix block is subdivided into smaller grid blocks, and pressure distribution within the matrix block is solved. The goal is to remove the pseudo-steady state assumption. The model assumes sequential flow; i.e., under the pressure depletion scenario, hydrocarbon flows from matrix to natural fracture and then to hydraulic fracture (discrete fracture). Due to the use of MINC, flow between matrix blocks is ignored in this model.

2.2.2 Gas Adsorption / Desorption

One of the most commonly used gas sorption isotherms is Langmuir (Manik et al., 2002). Let $V_a$ be adsorption capacity, $V_L$ be sorption volume, $P_L$ be sorption pressure, and $P$ be pressure. Eq. (2.1) gives the Langmuir Isotherm.

$$V_a = \frac{V_L P}{P_L + P}$$

(2.1)

Langmuir isotherm represents the component adsorption capacity at a given pressure. As the production continues, reservoir pressure decreases. At low pressure, gas starts to desorb from the
shale surface to matrix and flows from matrix to fracture. The amount of gas released per ton of shale is equal to the difference in gas adsorption capacity between initial and final conditions during a given interval. Under the same pressure difference, the amount of gas released is greater at lower pressure. When adsorbed gas is considered, the overall flowing mechanism of gas is as shown in Figure 2-1. Although the scheme in Figure 2-1 was developed for coalbed methane reservoirs, it can be used to explain a similar flow mechanism of fluid in shale reservoirs. Starting from left to right in Figure 2-1, gas is desorbed from shale surface to matrix pores. Gas then flows from shale matrix to fractures. In an ultra-low permeability system, flow is diffusion dominated. Gas then subsequently flows through fracture networks to the wellbore.

![Flow mechanism of coalbed methane and shale gas (Remner, 1986)](image)

**Figure 2-1: Flow mechanism of coalbed methane and shale gas (Remner, 1986)**

### 2.3 Effect of Nano-pore Capillary Pressure on Phase Behaviors

Pore sizes of tight rocks are in the range of nanometers, typically 50 nm or smaller (Kuila and Prasad, 2011). The presence of small pores in shale reservoirs has been verified using ultra-high-pressure mercury injection, back-scattered scanning, electron microscopy, and atomic force microscopy (Javadpour, 2009; Javadpour et al., 2007; Katsube, 2000). Capillary pressure between gas and oil in these nano-pores can be several hundreds of pounds per square inch (psi) or more,
depending on the gas-oil interfacial tension. The increase in capillary pressure leads to a very large change in fluid properties such as phase density and viscosity.

Sigmund et al. (1973) investigated the effect of porous media on phase behavior of binary hydrocarbons. In their experimental work, 30- to 40-US-mesh glass-bead packs were used to model the porous media, but their pores were larger than typically found in reservoir shales.

A thermodynamic model was used to study the effect of capillary pressure on phase equilibrium of a multi-component system (Brusilovsky, 1992). This paper showed the results of mathematical simulations of dew- and bubble-point pressures for multi-component systems under the influence of capillary forces. As pores became smaller, surface curvature increased. Consequently, the bubble point decreased while dew-point increased. In his study, the system reached bubble point first in the larger pores, while dew-points were reached first in smaller pores.

The effect of capillary pressure on phase behavior was explored in more detail over a full range of temperatures and pressures using a cubic equation of state in Nojabaei et al. (2013). They studied the effect of capillary pressure on phase behavior for binary mixtures and middle Bakken reservoir fluid. They found that densities and viscosities decreased with smaller pore sizes when capillary pressure was considered in flash calculations in water-wet rocks. Capillary pressure also decreased the bubble-point pressure significantly for the Bakken fluid at reservoir temperature. Nojabaei et al. (2013) further compared the expected produced gas-oil ratio with and without capillary pressure to Bakken well production data, and hypothesized that the constant gas-oil ratio in Bakken that exists for an extended period is likely the result of capillary pressure. Later, Nojabaei et al. (2014) studied the effect of saturation dependency of capillary pressure using a compositionally extended black-oil formulation and compared the production results from that model to those from a fully compositional formulation that considered seven components. The increase in cumulative oil production with pore-size distribution was approximately 12%
lower compared to the case with fixed pore-size. The results from the compositional formulation agreed well with those from the black-oil formulation.

Nojabaei et al. (2012) showed that ultra-low permeability of shale affects capillary pressure between phases and consequently the phase behavior of reservoir fluids. When capillary pressure was included in phase behavior calculation, they found a decrease in bubble-point pressure and either an increase or decrease in dew-point pressure depending on the location of interest in the phase envelope.

Phase equilibrium is achieved when fugacity of each phase is equal at a given pressure and temperature. In the case of two-phase liquid-vapor equilibrium calculation, the fugacity of each component in liquid and vapor phases must be equal (Firoozabadi, 1999). Thus, we can write:

\[ f_i^L = f_i^V \quad \text{for } i = 1, 2, \ldots, N_C \]  

(2.2)

Note that superscript \( L \) and \( V \) in Eq. (2.2) refer to liquid (oil) phase and vapor (gas) phase, respectively. Fugacity of each phase is a function of phase pressure, temperature, and phase compositions. Conventional flash calculation assumes that phase pressures are equal (i.e., capillary pressure is negligible). However, this assumption is not accurate as capillary pressure between two hydrocarbon phases can be several hundreds of pounds per square inch or more. Let \( P_o, P_g, T, x_i, \text{ and } y_i \) be liquid (oil) phase pressure, vapor (gas) phase pressure, reservoir temperature, liquid phase composition, and vapor phase composition, respectively. Thus, Eq. (2.2) can be rewritten:

\[ f_i^L(P_o, T, x_i, \ldots, x_{N_C}) = f_i^V(P_g, T, y_i, \ldots, y_{N_C}) \quad \text{for } i = 1, 2, \ldots, N_C \]  

(2.3)

In addition to fugacity constraints, the difference in phase pressures must be equal to the capillary pressure between two phases at equilibrium. This can be described by the Young-Laplace equation of capillarity in Eq. (2.4).
\[ P_g - P_o = P_{cgo} \left( S_g \right) = \frac{2\sigma_{go}}{r_{go}} \]  (2.4)

where \( P_g, P_o, P_{cgo}, \sigma_{go} \) and \( r_{go} \) are vapor (gas) phase pressure, liquid (oil) phase pressure, capillary pressure, interfacial tension, and pore radius, respectively. The Macleod and Sugden correlation is used to calculate interfacial tension as a function of compositions and phase densities (Pederson, 2007):

\[
\sigma_{go} = \left[ \sum_{i=1}^{N_c} \chi_i \left( x_i \tilde{\rho}_o - y_i \tilde{\rho}_g \right) \right]^4 
\]  (2.5)

where \( \chi_i, x_i, y_i, \tilde{\rho}_o, \) and \( \tilde{\rho}_g \) are parachor of component \( i \), liquid mole fraction of component \( i \), vapor mole fraction of component \( i \), liquid density, and vapor density, respectively. Parachor (\( \chi_i \)) of component \( i \) can be defined as follows.

\[
\chi_i = \frac{MW_i \cdot \gamma^{\frac{1}{4}}}{\rho_i} 
\]  (2.6)

where \( MW_i, \gamma, \) and \( \rho_i \) are molecular weight of component \( i \), surface tension, and density of component \( i \), respectively. Alternatively, parachors of common components have been tabulated and can be used directly. The system of equations is solved using successive substitution followed by the minimum-variable Newton-Raphson method.

The effect of capillary pressure can be extended for three-phase equilibrium between oil, gas, and water. To apply the effect of nano-pore capillary pressure, the phase equilibrium calculation and three-phase capillary pressure model will be modified. For three-phase equilibrium calculation, the fugacity constraint in Eq. (2.2) has been modified.

\[
f_i^j = f_i^r \quad \text{for} \quad i = 1, 2, \ldots, N_C; \quad \text{for} \quad j = 1, 2, \ldots, N_p; \quad j \neq r 
\]  (2.7)

Eq. (2.7) can be written \( N_C(N_p-1) \) times. For the three-phase equilibrium calculation, \( N_p \) is equal to 3, and \( 2N_C \) fugacity equations have to be solved. Similarly, nano-pore capillary pressure
between liquid and aqueous phase has to be considered. Eqs. (2.4) and (2.5) are modified for liquid and aqueous phase as follows.

\[
P_o - P_w = P_{c_{ow}} (S_o) = \frac{2\sigma_{ow}}{r_{ow}} \tag{2.8}
\]

\[
\sigma_{ow} = \left[ \sum_{i=1}^{N_c} \chi_i \left( w_i \tilde{\rho}_w - x_i \tilde{\rho}_n \right) \right]^4 \tag{2.9}
\]

where \( w_i \) and \( \tilde{\rho}_w \) are aqueous phase mole fraction of component \( i \) and aqueous phase density, respectively.

Wang et al. (2013) developed a compositional model incorporating the effect of capillary pressure on phase behavior for tight oil reservoirs. In their model, the Leverett J-function is used for capillary pressure. The change in porosity and permeability with effective stress was considered in the work. No discrete fractures were used, however, in the simulations.

Jin et al. (2013) studied the effect of molecular-pore wall interaction in shale formations. Two methods were used in their study: modified flash calculations to account for capillary pressure, and modified critical properties of pure components to account for the effect of confinement based on the molecular simulation study. From both methods, the phase envelope shrinks when capillary pressure is considered. In addition, when critical properties are modified, the location of the critical point changes. However, the critical point remains the same when modified flash calculation is used.

To determine the number of phases that co-exist in equilibrium, phase stability analysis is often performed in which capillary pressure is neglected. Rezaveisi et al. (2015) studied the conventional tangent plane distance for phase stability analysis and found that the method is not applicable when capillary pressure on phase behavior is considered. They proposed a new method to determine phase stability with capillary pressure and demonstrated that a limiting (maximum) capillary pressure exists at which phase equilibrium can be achieved. Beyond that limit,
equilibrium using the cubic equation-of-state is not possible. Rezaveisi et al. (2015) compared oil recoveries from three cases including gas condensates, but in all cases they did not consider discrete fractures.

2.4 Embedded Discrete Fracture Model

Simulation of discrete fractures typically requires the use of local grid refinement, unstructured grids, or a fine-grid model to capture the geometry, orientation, and size of the fractures. The aforementioned methods can be computationally expensive, especially in full-field simulation. The discrete fracture model (DFM) is commonly used to model naturally fractured reservoirs when information of individual fracture is available. The advantage of the model is that fractures are explicitly represented and the flow behavior is accurately captured. However, DFM requires the use of unstructured grid or high-resolution structured grid. Unstructured grid posts a complicated grid generation, while high-resolution structured grid can slow down the simulation dramatically. In addition, strong contrast in grid block size and transmissibility between hydraulic fracture blocks and surrounding blocks can be large. This increases computational time because small time step size must be used to guarantee the stability of finite-difference formulation, and additional grid blocks must be added to gradually reduce dispersion between hydraulic fracture blocks and reservoir blocks. In many cases, instability may occur and cause the simulation to fail to converge. Thus, methods have been developed recently to speed up numerical simulation while preserving the essential features of discrete fractures.

Lee et al. (2001) developed a hierarchical method to model fluid flow in naturally fractured formations with multiple-length fractures. The effects of different scales of fracture length are handled in a hierarchical manner. In the paper, short-scale fractures enhance matrix permeability only and are not modeled explicitly. The boundary element method is used to
calculate the effective matrix permeability of a medium-length fracture. Long-scale fractures are modeled explicitly as fluid transport conduits. These fractures are embedded in the grid block using well model-like equations to represent matrix-fracture fluid transfer. The method is later termed the embedded discrete fracture model (EDFM). Li and Lee (2008) adopted the method presented by Lee et al. (2001) to include modeling of a discrete fracture as a two-dimensional plane, and its corresponding well-fracture intersections. Li and Lee (2008) implemented this method in their black-oil reservoir simulator. The advantage of EDFM is its applicability and ease of implementation using a Cartesian grid. EDFM can explicitly and accurately capture the fracture orientations, width, height, anisotropy, and preferential channeling of hydrocarbons in the reservoir. Each fracture segment communicates with the matrix block through a well-like source term. Fracture segments also communicate with adjacent fracture segments in a similar manner as two grid blocks communicating with each other in a two-dimensional reservoir. Each block in the computational domain represents a matrix block in the reservoir domain. Each fracture is explicitly modeled and solved in the simulation. In the study, simulation of fractured reservoir using EDFM yields similar results to fine-grid simulation but at a much faster speed.

Previous research on EDFM has some limitations on the orientation of fractures. Moinfar et al. (2012) extended the method proposed by Li and Lee (2008) to model slanted fractures and applied the technique in a multi-phase compositional model. The work focused on memory allocation of fractures and calculation of transmissibility between matrix-fracture and two different intersecting fracture segments. EDFM was verified against analytical solutions, which showed that larger Cartesian grid blocks could be used to represent accurately the pressure response. The concept of non-neighboring connection (NNC) is introduced to explain the memory allocation and connection between matrix block and fracture segment.

In EDFM, the fluid transfer between matrix and discrete fracture is calculated from a well-like source term, and the expression for source/sink term is shown in Eq. (2.10).
\[
M_i = \sum_{n_{mnc}}^{N_{mnc}} \left\{ A_{m}^{mnc} \sum_{j=1}^{N_{p}} k_{m}^{mnc} k_{ij}^{mnc} \frac{\bar{\rho}_{j}}{\mu_{j}} \frac{1}{d_{m}^{mnc}} \left[ \left( P_{j} - \frac{1}{144} g_c \rho_{j} G \right) - \left( P_{j} - \frac{1}{144} g_c \rho_{j} G \right)_{m}^{mnc} \right] \right\}
\]  

(2.10)

where \( M_i \), \( N_{mnc} \), \( A_{m}^{mnc} \), \( N_{p} \), \( k_{m}^{mnc} \), \( k_{ij}^{mnc} \), \( \bar{\rho}_{j} \), \( \mu_{j} \), \( \omega_{ij} \), \( \frac{1}{d_{m}^{mnc}} \left[ \left( P_{j} - \frac{1}{144} g_c \rho_{j} G \right) - \left( P_{j} - \frac{1}{144} g_c \rho_{j} G \right)_{m}^{mnc} \right] \), and \( d_{m}^{mnc} \) are molar exchange of component \( i \) through NNC, number of non-neighboring connections, area open to flow, number of phase, harmonic average of permeability of non-neighboring blocks, relative permeability of phase \( j \), viscosity of phase \( j \), molar density of phase \( j \), mole fraction of component \( i \) in phase \( j \), potential of non-neighboring block, and characteristic distance, respectively. Thus, the transmissibility term \( \frac{A_{m}^{mnc} \times k_{m}^{mnc}}{d_{m}^{mnc}} \) is calculated based on types of intersections. Note that Eq. (2.10) does not consider diffusion in the transport. A fracture can intersect the matrix block, another fracture, and the wellbore. Li and Lee (2008) and Hajibeygi et al. (2011) assumed that the pressure varies linearly in the normal direction to each fracture in a grid block. Thus, the average normal distance \( d_{m}^{mnc} \) must be calculated using the following equation.

\[
d_{m}^{mnc} = \frac{\int v \cdot d\nu}{V}
\]  

(2.11)

When reservoir pressure drops, fracture closures occur that result in a decrease in fracture permeability. Ozkan et al. (2010) proposed a stress-dependent permeability relationship.

\[
k_f = k_f^o \exp \left[ -d_f \left( P_{f,i} - P_f \right) \right]
\]  

(2.12)

To model natural fractures using EDFM, similar to that of the dual-continuum model, small randomly generated fractures must be introduced to the reservoir. Effective reservoir properties such as permeability tensor are used to represent permeability of the matrix blocks containing natural fractures.
2.5 Stimulated Reservoir Volume Model

Fractures in hydraulically fractured reservoirs are commonly modeled by two methods: discrete fracture model (DFM) and stimulated reservoir volume model (SRVM). The first method was discussed in Section 2.4. From microseismic data, hydraulic fracturing creates a massively fractured area around the wellbore. In the stimulated reservoir volume model, the massively fractured area has relatively higher permeability. Additionally, the stimulated zone in the dual-porosity model also has smaller fracture spacing. The smaller fracture spacing allows for higher fluid transport from matrix blocks to fracture and vice versa. These fractures serve as high-permeability pathways for hydrocarbon to flow to the wellbore. This stimulated reservoir volume can be modeled with an ellipsoid in three-dimensional models, as shown in Figure 2-2.

![Figure 2-2: Stimulated reservoir volume around a horizontal well in a thick formation](image)

Several researchers use SRV to represented hydraulically fractured zone in their simulation of unconventional reservoirs (Mayerhofer et al. 2010; Du et al. 2011; Darishchev et al. 2013; Ding et al. 2014). The stimulated reservoir volume concept was also studied by Siripatrachai and Ertekin (2012) for hydraulically fractured shale gas reservoirs. In the model, the stimulated zone is an ellipsoid covering the entire thickness of the two-dimensional reservoir. In a three-dimensional model, the stimulated reservoir volume can be modeled with the elliptic
equation shown in Eq. (2.13) where $a$, $b$, and $c$ are axis lengths of the ellipsoid in $x$, $y$, and $z$-direction, respectively.

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$$  \hspace{1cm} (2.13)

Once the stimulated reservoir volume has been identified, grid blocks are created to match the shape of the ellipsoid. Both the inner region (stimulated zone) and outer region (unstimulated zone) are modeled with a dual-porosity, dual-permeability model. The fracture permeability of the inner region is adjusted to have relatively higher permeability compared to the outer region. Conversely, the fracture spacing in the inner region will be smaller compared to the outer region. The advantage of SRVM is that a relatively larger grid block size compared to DFM can be used. This larger grid block allows a larger time step size, especially at the beginning of the simulation. However, the challenge of SRVM lies in the characterization of the reservoir properties in the stimulated zone and the time scale for flow could be inaccurate.

### 2.6 Highlights of the Chapter

In this chapter, a review of literature related to the development of the compositional model for unconventional reservoirs is presented and can be summarized as follows:

- Various compositional formulations are reviewed. Based on total number of Newton iterations for various study cases, Coats (1980) fully implicit compositional formulation outperforms other formulations and is selected in the development of the model in this research.
- Flow in naturally fractured reservoirs is typically captured by dual-porosity or multi-porosity models. Various models are discussed. EDFM is an efficient method in modeling discrete fractures and can be easily implemented in Cartesian grid. Hydraulic
fracturing creates a stimulated zone of high permeability which allows for flow of oil and gas. In this research, natural fractures and matrix blocks are modeled by dual-porosity, dual-permeability model. Hydraulic fractures are modeled by the EDFM. The flow in the proposed is fully coupled and occurs simultaneously in all porosity types.

- Large capillary pressure in tiny pores can suppress bubble point and alter fluid properties. The interfacial tension is estimated using Macleod and Sugden correlation and used in the calculation of capillary pressure. Phase fugacity calculation is modified to account for large capillary pressure between oil and gas.
Chapter 3

Problem Statement

The current challenge in compositional simulation for unconventional reservoirs lies in the robustness, accuracy, and efficiency of the simulator. This is primarily due to the complexities of the transport phenomena, fluid phase behaviors, and nature of formations. In addition, these complexities are not well understood and are not accurately modeled by the current simulators. During production or injection, gas may release or adsorb on shale surface, causing the shale to shrink or swell due to increase or decrease in formation pressure. Shale has the capability to adsorb gas on its surface. These mechanisms and phase behaviors of the fluid affect the accuracy of the simulation results if they are not considered during simulations. In addition, modeling discrete fractures using small grid blocks is not computationally efficient to model all small-scale natural fractures. Therefore, having a simulator that can effectively and efficiently capture and model the aforementioned complex mechanisms and phase behaviors is of utmost importance.

Multi-porosity simulation has been developed to capture the heterogeneity and flow behavior in different porosity domains. Unfortunately, the most current compositional reservoir simulators assume sequential flow from one porosity type to another. An enhanced matrix permeability on the grid block that hosts short-scale fractures is commonly used. In many multi-porosity models, flows between different porosity types are not fully coupled. Furthermore, most prior research on tight formations has focused on capillary pressure and its impact on phase behavior. Very few compositional simulations have been made to consider a variety of cases. Further, no compositional simulations have been made that couple the effect of capillary pressure on phase behavior with discrete fractures. Ignoring this effect can impact the oil-in-place
calculation as well as the production forecast. Therefore, a multi-porosity compositional reservoir simulator that fully couples flows between porosity types will efficiently capture flow behaviors by using the advantages of both EDFM and dual-continuum models. Furthermore, incorporation of the capillary pressure in modeling phase behavior is needed to accurately model fluid transport and phase behavior in tight rocks and shale.

The objective of this research is to develop an advanced multi-mechanistic triple-porosity, triple-permeability compositional reservoir simulator that couples the effect of capillary pressure on phase behavior with EDFM to investigate the impact on original oil-in-place and production in tight rocks and hydraulically fractured shale reservoirs. The importance of incorporating the effect of capillary pressure on phase behavior on original oil-in-place estimation and cumulative oil production is studied using both the Bakken and Eagle Ford crudes. Then, various cases of production from hydraulically fractured wells using the two fluids are demonstrated.

The developed reservoir simulator can accurately model the aforementioned complex mechanisms and phase behavior of hydrocarbons in shale and tight reservoirs during the production and EOR processes. Flows between three porosity types are fully coupled without making the assumption of sequential flow from matrix to natural fracture and, finally, hydraulic fractures. In this research, the embedded discrete fracture model is implemented to effectively and efficiently capture heterogeneity and orientation of fractures. Existence of natural fractures or short-scale fractures is handled through the use of the dual-porosity model without lumping these fractures into matrix blocks by enhancing the permeability of the matrix blocks. In addition, by considering the effect of capillary pressure in nano-pores on phase behavior and integrating a multi-mechanistic flow model and adsorption, we can expect a more realistic and accurate prediction of hydrocarbon from the simulator. Phase behavior of hydrocarbon, which affects the original oil-in-place and cumulative oil production is studied. The developed triple-porosity
model is used to study production from hydraulically fractured tight rock and shale under high capillary pressure as well as inter-porosity fluid transport.
Chapter 4

Formulation of the Compositional Model

This section describes the governing flow equation for the compositional model. More detailed derivation of the formulation can be found in Appendix A.

4.1 Governing Flow Equations

In the development of the model, the following assumptions are made:

- The porous medium is preferentially wetted by water or oil phase
- Hydrocarbon components can be both in the liquid and the gas phases
- Instantaneous equilibrium is reached at any point and time in the reservoir
- A cubic equation of state (EoS) is applicable to model thermodynamic equilibrium of hydrocarbon at a given pressure, temperature, and overall composition. Pore sizes are therefore assumed to be greater than 10 nm
- Reservoir is isothermal and geothermal gradients are negligible
- Flow of fluids in the reservoirs follow Darcy’s law and Fick’s law
- Multi-phase Darcy’s law is applicable
- Diffusion is only considered in gas phase
- A maximum of three mobile phases (oil, gas, water) exist in the reservoir at any time
- Water is isolated from the hydrocarbon component (i.e., water does not appear in both gas and oil phase)
- Source terms are used to express injection and production of fluids in the reservoir
- Peaceman’s well model is applicable for calculation of production/injection source terms
- No flow boundaries
- No chemical reactions
4.1.1 Overall Compositional Balance

Starting from a mass (or molar) conservation equation for any coordinates in an arbitrary control volume for component \( i \), we arrive at the overall compositional balance equation by summing each term in the mass conservation equation for each phase \( j \):

\[
\nabla \cdot \left( \sum_{j=1}^{N_\text{ph}} \left( \omega_{ij} \rho_j \frac{k_j}{\mu_j} \nabla \Phi_j + \phi S_j D_{\text{eff}} \cdot \nabla \left( \omega_{ij} \rho_j \right) \right) \right) + \left( \sum_{j=1}^{N_\text{ph}} \phi S_j r_{ij} \right) + \sum_{j=1}^{N_\text{ph}} Q_{ij} = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_\text{ph}} \phi S_j \rho_j \omega_{ij} \right)
\]

(4.1)

The terms in Eq. (4.1) from left to right represent rate of mass transport, rate of mass generation via chemical reaction, production/injection rate source term, and rate of mass accumulation in the control volume. Note that all terms in Eq. (4.1) have the unit of mass of component \( i \) per bulk volume per time \( \left( \frac{\text{mass}}{V_b \cdot \text{time}} \right) \).

4.1.2 Conservation Equations in Cartesian Coordinates

From Eq. (4.2), by assuming that diffusion is governed by Fick’s law, we can write conservation equations in Cartesian coordinates for component \( i \):

\[
\frac{\partial}{\partial x} \left( \sum_{j=1}^{N_\text{ph}} \omega_{ij} \rho_j A_x k_j \frac{\partial \Phi_j}{\partial x} + \phi S_j A_x D_{\text{eff}} \frac{\partial}{\partial x} \left( \omega_{ij} \rho_j \right) \right) \Delta x
\]

\[
+ \frac{\partial}{\partial y} \left( \sum_{j=1}^{N_\text{ph}} \omega_{ij} \rho_j A_y \frac{k_j}{\mu_j} \frac{\partial \Phi_j}{\partial y} + \phi S_j A_y D_{\text{eff}} \frac{\partial}{\partial y} \left( \omega_{ij} \rho_j \right) \right) \Delta y
\]

\[
+ \frac{\partial}{\partial z} \left( \sum_{j=1}^{N_\text{ph}} \omega_{ij} \rho_j A_z \frac{k_j}{\mu_j} \frac{\partial \Phi_j}{\partial z} + \phi S_j A_z D_{\text{eff}} \frac{\partial}{\partial z} \left( \omega_{ij} \rho_j \right) \right) \Delta z
\]

\[
+ \sum_{j=1}^{N_\text{ph}} \phi S_j r_{ij} V_b + \sum_{j=1}^{N_\text{ph}} Q_{ij} = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_\text{ph}} \phi S_j \rho_j \omega_{ij} V_b \right)
\]

(4.2)
4.1.3 Three-phase (Oil, Gas, Water) N_C-Component Flow Equations

Chemical reaction in the control volume is assumed to be negligible. Additionally, it is assumed that hydrocarbon components can form up to two phases in equilibrium. The flow equation for hydrocarbon component in Cartesian coordinates is shown in Eq. (4.3).

\[
\frac{\partial}{\partial x} \left( x_i \tilde{\rho}_o A_x \frac{k_{k_{ro}}}{\mu_o} \frac{\partial P}{\partial x} + y_i \tilde{\rho}_g A_x \frac{k_{k_{rg}}}{\mu_g} \frac{\partial P_g}{\partial x} + y_i \phi S_i A_x \frac{D_{eff}}{5.615} \frac{\partial \tilde{P}_g}{\partial x} \right) \Delta x \\
- \frac{\partial}{\partial x} \left( \frac{1}{144 g_c} \rho_o x_i \tilde{\rho}_o A_x \frac{k_{k_{ro}}}{\mu_o} \frac{\partial G}{\partial x} + \frac{1}{144 g_c} \rho_g x_i \tilde{\rho}_g A_x \frac{k_{k_{rg}}}{\mu_g} \frac{\partial G}{\partial x} \right) \Delta x \\
+ \frac{\partial}{\partial y} \left( x_i \tilde{\rho}_o A_y \frac{k_{k_{ro}}}{\mu_o} \frac{\partial P}{\partial y} + y_i \tilde{\rho}_g A_y \frac{k_{k_{rg}}}{\mu_g} \frac{\partial P_g}{\partial y} + y_i \phi S_i A_y \frac{D_{eff}}{5.615} \frac{\partial \tilde{P}_g}{\partial y} \right) \Delta y \\
- \frac{\partial}{\partial y} \left( \frac{1}{144 g_c} \rho_o x_i \tilde{\rho}_o A_y \frac{k_{k_{ro}}}{\mu_o} \frac{\partial G}{\partial y} + \frac{1}{144 g_c} \rho_g x_i \tilde{\rho}_g A_y \frac{k_{k_{rg}}}{\mu_g} \frac{\partial G}{\partial y} \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( x_i \tilde{\rho}_o A_z \frac{k_{k_{ro}}}{\mu_o} \frac{\partial P}{\partial z} + y_i \tilde{\rho}_g A_z \frac{k_{k_{rg}}}{\mu_g} \frac{\partial P_g}{\partial z} + y_i \phi S_i A_z \frac{D_{eff}}{5.615} \frac{\partial \tilde{P}_g}{\partial z} \right) \Delta z \\
- \frac{\partial}{\partial z} \left( \frac{1}{144 g_c} \rho_o x_i \tilde{\rho}_o A_z \frac{k_{k_{ro}}}{\mu_o} \frac{\partial G}{\partial z} + \frac{1}{144 g_c} \rho_g x_i \tilde{\rho}_g A_z \frac{k_{k_{rg}}}{\mu_g} \frac{\partial G}{\partial z} \right) \Delta z \\
+ M_i = \frac{V_b}{5.615} \frac{\partial}{\partial t} \left( \phi S_i \tilde{\rho}_o x_i + \phi S_g \tilde{\rho}_g y_i \right)
\] (4.3)

Similarly, flow equation for water component in Cartesian coordinates is shown in Eq. (4.4).

\[
\frac{\partial}{\partial x} \left( A_w \frac{k_{k_{rw}}}{\mu_w B_w} \frac{\partial P_w}{\partial x} - \frac{1}{144 g_c} \rho_w A_w \frac{k_{k_{rw}}}{\mu_w B_w} \frac{\partial G}{\partial x} \right) \Delta x + \frac{\partial}{\partial y} \left( A_w \frac{k_{k_{rw}}}{\mu_w B_w} \frac{\partial P_w}{\partial y} - \frac{1}{144 g_c} \rho_w A_w \frac{k_{k_{rw}}}{\mu_w B_w} \frac{\partial G}{\partial y} \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( A_w \frac{k_{k_{rw}}}{\mu_w B_w} \frac{\partial P_w}{\partial z} - \frac{1}{144 g_c} \rho_w A_w \frac{k_{k_{rw}}}{\mu_w B_w} \frac{\partial G}{\partial z} \right) \Delta z + q_w^e = \frac{V_b}{5.615} \frac{\partial}{\partial t} \left( \phi S_w \right)
\] (4.4)
4.2 Phase Behavior Model

4.2.1 Generalized Cubic Equation of State

An Equation of State (EoS) is often used to perform fluid equilibrium calculations and property predictions. The generalized cubic equation of state in the Z form is shown in Eq. (4.5).

\[ Z^3 + \left[ (m_1 + m_2 - 1)B - 1 \right]Z^2 + \left[ A + m_1m_2B^2 - (m_1 + m_2)B(B+1) \right]Z \]
\[ - \left[ AB + m_1m_2B^2(B+1) \right] = 0 \]  
(4.5)

The coefficient \( m_1 \) and \( m_2 \) are used based on the selected EoS. The coefficients \( A \) and \( B \) can be calculated using Eqs. (4.6) and (4.7).

\[ A = \sum_{i=1}^{N_c} \sum_{j=1}^{N_c} c_{i,j} A_{ij} \]  
(4.6)

\[ B = \sum_{i=1}^{N_c} c_i B_i \]  
(4.7)

The parameters \( A_{ij}, A_i, B_i, P_{ri}, \) and \( T_{ri} \) can be calculated as follow.

\[ A_{ij} = (1-\delta_{ij})(A_i A_j)^{0.5} \]  
(4.8)

\[ A_i = \Omega_i^r \left[ 1 + m_i \left( 1 - T_{ri}^{0.5} \right) \right]^{2} \frac{P_{ri}}{T_{ri}^2} \]  
(4.9)

\[ B_i = \Omega_i^r \frac{P_{ri}}{T_{ri}} \]  
(4.10)

\[ P_{ri} = \frac{P}{P_{ci}} \]  
(4.11)

\[ T_{ri} = \frac{T}{T_{ci}} \]  
(4.12)
where $\delta_{ij}$ is binary interaction parameter between component $i$ and $j$. The EoS constant $m_1, m_2$, co-volume parameter ($\Omega_{ai}^o$), and attraction parameter ($\Omega_{bi}^o$) are used based on choice of EoS and are shown in Table 4-1. In some instance, the attraction and co-volume parameters can be component-dependent.

Table 4-1: Equation of State constant parameters

<table>
<thead>
<tr>
<th>Equation of State</th>
<th>$m_1$</th>
<th>$m_2$</th>
<th>$\Omega_{ai}^o$</th>
<th>$\Omega_{bi}^o$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peng-Robinson (Peng and Robinson, 1976)</td>
<td>$1 + \sqrt{2}$</td>
<td>$1 - \sqrt{2}$</td>
<td>0.45724</td>
<td>0.07780</td>
</tr>
<tr>
<td>Soave-Redlich-Kwong (Soave, 1972)</td>
<td>0</td>
<td>1</td>
<td>0.42747</td>
<td>0.08664</td>
</tr>
</tbody>
</table>

For PR-EoS,

$$m_i = \begin{cases} 
0.374640 + 1.54226\omega_i - 0.26992\omega_i^3 & \text{if } \omega_i \leq 0.49 \\
0.379642 + 1.48503\omega_i - 0.164423\omega_i^2 + 0.016666\omega_i^3 & \text{if } \omega_i > 0.49 
\end{cases} \quad (4.13)$$

For SRK-EoS,

$$m_i = 0.48 + 1.574\omega_i - 0.176\omega_i^2 \quad (4.14)$$

The parameter $c_i$ in Eq. (4.8) and (4.9) represents compositions of the phase or mixture of our interest.

4.2.2 Rachford-Rice Objective Function

Rachford and Rice (1952) performed two-phase split calculations. The objective function is in a form of molar balance for two-phase system in equilibrium.

$$g(V) = \sum_{i=1}^{N_c} \frac{c_i (K_i - 1)}{1 + V (K_i - 1)} = 0 \quad (4.15)$$

Eq. (4.15) is solved for $V$ which is the molar fractional amount of vapor that is found in the system equilibrium at given conditions. The $K_i$ values are the ratio between the mole fraction of
vapor phase of the \( i \)th component and the mole fraction of the liquid phase of the same component as can be seen in Eq. (4.16):

\[
K_i = \frac{y_i}{x_i}. \tag{4.16}
\]

Initial estimates of \( K_i \)-values in the iterative procedure are based on the Wilson’s correlation (1968) described in Eq. (4.17) is used.

\[
K_i = \frac{1}{P_{ri}} \exp \left[ 5.37 \left( 1 + \omega_i \right) \left( 1 - \frac{1}{T_{ri}} \right) \right] \tag{4.17}
\]

where \( P_{ri} \) and \( T_{ri} \) are reduced pressure and temperature, respectively and \( \omega_i \) is Pitzer’s acentric factor.

### 4.2.3 Successive Substitution Method

Fugacity of the component in each phase is used as a criterion for thermodynamic equilibrium. Equilibrium ratio \((K_i)\) is directly related to the fugacity coefficients as follows:

\[
K_i = \frac{f_i^L}{\phi_i} = \frac{y_i}{x_i} \frac{f_i^L}{f_i^V} = \frac{y_i}{x_i} \frac{f_i^L}{f_i^V}. \tag{4.18}
\]

The updated to find \( K_i \)-values are calculated through Successive Substitution Method (SSM):

\[
K_i^{n+1} = \left( \frac{y_i}{x_i} \right)^n \left( \frac{f_i^L}{f_i^V} \right)^n \tag{4.19}
\]

\[
K_i^{n+1} = K_i^n \left( \frac{f_i^L}{f_i^V} \right)^n \tag{4.20}
\]

Successive Substitution (SS) updates all previous equilibrium ratios \((K_i)\) using the fugacities predicted by the equation of state in the previous iteration. The iteration requires initial estimates
of the \( K_i \) values. Wilson’s correlation (Eq. (4.17)) or \( K_i \) values from previous iteration or time step are used to initialize the \( K_i \) values. Convergence criteria are achieved when fugacity ratios of all the components in the systems are close to unity as described in Eq. (4.21).

\[
\max \left| \ln \left( f_i^L \right) - \ln \left( f_i^V \right) \right| < 10^{-10} \quad \text{for} \quad i = 1, 2, 3, \ldots, N_C \quad (4.21)
\]

When a component mole fraction is tiny (\(<10^{-7}\)), the component is excluded from consideration of the convergence criteria in Eq. (4.21).

Successive Substitution is well known for its robustness. However, this technique has a linear convergence rate. On the other hand, Newton-Raphson method has a quadratic convergence rate, but it has a smaller radius of convergence. Therefore, it is suggested that a combination of SS steps followed by Newton-Raphson method (Pan and Firoozabadi, 2001; Whitson and Brule, 2000; Gorucu, 2013). SS method is performed to get closer to the solution. After a switching criterion is met, the solution technique is switched to Newton-Raphson method. This study follows this approach. The switch criterion shown in Eq. (4.22) is used here (Gorucu, 2013).

\[
\max \left| \ln \left( f_i^L \right) - \ln \left( f_i^V \right) \right| < 10^{-4} \quad \text{for} \quad i = 1, 2, 3, \ldots, N_C \quad (4.22)
\]

Using initial estimates from Wilson’s correlation, a typical flash calculation takes 10-12 SS steps followed by 3-4 NR steps. The Newton-Raphson method is discussed in the next section.

### 4.2.4 Minimum-variables Newton-Raphson Algorithm

To accelerate the convergence of flash calculations, Michelsen’s minimum-variables Newton-Raphson (MVNR) protocol is used when the switching criterion (Eq. (4.22)) is met. Let \( L \) and \( V \) superscripts be liquid and vapor phase identifications, respectively. The fugacity residual equation can be described as follows.
\[ R_i = \ln f_i^L - \ln f_i^V \]  

(4.23)

Differentiating Eq. (4.23) with respect to liquid mole number \( n_i^L \) yields

\[ \frac{\partial R_i}{\partial n_i^L} = \frac{\partial \ln f_i^L}{\partial n_i^L} - \frac{\partial \ln f_i^V}{\partial n_i^L} \]  

(4.24)

\[ \frac{\partial R_i}{\partial n_i^L} = \frac{\partial \ln (x_i \phi_i^L)}{\partial n_i^L} - \frac{\partial \ln (y_i \phi_i^L)}{\partial n_i^L} \]  

(4.25)

The total moles of a component must be conserved. For component \( k \), the total mole is the sum of moles of component \( k \) in liquid phase and vapor phase.

\[ n_k^L + n_k^V = n_k^{\text{total}} \]  

(4.26)

In differential form, Eq. (4.26) can be written as follows.

\[ \partial n_k^L + \partial n_k^V = \partial n_k^{\text{total}} = 0 \]  

(4.27)

Thus,

\[ \partial n_k^L = -\partial n_k^V \]  

(4.28)

Substituting Eq. (4.28) into Eq. (4.25) yields:

\[ \frac{\partial R_i}{\partial n_i^L} = \frac{\partial \ln (x_i \phi_i^L)}{\partial n_i^L} + \frac{\partial \ln (y_i \phi_i^L)}{\partial n_i^L} \]  

(4.29)

For \( i = k \),

\[ \frac{\partial R_k}{\partial n_k^L} = \left( \frac{\partial \ln \phi_k^L}{\partial n_k^L} + \frac{1}{x_k \beta_L} - \frac{1}{\beta_L} \right) + \left( \frac{\partial \ln \phi_k^V}{\partial n_k^L} + \frac{1}{y_k \beta_v} - \frac{1}{\beta_v} \right) \]  

(4.30)

For \( i \neq k \),

\[ \frac{\partial R_i}{\partial n_k^L} = \left( \frac{\partial \ln \phi_k^L}{\partial n_k^L} - \frac{1}{\beta_L} \right) + \left( \frac{\partial \ln \phi_i^V}{\partial n_k^L} - \frac{1}{\beta_v} \right) \]  

(4.31)

More details on analytic derivative of \( \frac{\partial \ln \phi_i^L}{\partial n_i^L} \) can be found in Appendix B.2.
A sample Jacobian matrix for MVNR protocol for a 3-component system is shown below.

\[
\begin{bmatrix}
\frac{\partial \ln \phi^L_i}{\partial n^L_i} + \frac{1}{x_i \beta_L} - \frac{1}{\beta_L} + \frac{1}{x_i \beta_L} - \frac{1}{y_i \beta_v} - \frac{1}{\beta_v} \\
\frac{\partial \ln \phi^V_i}{\partial n^V_i} + \frac{1}{y_i \beta_v} - \frac{1}{\beta_v} + \frac{1}{x_i \beta_L} - \frac{1}{\beta_L} + \frac{1}{x_i \beta_L} - \frac{1}{y_i \beta_v} - \frac{1}{\beta_v} \\
\frac{\partial \ln \phi^L_i}{\partial n^L_i} + \frac{1}{x_i \beta_L} - \frac{1}{\beta_L} + \frac{1}{y_i \beta_v} - \frac{1}{y_i \beta_v} - \frac{1}{\beta_v} + \frac{1}{x_i \beta_L} - \frac{1}{\beta_L} + \frac{1}{x_i \beta_L} - \frac{1}{y_i \beta_v} - \frac{1}{\beta_v} \\
\end{bmatrix}
\]

4.2.5 Fugacity

In order for a fluid to be in equilibrium, the temperature, pressure, chemical potential must be equal in all phases. Since the system has constant pressure and temperature, the chemical potential must be the same at equilibrium. In other words, fugacities of all components in each phase must be equal as shown in Eq. (4.32).

\[f^L_i = f^V_i \quad \text{for } i = 1, 2, 3, \ldots, N_C\]  \hspace{1cm} (4.32)

where \(f^L_i\) and \(f^V_i\) are fugacities of component \(i\) in liquid phase and vapor phase, respectively. If the system has equal fugacities for a component in both phases, the system is said to have zero net transfer of a component, and equilibrium has been established. Fugacity is calculated from fugacity coefficient (\(\phi\)) as follows:

\[\phi^V_i = \frac{f^V_i}{y_i P_s} \rightarrow f^V_i = y_i P_s \phi^V_i\]  \hspace{1cm} (4.33)
where $\phi^e_i$ and $\phi^l_i$ are fugacity coefficients of component $i$ in vapor and liquid phases, respectively. The fugacity of component $i$ in phase $j$ can be calculated from the following equation.

$$
\ln \phi^j_i = -\ln \left(Z_j - B_j \right) + \frac{A_j}{(m_1 - m_2)B_j} \left(\frac{2\sum_{k=1}^{n_c} A_k c_k}{A_j} - \frac{B_1}{B_j} \ln \left[ \frac{Z_j + m_2 B_j}{Z_j + B_j} \right] + \frac{B_1}{B_j}(Z_j - 1) \right)
$$

(4.35)

Using Eqs. (4.33), (4.34), and (4.35), the updated $K_i$’s can be calculated as follows from Eq. (4.18). An iterative procedure is used to determine the exact value of $K_i$ at equilibrium.

### 4.2.6 Phase Stability

At a given reservoir condition and fluid composition, we need to determine whether a given fluid composition under a given pressure and temperature will split into two phases or remain stable as single phase. Michelsen (1982) suggests creating a second-phase inside any given mixture to then verify whether such a system is stable or not. The procedure is performed for liquid-like and vapor-like phases since two possibilities can occur (i.e., second phase can be liquid-like or vapor-like). To have a successful test, the $Z$ factor that minimizes Gibbs free energy must be selected from the cubic polynomial equation. The following procedure is used in the phase stability analysis (Ayala, 2004):

1. Calculate vapor-like second-phase mole number $Y_j$:

   $$
   Y_j = z_j K_i
   $$

   (4.36)

2. Calculate the sum of mole numbers $S_{Vj}$:
3. Normalize the second-phase mole number to obtain the mole fraction:

\[ y_i = \frac{Y_i}{S_v} \]  

(4.38)

4. Calculate the second-phase fugacity

5. Calculate the correction for \( K_i \)-values

\[ f_i = \frac{f_{zi}}{f_{yi}} \cdot \frac{1}{S_v} \]  

(4.39)

\[ K_i^{n+1} = K_i^n \cdot f_i \]  

(4.40)

6. Check whether convergence is achieved or a trivial solution is approached using the following equations:

Convergence:

\[ \sum_{i=1}^{N_c} (R_i - 1)^2 < 10^{-10} \]  

(4.41)

Trivial solution:

\[ \sum_{i=1}^{N_c} (\ln K_i)^2 < 10^{-4} \]  

(4.42)

The procedure is stopped when either convergence is achieved or a trivial solution is approached.

Create a liquid-like second phase by following the same previous steps (1-6) by replacing Eq. (4.36) to Eq. (4.39) with Eq. (4.43) to Eq. (4.46), respectively. The same \( K_i \) updating scheme (Eq. (4.40)), convergence criteria (Eq. (4.41)), and trivial solution criteria (Eq. (4.42)) are used for liquid-like second phase.

\[ Y_i = \frac{z_i}{K_i} \]  

(4.43)

\[ S_L = \sum_{i=1}^{N_c} Y_i \]  

(4.44)
\[ y_i = \frac{Y_i}{S_L} \]  

(4.45)  

\[ R_i = \frac{f_{si}}{f_{zi}} S_L \]  

(4.46)

Once step 1-6 has been completed, the results are classified as discussed below:

1. Stable (single-phase condition) if:
   a. Both tests yield \( S \leq 1 \) (\( S_L < 1 \) and \( S_V < 1 \))
   b. Both tests converge to a trivial solution
   c. One test converges to a trivial solution and the other gives \( S \leq 1 \)

2. Unstable (two-phase condition) if one test yields \( S > 1 \)

It should be noted that phase stability analysis is only called when capillary pressure is not considered in phase behavior calculation. In contrast, a modified negative flash is used instead to determine the number of phases in equilibrium when capillary pressure is considered.

### 4.3 Compressibility of Formation

Porosity reduction as a result of compaction can be expressed as a function of change in pressure and compressibility of formation. Let \( c_{f, \phi} \) be compressibility of formation on porosity. Pressure-dependency equation for compressibility of formation can be expressed in Eq. (4.47).

\[ \phi = \phi^\circ \exp \left[ c_{f, \phi} \left( P_o - P_{ref} \right) \right] \]  

(4.47)

Applying Taylor’s series expansion, the first approximation compressibility of formation can be obtained.

\[ \phi = \phi^\circ \left[ 1 + c_{f, \phi} \left( P_o - P_{ref} \right) \right] \]  

(4.48)

Rearrangement of Eq. (4.48) gives:
\[ \frac{\phi}{\phi^o} = 1 + c_{f,\phi} \left( P_o - P_{ref} \right) \] (4.49)

Reiss (1980) relates permeability and porosity.

\[ \frac{k}{k^o} = \left( \frac{\phi}{\phi^o} \right)^3 \] (4.50)

By combining the definition of compressibility of formation, we obtain:

\[ \frac{k}{k^o} = \left( \frac{\phi}{\phi^o} \right)^3 = \left[ 1 + c_{f,\phi} \left( P_o - P_{ref} \right) \right]^3 \] (4.51)

where \( k^o, \phi^o \), and \( P_{ref} \) are permeability, porosity at initial condition, and reference pressure, respectively, and \( c_{f,\phi} \) is the compressibility of formation on porosity. Thus, the porosity and permeability changes by the effect of compressibility of formation are shown below.

\[ k = k^o \left[ 1 + c_{f,\phi} \left( P_o - P_{ref} \right) \right]^3 \] (4.52)

In the case that compaction impacts the permeability at different rate compared to porosity, one can assign a different value of compressibility of formation on permeability. This can be seen in Eq. (4.53) where \( c_{f,k} \) is compressibility of formation on permeability and \( \kappa \) is an exponent for pressure-dependency compressibility of formation.

\[ k = k^o \left[ 1 + c_{f,k} \left( P_o - P_{ref} \right) \right]^\kappa \] (4.53)

Eq. (4.53) allows us to be flexible with pressure-dependent compressibility in simulation. When \( c_{f,k} \) is equal to \( c_{f,\phi} \), and \( \kappa \) is equal to 3, Eq. (4.53) collapses to Eq. (4.52).
4.4 Capillary Pressure

Leverette J-function is a dimensionless parameter often used to calculate capillary pressure for a given rock that are similar in pore structure but different in permeability, porosity and wetting properties. It is described by the following equation. For air-mercury system permeability \( k_{lab} \) and porosity \( \phi_{lab} \) are obtained from the core sample.

\[
J_{a-Hg} = \frac{P_{ij}}{\sigma \cos \theta} \sqrt{\frac{k_{lab}}{\phi_{lab}}} \tag{4.54}
\]

J-function can be used to relate capillary pressure between gas-oil and water-oil in a water-wet system as a function of J-function and wetting phase saturation as shown in Eq. (4.55) and Eq. (4.56).

\[
P_{cgo} = J_{a-Hg} \cdot (\sigma \cos \theta)_{go} \sqrt{\frac{\phi_{resv}}{k_{resv}}} = f(S_{wet}) = f(S_w + S_o) \tag{4.55}
\]

\[
P_{cow} = J_{a-Hg} \cdot (\sigma \cos \theta)_{ow} \sqrt{\frac{\phi_{resv}}{k_{resv}}} = f(S_{wet}) = f(S_w) \tag{4.56}
\]

The general form of capillary pressure relationship is described as follows.

\[
P_c = P_{\text{wet}} - P_{\text{non-wet}} \tag{4.57}
\]

4.5 Wettability

Reservoirs may be water wet or oil wet based on type of formation. For the case of water-wet reservoir, water is the wetting phase, oil is the intermediate phase, and gas is the non-wetting phase. On the other hand, when the reservoir is oil wet, oil is the wetting phase, gas is the intermediate phase, and water is the non-wetting phase as can be seen in Figure 4-1 (Zhou and Blunt, 1998). Note that oil phase pressure is used as the principal unknown.
4.5.1 Water-wet Reservoir

The capillary pressure relationship between oil and water and between gas and oil can be described by Eq. (4.58) and Eq. (4.59), respectively.

\[ P_{cow} = P_o - P_w \rightarrow P_w = P_o - P_{cow} \]  
\[ (4.58) \]

\[ P_{cgo} = P_g - P_o \rightarrow P_g = P_o + P_{cgo} \]  
\[ (4.59) \]

Note that \( P_{cow} = f(S_w) \) and \( P_{cgo} = f(S_g) \).

4.5.2 Oil-wet Reservoir

The capillary pressure relationship between oil and gas and between gas and water can be described by Eq. (4.60) and Eq. (4.61), respectively.

\[ P_{cgo} = P_g - P_o \rightarrow P_g = P_o + P_{cgo} \]  
\[ (4.60) \]

\[ P_{cwg} = P_w - P_g \rightarrow P_w = P_g + P_{cwg} \]  
\[ (4.61) \]
Combining Eq. (4.60) and Eq. (4.61) gives the expression of \( P_w \) in terms of oil phase pressure and capillary pressure.

\[
P_w = P_o + P_{cwg} + P_{egw}
\] (4.62)

Note that \( P_{egw} = f(S_o) \) and \( P_{cwg} = f(S_w) \).

4.6 Relative Permeability

Relative permeability is assumed to be a function of saturation. Stone’s Three-phase Model II (Stone, 1973) is used to calculate the intermediate phase relative permeability. Assuming oil is an intermediate phase, the oil relative permeability can be calculated from Eq. (4.63):

\[
\frac{k_{ro}}{k_{row}} = \left( \frac{k_{row}}{k_{row} + k_{rw}} \right) \left( \frac{k_{rgw} + k_{rg}}{k_{row} + k_{rg}} \right) - \left( k_{rw} + k_{rg} \right)
\] (4.63)

Note that Eq. (4.63) is written for a water-wet reservoir. When the reservoir is oil wet, a different calculation has to be made. Stone’s II method is used to determine the relatively permeability of the gas phase. In oil-wet reservoir, \( k_{rw} = f(S_w) \), \( k_{ro} = f(S_o) \), and \( k_{rg} = f(S_o, S_w) \).

\[
\frac{k_{rg}}{k_{rgo}} = \left( \frac{k_{rgo}}{k_{rgo} + k_{ro}} \right) \left( \frac{k_{rgw} + k_{rw}}{k_{rgo} + k_{rw}} \right) - \left( k_{ro} + k_{rw} \right)
\] (4.64)

4.7 Diffusion

Darcy’s law is used to relate fluid flow in porous media to pressure gradient. However, in tight formation such that \( k < 0.1 \) mD, flow is no longer dominated by Darcian flow. Ertekin et al. (1986) suggests that flow occurs by pressure gradients and concentration gradients (i.e.,
diffusion) also known as multi-mechanistic flow. Different diffusion mechanisms (molecular self-diffusion, Knudsen diffusion, surface diffusion) can take place in porous media (Smith and Williams, 1984; Ertekin et al., 1986; da Silva and Belery, 1989; Ayala, 2004). Molecular self-diffusion is the diffusion of a phase due to imbalanced molecule-to-molecule collisions in regions of different concentrations. Knudsen diffusion is a type of diffusion which dominates in a tight formation where pore diameter is comparable to or smaller than the mean free path of the particles. The molecules collide with pore walls more than with each other. In this scenario, molecule-wall collisions dominate the diffusion process. Surface diffusion occurs when adsorption takes place. This type of diffusion is the transport of adsorbed gas molecules along the surface of the rock or the interface between gas and fluid.

In this research, two options of diffusion coefficient are used. First, the concept of effective diffusion coefficient as suggested by Ayala (2004) is used to represent net flow of gas via diffusion as a group. For flexibility, when the diffusion coefficient is assumed to be the property of a component, one can assign to each component a diffusion coefficient. Here, the same value of diffusion coefficient is used for all components. The transport term in x-direction with diffusion in the gas phase is shown in Eq. (4.65).

$$\frac{\partial}{\partial x} \left( \phi S_g A_g \frac{D_{\text{eff}}}{5.615} \frac{\partial\left(y_i \tilde{\rho}_g\right)}{\partial x} \right) \Delta x$$

(4.65)

From Eq. (4.65), one can assumes that $y_i$ is constant spatially and therefore can be taken out of the partial derivative.

$$\frac{\partial}{\partial x} \left( y_i \phi S_g A_g \frac{D_{\text{eff}}}{5.615} \frac{\partial\tilde{\rho}_g}{\partial x} \right) \Delta x$$

(4.66)
4.8 Adsorption

4.8.1 Gas Sorption Rate

Non-equilibrium sorption rate model for calculating the gas sorption is proposed by King et al. (1986). Eq. (4.67) shows the non-equilibrium sorption model. The model is pressure and time dependent and is derived based on the rate of gas adsorbed in the coal.

\[
\frac{dV_{a,i}}{dt} = \frac{1}{\tau}(V_{a,i} - V_{e,i})
\]  

(4.67)

where \( V_{a,i}, V_{e,i}, \) and \( \tau \) are the amount of gas adsorbed of gas component \( i \), gas desorption capacity of the gas component \( i \), and pseudo-steady state sorption time constant, respectively. The pseudo-steady state sorption time constant (\( \tau \)) represents the time delay of sorbed gas transport through the micropores in the coal matrix. Rearranging Eq. (4.67) gives:

\[
\frac{dV_{a,i}}{V_{a,i} - V_{e,i}} = \frac{dt}{\tau}
\]  

(4.68)

In order for the sorption rate formulation to be applicable for the instantaneous sorption process, Manik et al. (2002) proposed that the adsorption capacity, \( V_{e,i} \), be evaluated at the time level \( n+1 \). By integrating both sides of Eq. (4.68), we can obtain the non-equilibrium sorption rate formulation:

\[
\int_{V_{a,i}^{n+1}}^{V_{a,i}^{n+2}} \frac{dV_{a,i}}{V_{a,i} - V_{e,i}} = \int_{t^n}^{t^{n+1}} \frac{dt}{\tau}
\]  

(4.69)

\[
V_{a,i}^{n+1} = V_{a,i}^{n} \exp \left(-\frac{\Delta t}{\tau}\right) + V_{e,i}^{n+1} \left[1 - \exp \left(-\frac{\Delta t}{\tau}\right)\right]
\]  

(4.70)

If the sorption process reaches equilibrium instantaneously, the pseudo-steady state sorption time constant (\( \tau \)) approaches zero and Eq. (4.70) reduces to Eq. (4.71).
\[ V_{a,i}^{n+1} = V_{e,i}^{n+1} \]  
\[ (4.71) \]

On the other hand, if the pseudo-steady state sorption time constant (\( \tau \)) approaches infinity, no adsorption occurs, and Eq. (4.70) reduces to Eq. (4.72).

\[ V_{a,i}^{n+1} = V_{a,i}^{p} \]  
\[ (4.72) \]

Finally, the gas sorption rate for gas component \( i \) can be calculated from Eq. (4.73). The term \( M_{i}^{spr} \) has the unit of \( \text{lbmol STB day scf} \).

\[ M_{i}^{spr} = \frac{1}{5.615} \frac{V_{a,i}^{n+1} - V_{a,i}^{p}}{\Delta t} \]  
\[ (4.73) \]

### 4.8.2 Multi-component Sorptions

In this research, multi-component sorption capacity is calculated based on thermodynamic equilibrium between gas components in free and adsorbed phase (Myers and Prausnitz, 1965). From an ideal adsorbed solution model, one can establish equilibrium relations between gas compositions in the free phase (\( y_i \)) and adsorbed phase (\( a_i \)) by representing fugacity of the adsorbed phase as a function of free phase at standard condition.

\[ f_{i}^\text{free} = f_{i}^\text{ads} = f_{i}^o a_i \]  
\[ (4.74) \]

\[ P y_i \phi_i = P^o a_i \phi_i^o \]  
\[ (4.75) \]

where \( f_{i}^o \) is fugacity of pure component \( i \) at standard condition, \( P^o \) is pressure at standard condition, and \( \phi_i^o \) is fugacity coefficient of pure component at standard condition. The spreading
pressure group of component $i$ at standard state ($\psi_i^{o}$) can be defined as an integral of pure component adsorption capacity ($n_i^{o}$) and fugacity of adsorbed phase ($f_i$):

$$\psi_i^{o} = \frac{\pi_i^{o} A}{RT} = \int_0^{f_i^{o}} \frac{n_i^{o}}{f_i} df_i$$

(4.76)

Manik et al. (2002) proposed an iterative procedure to solve for adsorbed phase composition ($a_i$) using an objective function based on adsorbed composition constraint.

$$\mathcal{R}(\psi) = \sum_{i=1}^{N_c} a_i - 1 = \sum_{i=1}^{N_c} \left( \frac{f_i^{free}}{f_i^{o}} \right) - 1 = 0$$

(4.77)

$$\psi^{o,k+1} = \psi^{o,k} - \frac{\mathcal{R}(\psi^{o})}{d\mathcal{R}(\psi^{o})/d\psi^{o}}$$

(4.78)

The derivative term $\frac{d\mathcal{R}(\psi^{o})}{d\psi^{o}}$ in Eq. (4.78) can be calculated using Eq. (4.79).

$$\frac{d\mathcal{R}(\psi^{o})}{d\psi^{o}} = \frac{d}{d\psi^{o}} \left[ \sum_{i=1}^{N_c} \left( \frac{f_i^{free}}{f_i^{o}} \right) - 1 \right] = \sum_{i=1}^{N_c} \left[ - \frac{f_i^{free}}{(f_i^{o})^2} \frac{df_i^{o}}{d\psi^{o}} \right]$$

(4.79)

where $\frac{df_i^{o}}{d\psi^{o}}$ is obtained from taking the derivative on both side of Eq. (4.76) with respect to $\psi^{o}$.

$$\frac{df_i^{o}}{d\psi^{o}} = \frac{f_i^{o}}{n_i^{o}}$$

(4.80)

Substitution of Eqs. (4.79) and (4.80) into Eq. (4.78) gives the final equation for calculating the spreading pressure group for multi-component sorption.
\[
\psi^o |_{k+1}^k = \psi^o |^k - \left[ \frac{\sum_{i=1}^{N_c} \left( f_i^{\text{free}} \right) / f_i^o}{\sum_{i=1}^{N_c} \left( f_i^{\text{free}} / n_i^o \right) } \right]^k. \tag{4.81}
\]

Once the new \( \psi^o \) is obtained, \( f_i^o \) and \( n_i^o \) are updated using Eqs. (4.83) and (4.84). The convergence criteria for Eq. (4.81) is achieved when Eq. (4.82) is satisfied.

\[
\left| \psi^o |_{k+1}^k - \psi^o |^k \right| \leq 10^{-10} \tag{4.82}
\]

In the iterative procedure, the fugacity of component \( i \) in the free gas phase (\( f_i^{\text{free}} \)) is kept constant the entire process. Once the convergence is achieved, adsorption composition (\( a_i \)) and adsorption capacity (\( V_{a,i} \)) can be calculated from Eqs. (4.83) to (4.86).

\[
f_i^o = P_{L,i} \exp \left( \frac{\psi^o}{V_{L,i}} \right) - P_{L,i} \tag{4.83}
\]

\[
n_i^o = \frac{V_{L,i} f_i^o}{P_{L,i} + f_i^o} \tag{4.84}
\]

\[
a_i = \frac{f_i^{\text{free}}}{f_i^o} \tag{4.85}
\]

\[
V_{a}^{\text{total}} = \frac{1}{\sum_{i=1}^{N_c} \frac{a_i}{n_i^o}} \tag{4.86}
\]

Finally, one can calculate adsorption capacity of component \( i \) using Eq. (4.87).

\[
V_{a,i} = a_i V_{a}^{\text{total}} \tag{4.87}
\]

In Eq. (4.81), the initial estimated value of \( \psi^o \) can be calculated using the adsorption composition from the previous iteration/timestep and Eq. (4.88) and (4.89):
\[ \psi^a = \sum_{i=1}^{N_c} a_i \psi_i^a \]  \hspace{2cm} (4.88)

\[ \psi_i^a = V_{L,i} \ln \left( \frac{P_{L,i} + f_{i}^a}{P_{L,i}} \right) \]  \hspace{2cm} (4.89)

Langmuir volume and pressure for each component must be provided. Steps in iteratively solving for adsorption capacity and adsorbed composition are shown in Figure 4-2.

Alternatively, Manik et al. (2002) suggested a curve fitting method to represent other isotherms such as Toth and UNILAN in simpler forms (Eqs. (4.90) and (4.91)). Once curve fitting is done,
the coefficients \( c_{1,i}, c_{2,i}, c_{3,i} \) can be obtained and used in the iterative procedure described in this section.

\[
\begin{align*}
    n_i^o &= \frac{c_{1,i} f_i^o}{c_{2,i} + f_i^o} \\
    n_i^e &= \frac{c_{1,i} f_i^e}{\left( c_{2,i} + f_i^e \right)^{c_{3,i}}}
\end{align*}
\]  

(4.90)  

(4.91)

### 4.9 Phase Tracking

For a grid block that is initially single-phase oil, phase stability analysis is performed to determine if the fluid is still stable under an updated reservoir condition. If the fluid is unstable at the given condition, flash calculation is performed to determine the phase saturations and phase compositions. If the reservoir is stable, the phase type (single-phase oil or single-phase gas) is assumed to be the same as the previous iteration/timestep. In other words, it is assumed that phase flip does not occur (i.e., single-phase oil at the beginning of the iteration does not change into single-phase gas at the end of the iteration and vice versa).

### 4.10 Highlights of the Chapter

In this chapter, the formulation of the compositional model is discussed. The topics covered in this chapter are summarized as follows:

- Starting from the overall compositional balance, the governing flow equations for hydrocarbon components and water are derived. The flow equations are written in Cartesian coordinates. Assumptions of the compositional model are discussed.
• Generalized cubic equation of state is used to perform fluid equilibrium calculations. Phase mole fractions and phase compositions are calculated by solving equilibrium constraints using successive substitution and Minimum-variables Newton-Raphson protocol. Phase stability analysis is used determine the number of phases that can exist in equilibrium. No phase flip is allowed in the model.

• The formation can be water wet or oil wet. When the reservoir is water wet, oil is an intermediate phase and gas is non-wetting phase. Conversely, when the reservoir is oil wet, gas is an intermediate phase and water is non-wetting phase. The capillary pressure and relative permeability relationships are derived based on wettability.

• As reservoir pressure changes, porosity and permeability can change due to compressibility of formation. The change in porosity and permeability is assumed to be a function of compressibility and difference in pressure between the reference state and the current state.

• In tight formation, diffusion is the dominating flow mechanism. In this research, diffusion only occurs in gas phase. Multi-mechanistic flow where flow is driven by pressure gradients and concentrations gradients is considered. Diffusion coefficient is treated as a single-valued constant for each component.

• Thermodynamic equilibrium between adsorbed gas phase and free gas phase for multi-component sorption model is implemented in the model. At equilibrium, adsorbed gas composition and total amount of adsorption are calculated. The rate of adsorption or desorption follows a non-equilibrium sorption model.
Chapter 5

Numerical Reservoir Simulation

In this chapter, numerical treatment of the governing equations is discussed. The topics to be covered in this chapter are as follows: First, the governing flow equations are approximated using finite difference formulation. The treatment of the transmissibility terms and well source/sink term in the finite difference approximation is presented. During the simulation, the number of hydrocarbon phases that co-exist in equilibrium has to be checked. Handling of phase appearance and disappearance is discussed. In the discretized model, original oil-, gas-, hydrocarbon-in-place in each grid block is summed for the entire reservoir to obtain the oil-in-place. Internal checks such as incremental and cumulative material balance checks and residual check have been implemented to ensure the convergence of the time step. Finally, linear solver used in the development of the model and time step control numerical control of the simulator is briefly discussed.

5.1 Finite Difference Formulation

The compositional molar flow differential equation Eq. (4.3) and water volume balance differential equation Eq. (4.4) can be rewritten to finite difference form by applying finite difference approximations. Central finite difference representation is used to approximate spatial derivatives while backward finite difference representation is used to approximate temporal derivatives. Applying backward-in-time, central-in-space finite difference approximations, we obtain finite difference compositional molar balance and water volume balance as shown in Eqs. (5.1) and (5.2), respectively.
\[ x \left( \frac{\tilde{\rho}_e A k k_m}{\Delta x \mu_o} \right) \left| _{x, y, z - \frac{1}{2}} \right| (P |_{x+1, y, z} - P |_{x, y, z}) - y \left( \frac{\tilde{\rho}_e A k k_m}{\Delta x \mu_o} \right) \left| _{x, y, z - \frac{1}{2}} \right| (P |_{x, y, z+1} - P |_{x, y, z}) \]
\[ + y \left( \frac{\tilde{\rho}_e A k k_m}{\Delta x \mu_o} \right) \left| _{x, y, z - \frac{1}{2}} \right| (P |_{x, y+1, z} - P |_{x, y, z}) - y \left( \frac{\tilde{\rho}_e A k k_m}{\Delta x \mu_o} \right) \left| _{x, y, z - \frac{1}{2}} \right| (P |_{x, y, z+1} - P |_{x, y, z}) \]
\[ + y \phi S_y \frac{D_{eff} A e}{5.615 \Delta x} \left( \tilde{\rho}_e |_{x, y, z+1} - \tilde{\rho}_e |_{x, y, z} \right) - y \phi S_y \frac{D_{eff} A e}{5.615 \Delta x} \left( \tilde{\rho}_e |_{x, y, z} - \tilde{\rho}_e |_{x, y, z-1} \right) \]
\[ - \left( \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} x_k m \right) \left| _{x, y, z+1} \right| (G |_{x+1, y, z} - G |_{x, y, z}) - \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} x_k m \left| _{x, y, z} \right| (G |_{x, y+1, z} - G |_{x, y, z}) \]
\[ - \left( \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} y_k m \right) \left| _{x, y, z+1} \right| (G |_{x+1, y, z} - G |_{x, y, z}) - \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} y_k m \left| _{x, y, z} \right| (G |_{x, y+1, z} - G |_{x, y, z}) \]
\[ + x \left( \frac{\tilde{\rho}_e A k k_m}{\Delta y \mu_o} \right) \left| _{y, z+1} \right| (P |_{x, y, z+1} - P |_{x, y, z}) - x \left( \frac{\tilde{\rho}_e A k k_m}{\Delta y \mu_o} \right) \left| _{y, z} \right| (P |_{x, y+1, z} - P |_{x, y, z}) \]
\[ + y \left( \frac{\tilde{\rho}_e A k k_m}{\Delta y \mu_o} \right) \left| _{y, z+1} \right| (P |_{x, y, z+1} - P |_{x, y, z}) - y \left( \frac{\tilde{\rho}_e A k k_m}{\Delta y \mu_o} \right) \left| _{y, z} \right| (P |_{x, y+1, z} - P |_{x, y, z}) \]
\[ + y \phi S_y \frac{D_{eff} A e}{5.615 \Delta y} \left( \tilde{\rho}_e |_{y, z+1} - \tilde{\rho}_e |_{y, z} \right) - y \phi S_y \frac{D_{eff} A e}{5.615 \Delta y} \left( \tilde{\rho}_e |_{y, z} - \tilde{\rho}_e |_{y, z-1} \right) \]
\[ - \left( \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} x_k m \right) \left| _{y+1} \right| (G |_{x, y+1} - G |_{x, y}) - \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} x_k m \left| _{y, z} \right| (G |_{x, y, z+1} - G |_{x, y, z}) \]
\[ - \left( \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} y_k m \right) \left| _{y+1} \right| (G |_{x, y+1} - G |_{x, y}) - \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} y_k m \left| _{y, z} \right| (G |_{x, y, z+1} - G |_{x, y, z}) \]
\[ + x \left( \frac{\tilde{\rho}_e A k k_m}{\Delta z \mu_o} \right) \left| _{z+1} \right| (P |_{x, y, z+1} - P |_{x, y, z}) - x \left( \frac{\tilde{\rho}_e A k k_m}{\Delta z \mu_o} \right) \left| _{z} \right| (P |_{x, y, z+1} - P |_{x, y, z}) \]
\[ + y \left( \frac{\tilde{\rho}_e A k k_m}{\Delta z \mu_o} \right) \left| _{z+1} \right| (P |_{x, y, z+1} - P |_{x, y, z}) - y \left( \frac{\tilde{\rho}_e A k k_m}{\Delta z \mu_o} \right) \left| _{z} \right| (P |_{x, y, z+1} - P |_{x, y, z}) \]
\[ + y \phi S_y \frac{D_{eff} A e}{5.615 \Delta z} \left( \tilde{\rho}_e |_{z+1} - \tilde{\rho}_e |_{z} \right) - y \phi S_y \frac{D_{eff} A e}{5.615 \Delta z} \left( \tilde{\rho}_e |_{z} - \tilde{\rho}_e |_{z-1} \right) \]
\[ - \left( \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} x_k m \right) \left| _{y+1} \right| (G |_{x, y+1} - G |_{x, y}) - \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} x_k m \left| _{y, z} \right| (G |_{x, y, z+1} - G |_{x, y, z}) \]
\[ - \left( \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} y_k m \right) \left| _{y+1} \right| (G |_{x, y+1} - G |_{x, y}) - \frac{1}{144} \frac{A k}{g} \frac{\rho \tilde{\rho}}{\mu_o} y_k m \left| _{y, z} \right| (G |_{x, y, z+1} - G |_{x, y, z}) \]
\[ + \frac{V}{5.615 \Delta t} \left[ (\phi S_y \rho \tilde{\rho} + \phi S_y \rho \tilde{\rho}) |_{y+1, z} \right] - (\phi S_y \rho \tilde{\rho} + \phi S_y \rho \tilde{\rho}) |_{y, z} \right) 
\]

(5.1)
And similarly, finite difference formulation for water equation can be derived.

\[
\frac{A_k k_w}{\Delta x \mu_w B_w} \left( P_n^{k_{x+1,y,z}} - P_n^{k_{x,y,z}} \right) - \frac{A_k k_w}{\Delta y \mu_w B_w} \left( P_n^{k_{x,y+1,z}} - P_n^{k_{x,y,z}} \right) - \frac{A_k k_w}{\Delta z \mu_w B_w} \left( P_n^{k_{x,y,z+1}} - P_n^{k_{x,y,z}} \right) - \frac{1}{144 \Delta z} \rho_w \left( G_{k_{x,y,z}}^{1,1} - G_{k_{x,y,z}}^{1,0} \right) - \frac{1}{144 \Delta y} \rho_w \left( G_{k_{x,y,z}}^{0,1} - G_{k_{x,y,z}}^{0,0} \right) + q_w^{well} = \frac{V_b}{5.615 \Delta t} \left( \phi S_w^{n+1} - \frac{\phi S_w^n}{B_w} \right)
\] (5.2)

Coats (1980) fully implicit compositional formulation is implemented in PennComp, our in-house simulator. In his formulation, “natural” variables are selected as principal unknowns.

The full set of unknowns is described as follows:

- \( P_o \), pressure of the oil phase,
- \( S_o \), saturation of the oil phase,
- \( S_g \), saturation of the gas phase,
- \( x_i \) for \( i = 1, 2, 3, ..., N_C - 1 \), liquid composition of the \( i^{th} \) species,
- \( y_i \) for \( i = 1, 2, 3, ..., N_C - 1 \), vapor composition of the \( i^{th} \) species

The selection of this set of unknowns generates a total of \( 2N_C + 1 \) principal unknowns in \( 2N_C + 1 \) equations (\( N_C \) hydrocarbon conservation equations, 1 water conservation equation, and \( N_C \) phase equilibrium constraints). All other remaining unknowns can be calculated using auxiliary
equations presented Chapter 4. If the grid block is single phase, one set of phase composition \(x_i\) or \(y_i\) for \(i = 1,2,3,...,N_C-1\) and one phase saturation \((S_o \text{ or } S_g)\) is eliminated, leaving \(N_C+1\) unknowns in the full set of principal unknowns. In Coats (1980) formulation, conservation equations and phase behavior constraints are solved simultaneously during Newton iteration. Negative flash calculation or phase stability analysis is performed at the end of the iteration for any grid block that is in single-phase condition to identify the forming of a second phase.

To reduce the size of the Jacobian matrix, one can perform local matrix manipulations to reduce the full set of \(2N_C+1\) unknowns to primary set of \(N_C+1\) unknowns. The primary unknowns are described below:

1. If both oil and gas phases are present,
   \[ P, S_o, S_g, y_i \quad \text{for} \quad i = 3,4,...,N_C \rightarrow N_C + 1 \text{ unknowns} \]

2. If only oil phase is present, \(P, S_o, x_i\) for \(i = 1,2,...,N_C-1 \rightarrow N_C + 1\) unknowns

3. If only gas phase is present, \(P, S_g, y_i\) for \(i = 1,2,...,N_C-1 \rightarrow N_C + 1\) unknowns

In all case, we will have \(N_C+1\) primary unknowns (listed above) in \(N_C+1\) primary equations (\(N_C\) hydrocarbon conservation equations and 1 water conservation equation) to solve. Detailed steps in solving systems of primary and secondary equations to reduce the size of the Jacobian matrix can be found in Cao (2002) and Schmall (2013). Although the method is not implemented in PennComp, the procedure is outlined as follows:

1. At the beginning of the iteration, identify which set of primary unknowns will be used based on presence of oil and gas.

2. Calculate entries in the Jacobian matrix and residual vector using analytical differentiation.

3. Store these entries based on type of unknowns and derivatives in a submatrix for each grid block (i.e., submatrix A, B, C, and D) as described in Cao (2002).
4. Locally solve the submatrix A, B, C, and D to reduce the size of the Jacobian matrix.

5. Solve the reduced linearized system of equations using linear solver (e.g., GMRES)

5.2 Calculation of the Inter-block Transmissibility

The conservation equation can be broken down into convection term and diffusive term. Typical inter-block transmissibility terms are shown in Eqs. (5.3) to (5.6) transmissibility in the x-direction.

\[
T_{xs}^{m+1} = \frac{A_x k_x}{\Delta x} \left. \right|_{x+\frac{1}{2}} \frac{\hat{\rho}_j^{m+1}}{\mu_j^{m+1}} \left. \right|_{x+\frac{1}{2}} \omega_j \left( k_j^{m+1} \right) \tag{5.3}
\]

\[
T_{wx}^{m+1} = \frac{A_x k_x}{\Delta x} \left. \right|_{x+\frac{1}{2}} \frac{1}{\mu_x B_x} \left. \right|_{x+\frac{1}{2}} k_{m}^{m+1} \tag{5.4}
\]

\[
T_{jk}^{m+1} = \frac{1}{144} \frac{g}{g_c} \rho_j^{m+1} T_{jk}^{m+1} \tag{5.5}
\]

\[
D_{st}^{m+1} = \frac{D_{eff}}{5.615} \frac{A_x \left. \right|_{x+\frac{1}{2}} \phi S_{st}^{m+1} y_{st}^{m+1}}{\Delta x} \tag{5.6}
\]

5.2.1 Constant Part of the Transmissibility

The constant part of the transmissibility at the interface of the two adjacent grid blocks is calculated using harmonic averaging technique, as shown in Eqs. (5.7) and (5.8).

\[
\frac{1}{A_x k_x \left. \right|_{x+\frac{1}{2}}} = \frac{1}{2} \left( \frac{1}{A_x k_x \left. \right|_{x}} + \frac{1}{A_x k_x \left. \right|_{x+1}} \right) \tag{5.7}
\]
Expanding the terms on the right hand side of Eqs. (5.7) and (5.8) gives:

\[
\frac{A_j k_x}{\Delta x_{x_+\frac{1}{2}}} = \frac{1}{2}\left(\frac{1}{A_j} + \frac{1}{A_j}ight)
\]  

(5.8)

\[
\frac{A_j k_x}{\Delta x_{x_+\frac{1}{2}}} = \frac{2\left(\frac{A_j k_x}{\Delta x_x}\right)}{\Delta x_{x_+\frac{1}{2}}} + \frac{\left(\frac{A_j k_x}{\Delta x_{x_+\frac{1}{2}}}ight)}{\Delta x_{x_+\frac{1}{2}}} = \frac{2\left(\frac{A_j k_x}{\Delta x_x}\right)}{\Delta x_{x_+\frac{1}{2}}} + \frac{\left(\frac{A_j k_x}{\Delta x_{x_+\frac{1}{2}}}ight)}{\Delta x_{x_+\frac{1}{2}}}
\]  

(5.9)

\[
\frac{D_{eff} A_j}{5.615\Delta x_{x_+\frac{1}{2}}} = \frac{2D_{eff} \left(\frac{A_j}{\Delta x_x}\right)}{5.615\left(\frac{A_j}{\Delta x_{x_+\frac{1}{2}}}ight)} + \frac{\left(\frac{A_j}{\Delta x_{x_+\frac{1}{2}}}\right)}{5.615\left(\frac{A_j}{\Delta x_{x_+\frac{1}{2}}}\right)} = \frac{2D_{eff} \left(\frac{A_j}{\Delta x_x}\right)}{5.615\left(\frac{A_j}{\Delta x_{x_+\frac{1}{2}}}\right)} + \frac{\left(\frac{A_j}{\Delta x_{x_+\frac{1}{2}}}\right)}{5.615\left(\frac{A_j}{\Delta x_{x_+\frac{1}{2}}}\right)}
\]  

(5.10)

In our model, Eqs. (5.9) and (5.10) are used to compute the constant part of the transmissibility for the convection and diffusive terms, respectively.

### 5.2.2 Non-linear Part of the Transmissibility

In this study, one-point upstream weighting is used to calculate all non-linearities in compositional simulation as suggested by Coats (1980) and Nghiem et al. (1981).

**Convection Term**

One-point upstream weighting is used for determination of property \( H \) of phase \( j \) at the interface between block for all non-linear properties.

\[
H_j \bigg|_{x_+\frac{1}{2}} = \begin{cases} 
H_j \bigg|_{x} & \text{if } \Delta \Phi_j \bigg|_{x} > \Delta \Phi_j \bigg|_{x+1} \\
H_j \bigg|_{x+1} & \text{if } \Delta \Phi_j \bigg|_{x} < \Delta \Phi_j \bigg|_{x+1}
\end{cases}
\]  

(5.11)

where \( \Delta \Phi_j \) determines the direction of flow

\[
\Delta \Phi_j \bigg|_{x_+\frac{1}{2}} = \left( P_j \bigg|_{x+1} - P_j \bigg|_{x} \right) - \gamma_j \bigg|_{x_+\frac{1}{2}} \left( G_{x+1} - G_x \right) = \Delta P_j - \gamma_j \bigg|_{x_+\frac{1}{2}} \Delta G
\]  

(5.12)
and the specific weight of phase $j$ at the interface in \( \frac{lb\text{f}}{ft^3} \) is defined as:

$$\gamma_j \bigg|_{i+ \frac{1}{2}} = \eta \gamma_j \bigg|_i + (1 - \eta) \gamma_j \bigg|_{i+1}$$  \hspace{1cm} (5.13)

where:

$$\eta = \frac{(V_p \gamma_p) \bigg|_i}{(V_p \gamma_p) \bigg|_i + (V_p \gamma_p) \bigg|_{i+1}}$$  \hspace{1cm} (5.14)

$$V_p = \phi V_b$$  \hspace{1cm} (5.15)

$$\gamma_p = \frac{1}{144} \frac{g}{g_c} \rho_p$$  \hspace{1cm} (5.16)

**Diffusive Term**

The non-linearities of the transmissibility in the diffusive flow term (\( \phi S_g \)) is computed using harmonic average as shown in Eq. (5.17).

$$\phi S_g \bigg|_{i+ \frac{1}{2}} = \frac{2(\phi S_g \bigg|_i)(\phi S_g \bigg|_{i+1})}{(\phi S_g \bigg|_i) + (\phi S_g \bigg|_{i+1})}$$  \hspace{1cm} (5.17)

**5.3 Treatment of Phase Disappearance and Reappearance**

In a grid block, there may be up to two hydrocarbon phases (oil and gas) co-existing in equilibrium. At the end of each iteration, the simulator must detect if a phase has disappeared or a new phase has formed.
5.3.1 Phase Disappearance

When a grid block has two phases, the condition must be monitored whether or not it will change into a single-phase condition at the end of the iteration. For each Newton iteration after the flow equations are solved for the unknowns \((P_o, S_o, S_g, x_i, y_i, \text{ for } i = 1,2,3,\ldots,N_C)\), if either \(S_o\) or \(S_g\) becomes negative, the corresponding hydrocarbon phase disappears. The negative saturation is set to zero before initializing for the next Newton iteration (Coats, 1980). If either \(S_o\) or \(S_g\) is still within 0 and 1 at the end of the iteration, both phases still co-exist in equilibrium and the grid block is initialized as a two-phase condition in the next Newton iteration by updating the properties of each phase.

5.3.2 Phase Appearance

At the end of each Newton iteration, for the grid block that has only a single-phase hydrocarbon, a phase stability analysis is performed on the grid block to determine the number of phases. Alternatively, a negative flash calculation can be used to determine whether the grid block has one phase or two phases (Nghiem et al., 1983). The role of the phase stability analysis and negative flash calculation is to determine whether the hydrocarbon fluid remains stable as single phase or splits into two phases. If the phase stability analysis indicates that the fluid is unstable and splits into two phases or a negative flash indicates that either liquid or gas phase mole fraction \((L \text{ or } V)\) is between 0 and 1, an additional phase appears. Flash calculation is then performed to determine the phase mole fraction and phase compositions of the grid block. Phase molecular weight, density, viscosity, saturation are then calculated. The grid block is marked as two-phase condition, and the calculation on the grid block continues as two phases in the next Newton iteration. On the other hand, if the fluid is found to be stable from the phase stability
analysis or the negative flash calculation gives either liquid or gas phase mole fraction that is outside the range of zero and one (i.e., \( L \) or \( V > 1 \) or \( L \) or \( V < 0 \)), the grid block remains single phase and is initialized as single-phase condition for the next Newton iteration. The type of phase, whether it is a single-phase gas or single-phase oil, is assumed to be the same as the previous iteration/timestep.

5.4 Source or Sink Terms

Source or sink terms are used to calculate production or injection from the reservoir. This section describes Peaceman’s well model (1983) and injection/production specifications implemented in PennComp.

5.4.1 Modeling of Production Wells

Modeling of well model follows Peaceman (1983). Well is treated as source or sink term. Two approaches for the well model are available: including capillary pressure in the well model (Eqs. (5.18) and (5.19)) and ignoring capillary pressure in the well model (Eqs. (5.20) and (5.21)).

Well model with different phase gradient:

\[
q_{ij} = -\alpha_j \bar{p}_j \frac{2\pi k_{ave} h}{\ln \left( \frac{r_j}{r_w} + S \right)} \frac{k_{ij}}{\mu_j} (P_j - P_{w_f}) \quad \text{where } j = o, g
\]  
(5.18)

\[
q_{w}^{\text{w}} = -\frac{2\pi k_{ave} h}{\ln \left( \frac{r_w}{r_w} + S \right)} \frac{k_{rw}}{\mu_w B_w} (P_w - P_{w_f})
\]  
(5.19)
Well model with equal phase gradient:

\[ q_j = -\omega_j \hat{p}_j \frac{2\pi k_{ave} h}{\ln\left(\frac{r}{r_w} + S\right)} \frac{k_{ij}(P_o - P_{wf})}{\mu_j} \quad \text{where} \quad j = o, g \quad (5.20) \]

\[ q_w^{sc} = \frac{2\pi k_{ave} h}{\ln\left(\frac{r}{r_w} + S\right)} \frac{k_{ro}(P_o - P_{wf})}{\mu_o} \quad (5.21) \]

For hydrocarbon component in two-phase system, Eq. (5.18) can be expressed as:

\[ M_i = -x_i\hat{p}_o \frac{2\pi k_{ave} h}{\ln\left(\frac{r}{r_w} + S\right)} \frac{k_{ro}(P_o - P_{wf})}{\mu_o} - y_i\hat{p}_g \frac{2\pi k_{ave} h}{\ln\left(\frac{r}{r_w} + S\right)} \frac{k_{rg}(P_g - P_{wf})}{\mu_g} \quad (5.22) \]

Let \( q_o \) and \( q_g \) be oil and gas production/injection rate at reservoir condition. Eq. (5.22) can be shortened to Eq. (5.23)

\[ M_i = x_i\hat{p}_o q_o + y_i\hat{p}_g q_g \quad (5.23) \]

where

\[ q_o = -\Omega \frac{k_{ro}}{\mu_o}(P_o - P_{wf}) \quad (5.24) \]

\[ q_g = -\Omega \frac{k_{rg}}{\mu_g}(P_g - P_{wf}) \quad (5.25) \]

Similarly, for water, Eq. (5.19) can be rewritten as:

\[ q_w^{sc} = \frac{q_w}{B_w} \quad (5.26) \]

where

\[ q_w = -\Omega \frac{k_{rw}}{\mu_w}(P_w - P_{wf}) \quad (5.27) \]
The term $\Omega$ is productivity index and is defined in Eq. (5.28):

$$\Omega = \frac{2\pi k_{ave} h}{\ln \left( \frac{r_e}{r_w} + S \right)}$$  \hspace{1cm} (5.28)

Whether one assumes equal phase gradient or not, average permeability ($k_{ave}$) and equivalent well block radius ($r_e$) are calculated from Eqs. (5.29) and (5.30).

$$k_{ave} = \sqrt{k_x k_y}$$  \hspace{1cm} (5.29)

$$r_e = 0.28 \sqrt{\left( \frac{k_y}{k_x} \right)^{0.5} (\Delta x)^2 + \left( \frac{k_x}{k_y} \right)^{0.5} (\Delta y)^2 \left( \frac{k_y}{k_x} \right)^{0.25} + \left( \frac{k_x}{k_y} \right)^{0.25}}$$  \hspace{1cm} (5.30)

### 5.4.1.1 Specification of Production at Reservoir Condition

When production rate of a phase at reservoir condition is specified, the corresponding bottom-hole pressure ($P_{w}$) is calculated and used in the production calculation of other phases. The molar production rate of component $i$ and water production rate at surface condition can be calculated from Eq. (5.31) and (5.32), respectively.

$$M_i = x_i \tilde{\rho}_i q_o + y_i \tilde{\rho}_k q_g$$  \hspace{1cm} (5.31)

$$q_{w,sc} = \frac{q_w}{B_w}$$  \hspace{1cm} (5.32)
5.4.1.2 Specification of Constant Bottom-hole Pressure

When bottom-hole pressure (or wellflow pressure) is specified, the hydrocarbon molar production rate \((M_i)\) can be computed directly using Eq. (5.22). Similarly, water production rate can be computed using Eq. (5.19) or (5.21).

5.4.2 Modeling of Injection Wells

Two methods of handling of mobility in injection well are available to model injection wells. Ayala (2002) assumes the mobility of the injection fluid is equal to injection fluid end-point mobility of the corresponding phase as shown in Eq. (5.33).

\[
q^{\text{inj}}_{j} = -\frac{2\pi k_{\text{ave}} h}{\ln \left( \frac{r_{e}}{r_{w}} + \frac{S}{r_{w}} \right)} \frac{k_{\text{max}}^{\text{ave}}}{\mu_{j}} \left( P_{j} - P_{wf} \right) \quad \text{where } j = o, g \tag{5.33}
\]

Chappelear and Williamson (1979) proposed the use of total mobility in the injection well.

\[
q^{\text{inj}}_{j} = -\frac{2\pi k_{\text{ave}} h}{\ln \left( \frac{r_{e}}{r_{w}} + \frac{S}{r_{w}} \right)} \lambda_{\text{total}} \left( P_{j} - P_{wf} \right) \quad \text{where } j = o, g \tag{5.34}
\]

\[
\lambda_{\text{total}} = \frac{k_{re}}{\mu_{o}} + \frac{k_{rg}}{\mu_{g}} + \frac{k_{rw}}{\mu_{w}} \tag{5.35}
\]

In this work, the modeled proposed by Chappelear and Williamson (1979) is implemented.
5.4.2.1 Water Injection

When water is injected into the reservoir, water goes directly into the water phase. By replacing phase \( j \) with \( w \) in Eqs. (5.33) and (5.34), we obtain Eq. (5.36). Total mobility can be calculated from Eq. (5.35).

\[
q_w^{\text{inj}} = -\frac{2\pi k_{\text{ave}} h}{\ln \left( \frac{r}{r_w} + S \right) B_w} \lambda_{\text{total}} \left( P_w - P_{wf} \right) 
\]  \hspace{1cm} (5.36)

5.4.2.2 Gas Injection

For gas injection, injecting solvent composition \( y_i^{\text{inj}} \) must be specified by the user. It is assumed that the injected fluid is in gas phase at surface and reservoir conditions. Gas is injected into the gas phase. The source term can be described by Eq. (5.37).

\[
M_i^{\text{inj}} = y_i^{\text{inj}} \frac{F_g^{\text{inj}}}{5.615} = -y_i^{\text{inj}} \tilde{\rho}_g^{\text{inj}} q_{\text{res},g}^{\text{inj}} = -y_i^{\text{inj}} \tilde{\rho}_g^{\text{inj}} \lambda_{\text{total}} \Omega \left( P_g - P_{wf} \right) \]  \hspace{1cm} (5.37)

The injected fluid molar density \( \tilde{\rho}_g^{\text{inj}} \) in \( \text{lbmol/ft}^3 \) is evaluated using injected fluid composition at grid block pressure and temperature.

5.4.2.2.1 Specification of Molar Injection Rate \( (F_g^{\text{inj}}, \text{lbmol/day}) \)

When molar injection rate is specified, the rate of each component can be computed directly by multiplying the molar rate by the injecting solvent composition as the compositional formulation is written in moles. Molar injection rate is divided by 5.615 to convert the unit into \( \text{lbmol RB day}^{-1} \text{ft}^{-3} \) so it is consistent with the compositional formulation.
5.4.2.2.2 Specification of Surface Volume Injection Rate \((q_{g,sc}^{inj}, Mscf/day)\)

When surface injection rate is specified, one can calculate the amount of moles being injected into the reservoir using Eq. (5.39). In specification of surface volume injection rate, it is assumed that gas is

\[
F_g^{inj} = \frac{P_{sc}}{T_{sc}} \frac{q_{g,sc}^{inj}}{0.01073}
\]  
(5.39)

Substituting \(F_g^{inj}\) into Eq. (5.37) gives:

\[
M_i^{inj} = y_i^{inj} \frac{F_g^{inj}}{5.615} = \frac{y_i^{inj} P_{sc}}{5.615} \frac{q_{g,sc}^{inj}}{T_{sc} 0.01073}
\]  
(5.40)

5.4.2.2.3 Specification of Gas Bottom-Hole Injection Pressure

When bottom-hole injection pressure is specified, the molar injection rate can be calculated by Eq. (5.41).

\[
M_i^{inj} = -y_i^{inj} \tilde{\rho}_g^{inj} \lambda_{total} \Omega \left( P_g - P_{wf} \right)
\]  
(5.41)

where \(\tilde{\rho}_g^{inj}\) is injected gas molar density evaluated at reservoir condition using well block pressure, \(lbmol/ft^3\).

5.5 Surface Production Rates in Compositional Simulation

In compositional simulation, it is common to express conservation equations in terms of mass or mole. However, it is more practical to express production rates from the reservoir in terms of volume of fluids occupy once they are brought to the surface. Molar production rates of each component from each perforation in a well are gathered at the surface. Well stream
composition \( z_i^{ws} \) can be calculated from the rate of each component \( (N_i) \) divided by the total rate from the well \( (N_t) \). The well stream composition can be calculated from Eq. (5.42).

\[
    z_i^{ws} = \frac{N_i}{N_t}
\]  

(5.42)

The overall well stream composition is flashed at the pressure and temperature of the first stage separator. In the subsequent stages, the liquid composition is flashed at the downstream stages. At each stage \( s \), we obtain the liquid mole fraction \( (f_{ml,s}) \). After the well stream composition is flashed through the last stage of separator (stock tank), we can calculate the overall liquid mole fraction \( (f_{so}) \) from Eq. (5.43).

\[
    f_{so} = \prod_{s=1}^{n_s} f_{ml,s}
\]  

(5.43)

Molar densities of oil and gas can be calculated as a function of compressibility factor of the oil and gas at surface condition (Eqs. (5.44) and (5.45)).

\[
    \tilde{\rho}_{sc,o} = \frac{P_{sc}}{Z_{o}^{sc}RT_{sc}}
\]  

(5.44)

\[
    \tilde{\rho}_{sc,g} = \frac{P_{sc}}{Z_{g}^{sc}RT_{sc}}
\]  

(5.45)

The volumetric production rate of oil and gas can be calculated from the total moles produced, phase mole fraction, and density at surface condition.

\[
    q_o^{sc} \left( \frac{STB}{day} \right) = 10.73 Z_{o}^{sc} \left( \frac{T_{sc}}{P_{sc}} \right) f_{so} N_t
\]  

(5.46)

\[
    q_g^{sc} \left( \frac{Mscf}{day} \right) = \frac{10.73 \cdot 5.615}{1000} \left( \frac{T_{sc}}{P_{sc}} \right) (1 - f_{so}) N_t
\]  

(5.47)
5.6 Original Fluid In Place

To assess the fluid recoveries from the reservoir, the original fluid-in-place (OHIP, OSIP, OOIP, and OGIP) must be determined. The original hydrocarbon-in-place depends on pore volume, phase fluid molar density, and the initial state of the reservoir fluid. The original hydrocarbon-in-place can be calculated by integrating the entire pore volume of the reservoir. Eq. (5.48) shows OHIP calculation when initial state of the reservoir is single-phase gas, single-phase oil, and two phases, respectively.

\[
OHIP = \begin{cases} 
\int V \phi (1 - S_w) dV & \text{for single-phase gas} \\
\int V \phi (1 - S_o) dV & \text{for single-phase oil} \\
\int V \phi (S_o \tilde{\rho}_o + S_g \tilde{\rho}_g) dV & \text{for two-phase condition}
\end{cases}
\] (5.48)

In a discretized reservoir, the integration term is calculated by adding the original hydrocarbon-in-place in all grid blocks making up the reservoir. The total original hydrocarbon-in-place (OHIP) can be calculated by Eq. (5.49):

\[
OHIP = \left( \sum_{z=1}^{N_z} \sum_{y=1}^{N_y} \sum_{x=1}^{N_x} V_b \cdot \phi (1 - S_w) \tilde{\rho}_g \right)_{x,y,z}^{i=0} \quad \text{for single-phase gas}
\]

\[
OHIP = \left( \sum_{z=1}^{N_z} \sum_{y=1}^{N_y} \sum_{x=1}^{N_x} V_b \cdot \phi (1 - S_o) \tilde{\rho}_o \right)_{x,y,z}^{i=0} \quad \text{for single-phase oil}
\]

\[
OHIP = \left( \sum_{z=1}^{N_z} \sum_{y=1}^{N_y} \sum_{x=1}^{N_x} V_b \cdot \phi \left( S_o \tilde{\rho}_o + S_g \tilde{\rho}_g \right) \right)_{x,y,z}^{i=0} \quad \text{for two-phase condition}
\] (5.49)

For the calculation of \(i^{th}\) original species-in-place (OSIP), the total amount of hydrocarbon-in-place can be split into different components. When the reservoir is in single-phase condition (either oil or gas), the initial reservoir fluid overall composition (\(z_i\) for \(i = 1,2,3,\ldots,N_C\)) is used. If the initial reservoir is in two-phase condition, phase saturations (\(S_o\) and \(S_g\)) and phase
compositions \((x_i, y_i)\) for \(i = 1, 2, 3, \ldots, N_c\) are used in the calculation instead as shown in Eq. (5.50).

\[
OSIP_i = \begin{cases} 
\sum_{x=1}^{N_x} \sum_{y=1}^{N_y} \sum_{z=1}^{N_z} V_z \cdot \phi(1 - S_w) z_i \tilde{\rho}_g \bigg|_{y_i,z_i} & \text{for single-phase gas} \\
\sum_{x=1}^{N_x} \sum_{y=1}^{N_y} \sum_{z=1}^{N_z} V_z \cdot \phi(1 - S_w) z_i \tilde{\rho}_o \bigg|_{y_i,z_i} & \text{for single-phase oil} \\
\sum_{x=1}^{N_x} \sum_{y=1}^{N_y} \sum_{z=1}^{N_z} V_z \cdot \phi \left( S_o \cdot x_i \tilde{\rho}_o + S_g \cdot y_i \tilde{\rho}_g \right) \bigg|_{y_i,z_i} & \text{for two-phase condition}
\end{cases}
\]

The first step in calculating original oil-in-place (OOIP in STB) and original gas-in-place (OGIP in Mscf) is to determine the initial state of the reservoir fluid. In this research, it is assumed that the entire hydrocarbon fluids in oil and gas phases are then sent through a separator train. If the reservoir is undersaturated, the calculation of OOIP is straight forward. The hydrocarbon composition is flashed at surface condition, and the OOIP and OGIP can be determined. Conversely, the calculation of OOIP for saturated reservoir is slightly more complicated. Oil at reservoir condition can split into gas and oil and surface condition. Similarly, gas at reservoir condition can split into gas and oil at surface condition. Therefore, the total OOIP is the sum of oil after gas is liberated at surface condition from the oil phase at reservoir condition and oil vaporized in the gas phase at reservoir condition, as shown in Eq. (5.51). Similarly in Eq. (5.52), the total OGIP is the sum of the gas after oil drops out from the free gas phase at reservoir condition and gas dissolved in the oil phase at reservoir condition. In Eqs. (5.51) and (5.52), the subscript “oil” and “gas” are used to signify the fluid coming out of the oil and gas phases at reservoir condition, respectively.

\[
OOIP_{\text{total}} = OOIP_{\text{oil}} + OOIP_{\text{gas}}
\]

\[
OGIP_{\text{total}} = OGIP_{\text{oil}} + OGIP_{\text{gas}}
\]
The initial state of the reservoir, composition, and pressure and temperature at each stage of the separator are used to calculate the value of liquid mole fraction of hydrocarbon at surface condition (\( f_{sc, o}^{\text{initial}} \)) and oil molar density (\( \tilde{\rho}_{sc, o} \)) as described in Eqs. (5.43) and (5.44), respectively.

\[
OOIP_{\text{total}} = \frac{f_{sc, o}^{\text{initial}} \cdot OHIP}{\tilde{\rho}_{sc, o} \cdot 5.615} \bigg|_{\text{oil zone}} + \frac{f_{sc, g}^{\text{initial}} \cdot OHIP}{\tilde{\rho}_{sc, g} \cdot 5.615} \bigg|_{\text{gas zone}}
\]

\[
OGIP_{\text{total}} = 0.01073 \left( \frac{T_{sc}}{P_{sc}} \right) f_{sc, o}^{\text{initial}} \cdot OHIP \bigg|_{\text{oil zone}} + 0.01073 \left( \frac{T_{sc}}{P_{sc}} \right) f_{sc, g}^{\text{initial}} \cdot OHIP \bigg|_{\text{gas zone}}
\]

Finally, the calculation of original water-in-place (OWIP) can be calculated by Eq. (5.55).

\[
OWIP = \sum_{z=1}^{N_z} \sum_{y=1}^{N_y} \sum_{x=1}^{N_x} \frac{V_x}{5.615} \cdot \phi \left( \frac{S_w}{B_w} \right)_{x,y,z}^{t=0}
\]

### 5.7 Material Balance Calculations

At the end of the time step, internal checks are performed to ensure the convergence is achieved. Two types of material balance checks were implemented in the simulator: incremental material balance and cumulative material balance. Incremental material balance is calculated by computing the change in fluid in the reservoir divided by the net produced or injected fluid within the time step. Cumulative material balance is calculated in a similar manner but this time, change in fluid in the reservoir since the start of the simulation is divided by net total produced or injected fluid. Ideally, the material balance checks must be close to unity.

For \( i^{th} \) component,
For water component,

\[
\text{IMB}_w = \frac{\sum_{z=1}^{N_z} \sum_{y=1}^{N_y} \sum_{x=1}^{N_x} V_{b,y,z}^x \left[ \phi\left( \frac{S_w}{B_w} \right)_{x,y,z}^{y+1} - \phi\left( \frac{S_w}{B_w} \right)_{x,y,z}^y \right]}{\sum_{t=1}^{N_t} (q_{i}^w + q_{f}^w) \cdot 5.615 \Delta t}
\]

(5.58)

\[
\text{CMB}_w = \frac{\sum_{z=1}^{N_z} \sum_{y=1}^{N_y} \sum_{x=1}^{N_x} V_{b,y,z}^x \left[ \phi\left( \frac{S_w}{B_w} \right)_{x,y,z}^{y+1} - \phi\left( \frac{S_w}{B_w} \right)_{x,y,z}^y \right]}{\sum_{t=0}^{t=n} \sum_{t=1}^{N_t} (q_{i}^w + q_{f}^w) \cdot 5.615 \Delta t}
\]

(5.59)

The same process is carried out in all porosity types considered in this work. In addition to material balance checks, residuals for conservation equations for hydrocarbon components and water and phase equilibrium equations for hydrocarbon components are calculated. The residual must be close to zero.

### 5.8 Generalized Newton-Raphson Procedure

Finite difference formulations for hydrocarbon component (Eq. (5.1)) and water (Eq. (5.2)) can be rearranged in the residual form by moving the accumulation term on the right hand side of the equations to the left side. Residual equation of hydrocarbon component and water is a
function of principal unknowns: \( P_o, \ S_o, \ S_g, \ x_i, \) and \( y_i \) for \( i = 1,2,\ldots,N_C - 1 \) of the grid block itself and adjacent grid blocks.

\[
R_{i,x,y,z}^{n+1} \left( P_o^{n+1}, S_o^{n+1}, S_g^{n+1}, x_i^{n+1}, \ldots, x_{N_C-1}^{n+1}, y_i^{n+1}, \ldots, y_{N_C-1}^{n+1} \right) = \\
f(P_o^{n+1}, S_o^{n+1}, S_g^{n+1}, x_i^{n+1}, \ldots, x_{N_C-1}^{n+1}, y_i^{n+1}, \ldots, y_{N_C-1}^{n+1}) = \\
f(P_o^{n+1}, S_o^{n+1}, S_g^{n+1}, x_i^{n+1}, \ldots, x_{N_C-1}^{n+1}, y_i^{n+1}, \ldots, y_{N_C-1}^{n+1}) = \\
(5.60)
\]

Similarly, residual equation for water can be written as follows:

\[
R_{i,x,y,z}^{n+1} \left( P_o^{n+1}, S_o^{n+1}, S_g^{n+1}, x_i^{n+1}, \ldots, x_{N_C-1}^{n+1}, y_i^{n+1}, \ldots, y_{N_C-1}^{n+1} \right) = \\
f(P_o^{n+1}, S_o^{n+1}, S_g^{n+1}, x_i^{n+1}, \ldots, x_{N_C-1}^{n+1}, y_i^{n+1}, \ldots, y_{N_C-1}^{n+1}) = \\
(5.61)
\]
Note that water component is isolated from hydrocarbon component. Therefore, the derivatives with respect to $x_i$ and $y_i$ only appear in the well specification when the specification is related to hydrocarbon component e.g. total rate specification or oil rate specification.

Newton-Raphson method linearizes system of non-linear equations and aims to minimize the residual to zero. Newton-Raphson linearization of Eq. (5.60) yields:

$$-R_{i}^{n+1} = \left( \frac{\partial R_{i,x,y,z}}{\partial P_{x,y,z}} \right) \Delta P_{x,y,z}^{n+1} + \left( \frac{\partial R_{i,x,y,z}}{\partial S_{x,y,z}} \right) \Delta S_{x,y,z}^{n+1} + \left( \frac{\partial R_{i,x,y,z}}{\partial g_{x,y,z}} \right) \Delta g_{x,y,z}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial x_{i}} \right) \Delta x_{i}^{n+1} + ... + \left( \frac{\partial R_{i,N_c-1,x,y,z}}{\partial x_{N_c-1}} \right) \Delta x_{N_c-1}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial y_{i}} \right) \Delta y_{i}^{n+1} + ... + \left( \frac{\partial R_{i,N_c-1,x,y,z}}{\partial y_{N_c-1}} \right) \Delta y_{N_c-1}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial P_{k+1,y,z}} \right) \Delta P_{k+1,y,z}^{n+1} + \left( \frac{\partial R_{i,x,y,z}}{\partial S_{k+1,y,z}} \right) \Delta S_{k+1,y,z}^{n+1} + \left( \frac{\partial R_{i,x,y,z}}{\partial g_{k+1,y,z}} \right) \Delta g_{k+1,y,z}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial x_{k+1,y,z}} \right) \Delta x_{k+1,y,z}^{n+1} + ... + \left( \frac{\partial R_{i,N_c-1,k+1,y,z}}{\partial x_{N_c-1}} \right) \Delta x_{N_c-1}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial y_{k+1,y,z}} \right) \Delta y_{k+1,y,z}^{n+1} + ... + \left( \frac{\partial R_{i,N_c-1,k+1,y,z}}{\partial y_{N_c-1}} \right) \Delta y_{N_c-1}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial P_{k-1,y,z}} \right) \Delta P_{k-1,y,z}^{n+1} + \left( \frac{\partial R_{i,x,y,z}}{\partial S_{k-1,y,z}} \right) \Delta S_{k-1,y,z}^{n+1} + \left( \frac{\partial R_{i,x,y,z}}{\partial g_{k-1,y,z}} \right) \Delta g_{k-1,y,z}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial x_{k-1,y,z}} \right) \Delta x_{k-1,y,z}^{n+1} + ... + \left( \frac{\partial R_{i,N_c-1,k-1,y,z}}{\partial x_{N_c-1}} \right) \Delta x_{N_c-1}^{n+1}$$

$$+ \left( \frac{\partial R_{i,x,y,z}}{\partial y_{k-1,y,z}} \right) \Delta y_{k-1,y,z}^{n+1} + ... + \left( \frac{\partial R_{i,N_c-1,k-1,y,z}}{\partial y_{N_c-1}} \right) \Delta y_{N_c-1}^{n+1} + ...$$
\[
\begin{align*}
... &+ \left( \frac{\partial R}{\partial P} \right)_{k,x,y,z}^{n+1} \Delta P_{k,x,y,z}^{n+1} + \left( \frac{\partial R}{\partial S} \right)_{k,x,y,z}^{n+1} \Delta S_{k,x,y,z}^{n+1} + \left( \frac{\partial R}{\partial S} \right)_{k,x,z}^{n+1} \Delta S_{k,x,z}^{n+1} + \\
&+ \left( \frac{\partial R}{\partial x} \right)_{k,x,y,z}^{n+1} \Delta x_{k,x,y,z}^{n+1} + \left( \frac{\partial R}{\partial x} \right)_{k,x,y,z}^{n+1} \Delta x_{k,x,y,z}^{n+1} + \left( \frac{\partial R}{\partial y} \right)_{k,x,y,z}^{n+1} \Delta y_{k,x,y,z}^{n+1} + \\
&+ \left( \frac{\partial R}{\partial y} \right)_{k,x,y,z}^{n+1} \Delta y_{k,x,y,z}^{n+1} + \left( \frac{\partial R}{\partial y} \right)_{k,x,y,z}^{n+1} \Delta y_{k,x,y,z}^{n+1} + \\
&+ \left( \frac{\partial R}{\partial z} \right)_{k,x,y,z}^{n+1} \Delta z_{k,x,y,z}^{n+1} + \left( \frac{\partial R}{\partial z} \right)_{k,x,y,z}^{n+1} \Delta z_{k,x,y,z}^{n+1} + \left( \frac{\partial R}{\partial z} \right)_{k,x,y,z}^{n+1} \Delta z_{k,x,y,z}^{n+1},
\end{align*}
\]

(5.62)
Similarly for Eq. (5.61),

\[-R_{1x,y,z}^{n+1} = \left( \frac{\partial R}{\partial P} \right)_{x,y,z}^{n+1} \Delta P_{1x,y,z}^{n+1} + \left( \frac{\partial R}{\partial S} \right)_{x,y,z}^{n+1} \Delta S_{1x,y,z}^{n+1} + \left( \frac{\partial R}{\partial g} \right)_{x,y,z}^{n+1} \Delta g_{x,y,z}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial x} \right)_{x,y,z}^{n+1} \Delta x_{1x,y,z}^{n+1} + \ldots + \left( \frac{\partial R}{\partial x_{N-1}} \right)_{x,y,z}^{n+1} \Delta x_{N-1}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial y} \right)_{x,y,z}^{n+1} \Delta y_{1x,y,z}^{n+1} + \ldots + \left( \frac{\partial R}{\partial y_{N-1}} \right)_{x,y,z}^{n+1} \Delta y_{N-1}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial P} \right)_{1x+1,y,z}^{n+1} \Delta P_{1x+1,y,z}^{n+1} + \left( \frac{\partial R}{\partial S} \right)_{1x+1,y,z}^{n+1} \Delta S_{1x+1,y,z}^{n+1} + \left( \frac{\partial R}{\partial g} \right)_{1x+1,y,z}^{n+1} \Delta g_{1x+1,y,z}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial x} \right)_{1x+1,y,z}^{n+1} \Delta x_{1x+1,y,z}^{n+1} + \ldots + \left( \frac{\partial R}{\partial x_{N-1}} \right)_{1x+1,y,z}^{n+1} \Delta x_{N-1}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial y} \right)_{1x+1,y,z}^{n+1} \Delta y_{1x+1,y,z}^{n+1} + \ldots + \left( \frac{\partial R}{\partial y_{N-1}} \right)_{1x+1,y,z}^{n+1} \Delta y_{N-1}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial P} \right)_{1x-1,y,z}^{n+1} \Delta P_{1x-1,y,z}^{n+1} + \left( \frac{\partial R}{\partial S} \right)_{1x-1,y,z}^{n+1} \Delta S_{1x-1,y,z}^{n+1} + \left( \frac{\partial R}{\partial g} \right)_{1x-1,y,z}^{n+1} \Delta g_{1x-1,y,z}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial x} \right)_{1x-1,y,z}^{n+1} \Delta x_{1x-1,y,z}^{n+1} + \ldots + \left( \frac{\partial R}{\partial x_{N-1}} \right)_{1x-1,y,z}^{n+1} \Delta x_{N-1}^{n+1} \]

\[+ \left( \frac{\partial R}{\partial y} \right)_{1x-1,y,z}^{n+1} \Delta y_{1x-1,y,z}^{n+1} + \ldots + \left( \frac{\partial R}{\partial y_{N-1}} \right)_{1x-1,y,z}^{n+1} \Delta y_{N-1}^{n+1} + \ldots \]
... + \left( \frac{\partial R_w}{\partial P} \right)_{i+1, y, z} \Delta P_{i+1, y, z}^{n+1} + \left( \frac{\partial R_w}{\partial S_o} \right)_{i+1, y, z} \Delta S_o^{n+1} + \left( \frac{\partial R_w}{\partial S_g} \right)_{i+1, y, z} \Delta S_g^{n+1}

+ \left( \frac{\partial R_w}{\partial x} \right)_{i+1, y, z} \Delta x_{i+1, y, z}^{n+1} + \left( \frac{\partial R_w}{\partial x} \right)_{i+1, y, z} \Delta x_{i+1, y, z}^{n+1} + \left( \frac{\partial R_w}{\partial y} \right)_{i+1, y, z} \Delta y_{i+1, y, z}^{n+1} + \left( \frac{\partial R_w}{\partial y} \right)_{i+1, y, z} \Delta y_{i+1, y, z}^{n+1}

+ \left( \frac{\partial R_w}{\partial z} \right)_{i+1, y, z} \Delta z_{i+1, y, z}^{n+1} + \left( \frac{\partial R_w}{\partial z} \right)_{i+1, y, z} \Delta z_{i+1, y, z}^{n+1} + \left( \frac{\partial R_w}{\partial w} \right)_{i+1, y, z} \Delta w_{i+1, y, z}^{n+1} + \left( \frac{\partial R_w}{\partial w} \right)_{i+1, y, z} \Delta w_{i+1, y, z}^{n+1}

\text{(5.63)}
When a grid block is in two-phase condition, additional phase equilibrium constraints must be solved. Recall that for a fluid to be in equilibrium, fugacity between liquid and vapor phase must be equal (Eq. (5.64)).

\[ \ln f_i^L = \ln f_i^V \quad \text{for} \quad i = 1, 2, 3, ..., N_C \]  

(5.64)

Rearranging Eq. (5.64) into residual form,

\[ R_i = \ln f_i^L - \ln f_i^V \quad \text{for} \quad i = 1, 2, 3, ..., N_C \]  

(5.65)

Fugacity of a phase is a function of pressure \((P_o)\), temperature \((T)\), and phase composition \((x_i, y_i, \text{for} \quad i = 1, 2, 3, ..., N_C)\) of the grid block only. Linearization of Eq. (5.65) gives:

\[-R_{ki}^{n+1} = \left( \frac{\partial R_i}{\partial P} \right)_{x,y,z} \Delta P_{k,y,z}^{n+1} + \left( \frac{\partial R_i}{\partial x_i} \right)_{x,y,z} \Delta x_i^{n+1} + \cdots + \left( \frac{\partial R_i}{\partial x_{N_C}} \right)_{x,y,z} \Delta x_{N_C-1}^{n+1} + \left( \frac{\partial R_i}{\partial y_i} \right)_{x,y,z} \Delta y_i^{n+1} + \cdots + \left( \frac{\partial R_i}{\partial y_{N_C}} \right)_{x,y,z} \Delta y_{N_C-1}^{n+1} \]  

(5.66)

The \(2N_C+1\) linearized expressions are shown in Eqs. (5.62), (5.63), and (5.66). The system of equations is solved simultaneously for every grid block in the discretized reservoir. Sample Jacobian submatrix for a block is discussed below. For a reservoir with \(N_C\) components and water, partial derivatives of flow equations with respect to principal unknowns in the Jacobian matrix can be calculated using numerical differentiation. The matrix shown below is a Jacobian submatrix for a block in the reservoir.
5.9 Analytical vs. Numerical Differentiation

This section aims to discuss the advantages and disadvantages of using analytical differentiation over numerical differentiation. The advantages of analytical differentiation are its speed compared to numerical differentiation and the computed derivatives are exact (i.e., the derivatives are not subject to the perturbation value). The disadvantage of analytical differentiation is its implementation. Any term that is added to the residual equation requires a derivation and check with numerical differentiation. For the case of numerical differentiation, the term can be directly added to the residual equation and the program can compute derivatives.

\[
\begin{bmatrix}
\frac{\partial R_1}{\partial S_o} & \frac{\partial R_2}{\partial S_o} & \frac{\partial R_3}{\partial S_g} & \cdots & \frac{\partial R_{n_c}}{\partial S_o} & \frac{\partial R_1}{\partial y_1} & \frac{\partial R_2}{\partial y_1} & \cdots & \frac{\partial R_{n_c}}{\partial y_1} & \frac{\partial R_1}{\partial x_1} & \cdots & \frac{\partial R_{n_c}}{\partial x_{n_c}} \\
\frac{\partial R_1}{\partial y_3} & \frac{\partial R_2}{\partial y_3} & \frac{\partial R_3}{\partial y_3} & \cdots & \frac{\partial R_{n_c}}{\partial y_3} & \frac{\partial R_1}{\partial y_2} & \frac{\partial R_2}{\partial y_2} & \cdots & \frac{\partial R_{n_c}}{\partial y_2} & \frac{\partial R_1}{\partial x_2} & \cdots & \frac{\partial R_{n_c}}{\partial x_{n_c}} \\
\frac{\partial R_1}{\partial y_{n_c}} & \frac{\partial R_2}{\partial y_{n_c}} & \frac{\partial R_3}{\partial y_{n_c}} & \cdots & \frac{\partial R_{n_c}}{\partial y_{n_c}} & \frac{\partial R_1}{\partial y_{n_c}} & \frac{\partial R_2}{\partial y_{n_c}} & \cdots & \frac{\partial R_{n_c}}{\partial y_{n_c}} & \frac{\partial R_1}{\partial x_{n_c}} & \cdots & \frac{\partial R_{n_c}}{\partial x_{n_c}} \\
\end{bmatrix}
\]
numerically. However, in compositional simulation, using numerical differentiation may significantly slow down the simulator as phase behavior calculation in numerical differentiation is extensive. For each grid block, two flash calculations are required to obtain one entry for an unknown in the Jacobian matrix. In our test case, the model with analytical differentiation is approximately 8 times faster as compared to model with numerical differentiation. In this study, all derivatives are calculated analytically.

5.10 Linear Solvers

Solving linearized system of equations is computationally expensive. In a large system, an iterative solver is more common. In this work, an iterative solver called Restarted Generalized Minimum Residual (GMRES) (Saad and Schultz, 1986; Saad, 2003; Kelly, 2004) is used. The incomplete LU decomposition is used as a preconditioner. The solver is developed by Lili Ju, University of South Carolina and John Burkardt, Florida State University. GMRES is an iterative linear solver applicable for non-symmetric system of linear equations. The solver uses restarts to control storage and computational requirement. The choice of number of inner iterations \( m \) is crucial to the success of the solver. Choosing a large value of \( m \) involves excessive work and requires more storage. On the other hand, choosing a too small value of \( m \) may cause GMRES to converge slowly or fail to converge. Examples show that the method stagnates and convergence is achieved only at the \( n^{th} \) step, where \( n \) is the order of Jacobian matrix.

5.11 Timestep Control

Fully implicit formulation is unconditionally stable. Therefore, the timestep can be of any size. However, larger time-step size is subject to large time discretization error and difficult
convergence in the Newton iterations. In practice, an appropriate time-step size is required to control the number of Newton iterations in each timestep. In PennComp, the specified maximum and minimum time-step sizes are used to ensure the time-step size suggested by the time-step adjustment algorithm is within the desired range. During the simulation, the time-step size must satisfy Eq. (5.67)

\[ \Delta t_{\text{min}} \leq \Delta t \leq \Delta t_{\text{max}} \]  

Aziz and Settari (1979) suggest the increasing or decreasing of time-step size from timestep \( n \) to \( n+1 \) based on the change in variables of previous timestep as described in Eq. (5.68).

\[ \Delta t_{n+1} = \Delta t^n \cdot \frac{1 + \omega}{\delta_x + \omega \eta_x} \sum_{i} \eta_x \]  

where \( i \) refers to the gridblock number, \( \eta_x \) is the specified desired change of variable \( x \), \( \delta_x \) is the change of variable \( x \) over the \( \Delta t^n \), and \( \omega \) is a tuning factor with a value between 0 and 1. Cao (2002) suggests typical values for \( \eta \) for different variables.

\[ \eta_p = 200 \text{ psia} \] for pressure

\[ \eta_s = 0.2 \] for saturations

\[ \eta_x = 0.02 \] for component mole fractions
5.12 Overall Flow Chart of the Simulator

Figure 5-1: Overall flow chart of the simulator

Figure 5-1 shows the overall flow chart of the simulator. After the program is launched, two input files are read ("input.dat" and "input_DF.dat"). Flash calculation is performed on every grid block to initialize the reservoir and determine the fluid initially in place. The system of equations is linearized using analytical differentiation. The linearized system is solved by the linear solver Restarted GMRES. Principal unknowns are updated and the next Newton iteration is initialized. The process is repeated until convergence is achieved. Material balance check and
residual check are performed as an internal check to ensure integrity of the solutions. Production and injection rates and cumulative productions are calculated and recorded. The next time step is initialized. The process continues until the final time step is reached.

The developed simulator follows Coats (1980) formulation. The full set of unknowns is solved simultaneously. The following sequence is used to update remaining unknown variables from the principal unknowns:

- Water saturation is calculated through the saturation constraints:
  \[ S_w = 1 - S_o - S_g \]

- Phase appearance and disappearance are checked.
  - For a block starting the iteration as single phase, phase stability analysis and flash calculation are performed to determine the number of phases at the end of the iteration.
  - For a grid block starting as two phases,
    - If either \( S_o \) or \( S_g \) becomes negative, the corresponding phase has disappeared and the overall composition is calculated before the next iteration is initialized. The composition and density of the phase that disappears are set to zero. The viscosity of the phase that disappears is set to one.
    - If both \( S_o \) and \( S_g \) stay positive, the next Newton iteration is initialized as two phases.
  - If a two-phase condition prevails, phase properties (phase compositions, compressibility factor, molecular weight, density, and viscosity) are calculated.
  - If the single-phase condition prevails, oil (or gas) properties are updated.
- Type of phase (single-phase oil, single-phase gas, or two-phase oil and gas) is stored for phase tracking purpose

- If capillary pressure is considered on phase behavior, $P_e$ and $P_w$ must be calculated using capillary pressure relationship prior to updating fluid properties.

\[
P_{cgo}(S_g) = P_g - P_o \quad \rightarrow \quad P_g = P_o + P_{cgo}
\]

\[
P_{cov}(S_w) = P_o - P_w \quad \rightarrow \quad P_w = P_o - P_{cov}
\]

- Water phase properties are calculated using the corresponding water phase pressure.

- Phase mole fraction and overall composition are calculated and stored for the next iteration.

\[
L = \frac{S_o \tilde{v}_g}{S_o \tilde{v}_g + S_g \tilde{v}_o}
\]

\[
z_i = L x_i + V y_i = L x_i + (1 - L) y_i
\]

- Porosity and permeability are updated from compressibility due to compaction of formation.

\[
\phi^{k+1} = \phi^o \left[ 1 + c_{f,\phi} \left( P_o - P_{ref} \right) \right]
\]

\[
k^{k+1} = k^o \left[ 1 + c_{f,k} \left( P_o - P_{ref} \right) \right]^\kappa
\]

- If capillary pressure on phase behavior is enabled, pore radius is updated using gas saturation of the grid block before fluid properties are updated.
5.13 Highlights of the Chapter

In this chapter, the numerical formulation of the compositional model is discussed. The topics covered in this chapter are summarized as follows:

- The hydrocarbon and water conservations are written in finite-difference forms. The calculations of constant and non-linear parts of the transmissibility in the finite formulations are discussed.

- During the simulation a hydrocarbon phase may appear and disappear. The phase reappearance is handled by phase stability analysis to determine if the gridblock still remains single phase at the end of the iteration. The disappearance of a phase is determined by the value of oil or gas saturation at the end of the iteration. If either $S_o$ or $S_g$ becomes negative, the phase disappears.

- Production and injection in the numerical model is handled by a source or sink term. The modeling of production and injection wells for various well constraints is discussed. In the case of a production well, the well stream composition calculated from the molar production rates is sent through a separator train. At the last stage of the separator, the oil and gas production rates at surface condition are obtained.

- At the beginning of the simulation, original fluid-in-place (oil, gas, water, hydrocarbon species) is calculated. The original fluid-in-place is used in the material balance check and recovery calculation. Residuals of conservation equations and phase equilibrium constraints are checked to ensure that convergence is achieved before moving to the next timestep.

- A generalized Newton-Raphson procedure is used to linearize the system of equations. The system of equations is then solved using Restarted GMRES. A brief discussion of the advantage of the analytical differentiation over numerical differentiation is presented.
Timestep control is implemented to ensure a proper time-step adjustment in the simulation.

- The overall flow chart of the simulator is presented. The sequence in updating unknown variables from the principal unknowns at the end of the iteration is discussed.
Chapter 6

Development of a Multi-mechanistic Triple-porosity Triple-permeability Compositional Model

In this chapter, the implementation of the effect of capillary pressure on phase behaviors and embedded discrete fracture model will be discussed. The formulation of the triple-porosity, triple-permeability model is then demonstrated.

6.1 Effect of Capillary Pressure on Phase Behaviors

Recall that Coats (1980) formulation couples both conservation equations (fluid transport) and phase behavior constraints in Newton iteration. In the implementation of the effect of capillary pressure on phase behavior, the derivatives of fugacity and properties of vapor phases are calculated using vapor phase pressure as shown in Eq. (6.1).

\[ f_i^L(P_g, T, x_1, \ldots, x_{N_C}) = f_i^V(P_v, T, y_1, \ldots, y_{N_C}) \quad \text{for } i = 1, 2, \ldots, N_C \] (6.1)

During the Newton iteration, the value of \( P_g \) is held constant (i.e., \( P_g \) comes 1 iteration behind). After solving the system of equations, gas phase pressure is updated.

The updating scheme for gas-oil capillary pressure depends on the number of phases of the grid block. For a grid block that has two hydrocarbon phases, capillary pressure between gas and oil phase (\( P_{cgo} \)) is calculated following the flow chart shown in Figure 6-1.
Because $P_{cgo}$ is calculated based on pore radius, oil and gas densities and compositions, and gas density is a function of gas phase pressure, an iterative procedure must be implemented. Initial $P_{cgo}$ from previous iteration is used as an initial guess in Newton iteration. The objective function is described in Eq. (6.2).

$$f(P_{cgo}) = P_{cgo} - \frac{2}{r} \sum_{i=1}^{N_c} Z_i \left( \tilde{\rho}_o x_i - \tilde{\rho}_g y_i \right)^4$$  (6.2)

$P_{cgo}$ is iterated until change from Newton iteration is negligible ($\sim 10^{-7}$). Once the convergence is achieved, $P_g$ is calculated by adding $P_{cgo}$ to $P_o$. Analytical derivatives for solving objective function in Eq. (6.2) are shown in Appendix C. Once gas phase pressure is updated, oil and gas phase properties can be computed directly using corresponding phase pressures.

When a grid block has only single hydrocarbon phase, a modified negative flash algorithm is implemented to account for the effect of capillary pressure on phase behavior. The flow chart is shown in Figure 6-2.
For every grid block in the reservoir, once a new value of gas saturation is obtained from Newton iteration, pore radius ($r$) is updated to reflect the temporal change in pore size over the course of the simulation. From the flow chart, pressure, temperature, overall composition, and updated pore radius are passed to the modified negative flash subroutine. Vapor-liquid equilibrium calculation is performed to determine phase mole fractions and phase compositions. Compressibility factor
and density of liquid and vapor are computed before they are used in the interfacial tension calculation using Young-Laplace equation. The equilibrium ratios \((K_i)\) are updated using successive substitution. The process is repeated until convergence is achieved (Eq. (4.21)). At convergence, fluid properties (compressibility factor, molecular weight, density, and viscosity) are calculated and used in the next Newton iteration. The modified negative flash is also used to determine the number of phases in equilibrium. If vapor mole fraction \((V)\) falls out of range 0 and 1, a single-phase condition is assumed. The modified negative flash subroutine is called for every grid block that has a single hydrocarbon phase.

In the Macleod and Sugden correlation, the parachor of each component must be known. Fanchi (1985) suggested the correlation for calculating parachor from critical temperature and critical volume of the component. Fanchi (1990) later updated his earlier correlation from 1985 with a new set of regression coefficients to expand the validity up to \(C_{20}\). Eq. (6.3) shows the correlation proposed by Fanchi (1990).

\[
\chi_i = a_0 + a_1 V_{c,i} + a_2 T_{c,i} + a_3 H_i + a_4 H_i^2 + a_5 H_i^3 + \frac{a_6}{H_i}
\]  

(6.3)

where \(H\) denotes Herzog’s parameters and is defined by Eq. (6.4)

\[
H_i = V_{c,i}^{5/6} T_{c,i}^{1/4}
\]  

(6.4)

The regression coefficients \(a_0, \ldots, a_6\) are shown in Table 6-1.

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a_0)</td>
<td>176.05005</td>
</tr>
<tr>
<td>(a_1)</td>
<td>-7,472.9807</td>
</tr>
<tr>
<td>(a_2)</td>
<td>-0.87458088</td>
</tr>
<tr>
<td>(a_3)</td>
<td>1,5604793</td>
</tr>
<tr>
<td>(a_4)</td>
<td>19.309439</td>
</tr>
<tr>
<td>(a_5)</td>
<td>0.05013801</td>
</tr>
<tr>
<td>(a_6)</td>
<td>-25.691718</td>
</tr>
</tbody>
</table>

Table 6-1: Regression coefficients for Fanchi (1990) correlation
6.2 Embedded Discrete Fracture Model

Embedded discrete fracture model (EDFM) relies on non-neighboring connection (NNC). NNC is a connection between grid blocks that are not next to each other in the computational domain. This NNC concept can be explained in Figure 6-3.

![Figure 6-3: Non-neighboring connection](image)

The reservoir model in Figure 6-3 contains one fracture (shown in red line) along the diagonal. The fracture intersects 8 matrix blocks. Each fracture segment is numbered and placed in the fracture domain. Red, green, and blue lines show examples of the connections between matrix blocks that connect to fracture segments (1, 2, and 3). The data structure for the fracture domain was proposed by Moinfar (2013). However, in our in-house reservoir simulator, a slightly different data structure is used to remove the limitation of a maximum number of fracture segments in the fracture domain. As we can see, the data structure proposed by Moinfar (2013) limits the number of fracture segments to the maximum number of matrix blocks. Memory is allocated for fracture domain to be exactly the same as the matrix domain. In our model, the memory we allocated is just enough for the fractures. The dimensions of the memory in fracture domain are $N_F \times N_{S,\text{max}}$ where $N_F$ and $N_{S,\text{max}}$ are the number of fractures in the model and the
number of fracture segments of the longest fracture in the model, respectively. This data structure allows us to optimize memory usage for fracture domain.

Recall fluid transport through non-neighboring connection. The source term is treated similarly to Peaceman’s well model as shown in Eq. (6.5).

\[
M^{nnc}_i = \sum_{m=1}^{N_{mnc}} A^{nnc}_m \sum_{j=1}^{N_{j}} \frac{k^{nnc}_{ij}}{\mu_j} \left( \frac{P_j - \frac{1}{144} \frac{g}{g_c} \rho_j G}{d^{nnc}_m} \right) - \left( \frac{P_j - \frac{1}{144} \frac{g}{g_c} \rho_j G}{d^{nnc}_m} \right)^m_{nnc} \\
+ \phi S^{nnc}_f \frac{D^{nnc}}{5.615 d^{nnc}_m} \left( y_i \rho_g - y_i \rho_{g, m}^{nnc} \right) 
\]

The fracture intersecting area and average normal distance between non-neighboring blocks are calculated from the pre-processor. One NNC is added for every connection between a matrix block and a fracture segment. It should be noted that only one NNC connection from a fracture segment to the matrix block exists, but one matrix block may contain more than one fracture segment. Therefore, multiple NNCs may be required for connection from a matrix block to multiple fracture segments. In the next paragraph, three types of NNCs, following Moinfar (2013), will be discussed. Note that, in triple-porosity model, NNC applies for matrix-hydraulic fracture and natural fracture-hydraulic fracture transmissibility.

6.2.1 Types of Non-neighboring Connections

6.2.1.1 NNC Type 1

This type of NNC applies to the NNC between different porosity domains (i.e., between natural fracture and hydraulic fracture porosities and between matrix and hydraulic fracture porosities). The connection between matrix and micro-fracture porosities are handled by dual-
continuum concept where each connection between matrix and micro-fracture has a one-to-one connection (i.e., block (2,3,1) in matrix domain connects to block (2,3,1) in natural fracture domain). Average normal distance \( d_m^{mc} \) is calculated using Eq. (2.11). Area open to flow \( A_m^{mc} \) is calculated from the geometry of the fracture segment that intersects the matrix block.

6.2.1.2 NNC Type 2

This type of NNC applies to the two intersecting fracture segments that are from two different fractures in EDFM. The transmissibility between the segments follows the approach presented by Karimi-Fard et al. (2004), and this transmissibility is shown below.

\[
\frac{k_n^{mc} A_n^{mc}}{d_n^{mc}} = \frac{T_1 T_2}{T_1 + T_2} \tag{6.6}
\]

\[
T_1 = \frac{k_f^1 \omega_f^1 L_{int}}{d_f^1}, \quad T_2 = \frac{k_f^2 \omega_f^2 L_{int}}{d_f^2} \tag{6.7}
\]

where \( L_{int} \) is the length of the intersection line between the two fracture segments bounded in a grid block, and \( T_1 \) and \( T_2 \) are transmissibility of the two fracture segments. Combining Eq. (6.6) with Eq. (6.7), we obtain.

\[
\frac{k_n^{mc} A_n^{mc}}{d_n^{mc}} = \frac{T_1 T_2}{T_1 + T_2} = \frac{\left( \frac{k_f^1 \omega_f^1 L_{int}}{d_f^1} \right) \left( \frac{k_f^2 \omega_f^2 L_{int}}{d_f^2} \right)}{\frac{k_f^1 \omega_f^1 L_{int}^2}{d_f^1} + \frac{k_f^2 \omega_f^2 L_{int}^2}{d_f^2}}
\]

\[
= \frac{k_f^1 \omega_f^1 L_{int} k_f^2 \omega_f^2 L_{int}}{k_f^1 \omega_f^1 L_{int} d_f^2 + k_f^2 \omega_f^2 L_{int} d_f^1} \tag{6.8}
\]
6.2.1.3 NNC Type 3

This type of NNC is similar to Type 2. However, this type of NNC applies to the fracture segments of the same fracture that are not neighbor in the computational domain. The calculation of the transmissibility term is similar to that of Type 2. In our data structure, this type of NNC is not required for horizontal fractures that are aligned with Cartesian coordinates and vertical fractures.

6.2.2 Well-Fracture Intersection

Because EDFM is developed to model large-scale fractures and hydraulic fractures, these fractures may intersect the well. Therefore, it is important to discuss well-fracture intersections. In this study, it is assumed that all fractures are perpendicular to the wellbore, and Peaceman’s well model is applicable to simulate production and injection from/to the reservoir. Each well-fracture intersection is treated as an additional perforation of the well. Fluid produced from the perforation is added to the well stream, which is used to compute well stream composition. The well stream composition is flashed at the surface condition to determine the volume of oil and gas. Figure 6-4 shows a blue fracture segment of height $h_f$, length $L_f$ and width $\omega_f$ intersecting a horizontal well. As can be seen from the figure, the fracture segment is simply a very thin grid block, and a well passes through the grid block.
Applying Peaceman’s well model, the well model for the fracture segment can be obtained as shown in Eqs. (6.9) and (6.10) for hydrocarbon and water components, respectively.

\[
q_{ij} = -\omega_{ij} \tilde{\rho}_j \frac{2\pi k_{ave} \alpha_f}{\ln \left( \frac{r_{e}}{r_w} + S \right)} \frac{k_j}{\mu_j} (P_j - P_{wf}) 
\text{ where } j = o, g \tag{6.9}
\]

\[
q_w = -\frac{2\pi k_{ave} \alpha_f}{\ln \left( \frac{r_e}{r_w} + S \right)} \frac{k_{rw}}{\mu_w B_w} (P_w - P_{wf}) \tag{6.10}
\]

where \( \alpha_f, k_{ave}, \) and \( r_e \) are fracture width in ft, harmonic average of the permeability of the fracture segment that intersects the well in mD, and equivalent well block radius for the rectangular fracture segment in ft, respectively. Average permeability and equivalent well block radius are calculated from Eqs. (6.11) and (6.12), respectively.

\[
k_{ave} = \sqrt{k_u \cdot k_v} \tag{6.11}
\]
As a special case, Eq. (6.12) can be reduced to Eq. (6.13) for an isotropic square fracture segment.

\[ r_c = 0.14 \sqrt{L_f^2 + h_f^2} \]  

(6.13)

6.3 Triple-porosity, Triple-permeability Compositional Formulation

Current multi-porosity compositional models assume sequential flow from matrix to natural fracture and then to hydraulic fracture. However, hydraulic fracturing either opens up existing natural fractures and/or shatters the formation (i.e., hydraulic fracturing creates new fractures). When hydraulic fractures create new fractures, a transmissibility between matrix and hydraulic fracture is needed. In addition, matrix block is not necessarily isolated from other matrix blocks as is assumed in Warren and Root (1963) model. Therefore, matrix-matrix and matrix-hydraulic fracture communications should not be ignored. In the proposed triple-porosity model, the three porosity types are matrix, natural fracture (micro fracture), and hydraulic fracture (macro fracture). Flow occurs simultaneously in all porosity types. This fully coupled triple-porosity model allows us to better accurately capture fluid flow through heterogeneous porous mediums in unconventional reservoirs that other models can’t. Our developed model removes the stated assumptions of sequential flow and enables us to capture the proper physic of the actual fractured reservoir as we allow fluid in different porosity types to directly communicate with each other. In Warren and Root (1963) dual-continuum model, fluid flows from matrix to fracture and from fracture to the wellbore. Fluid transfer between natural fractures and matrix is modeled
using shape factor. On the other hand, discrete fracture model (DFM) treats fractures explicitly. Small grid blocks are used to represent individual fractures. Transmissibility between matrix and fracture is directly calculated from the intersecting area between matrix and fracture. The proposed triple-porosity, triple-permeability compositional model will couple a dual-continuum model with embedded discrete fracture model (EDFM) to take advantage of both dual-continuum and discrete fracture models. The hydraulic fractures, which can be easily observed from microseismic data, are treated explicitly as is done in DFM. Natural fractures, which are likely to be uniformly distributed, are simplified and modeled with dual-continuum model. In this model, fluid can be stored in the matrix, natural fractures, and hydraulic fracture domains. Similarly, flow of fluids occurs within and between three porosity domains: matrix, natural fracture, and hydraulic fracture. This constitutes our fully coupled triple-porosity, triple-permeability model.

Darcy’s law is applied to mass conservation equation to obtain governing flow equations for hydrocarbon components and water in porous media. Water component is assumed to be isolated from hydrocarbon phases. Transport equations must be written for three domains: matrix, natural fracture, and hydraulic fracture. Let $M, f$, and $F$ subscripts be identifiers for matrix, natural fracture, and hydraulic fracture domains, respectively. Figure 6-5 shows the flow schematic of the proposed triple-porosity, triple-permeability model. As can be seen, each color represents flow within the same porosity type. The yellow arrows represent the inter-porosity fluid transfer.
The mass exchanges between the three domains are matrix-natural fracture, matrix-hydraulic fracture, and natural fracture-hydraulic fracture. Mass exchanges between matrix and natural fractures are calculated using a shape factor as is done in Warren and Root dual-continuum model. The source/sink term considers the Darcian flow and Fickian diffusion (for gas phase). Mass exchange between matrix and hydraulic fracture domains is handled by NNC source/sink term as shown in Eq. (6.5). The area open to flow is directly calculated and used in the mass exchange term. When hydraulic fractures exist in the model, hydraulic fractures can intersect with natural fractures. Since natural fractures in dual-porosity, dual-permeability model is a non-physical abstraction of actual natural fractures, the “effective” area open to flow between natural fractures and hydraulic fractures is approximated using matrix-hydraulic fracture intersecting area weighted by natural fracture porosity. This assumes the discrete fracture is a new fracture, not open up natural fractures. Natural fracture porosity is used in the in the inter-porosity flow because natural fracture porosity represents pore space of the medium which allows for flow. This effective area is used in NNC source term described in Eq. (6.5). This effective area can be adjusted if the discrete fracture is believed to open up natural fractures. The governing flow equations for different porosity types are discussed first followed by a more detailed discussion on inter-porosity flow.
Eq. (6.14) shows the governing flow equation for component $i$ in natural fracture. Note that diffusion is considered for components in vapor phase only. Gravitational effect is also included for both liquid and vapor phases.

$$
\frac{\partial}{\partial x}\left\{ x_i f \tilde{p}_{o,f} \frac{k_{s,f} k_{ro,f}}{\mu_{o,f}} \left( \frac{\partial P_{o,f}}{\partial x} - \frac{1}{144 g_c} \rho_{o,f} \frac{\partial G}{\partial x} \right) \right\} \Delta x + y_{i,f} \tilde{p}_{g,f} A_x \frac{k_{s,f} k_{rg,f}}{\mu_{g,f}} \left( \frac{\partial P_{g,f}}{\partial x} - \frac{1}{144 g_c} \rho_{g,f} \frac{\partial G}{\partial x} \right) + \phi_j S_{g,f} A_x D_{eff} \frac{\partial}{\partial x} \left( y_{i,f} \tilde{p}_{g,f} \right)
$$

$$
\frac{\partial}{\partial y}\left\{ x_j f \tilde{p}_{o,f} \frac{k_{s,j} k_{ro,f}}{\mu_{o,f}} \left( \frac{\partial P_{o,f}}{\partial y} - \frac{1}{144 g_c} \rho_{o,f} \frac{\partial G}{\partial y} \right) \right\} \Delta y + y_{i,f} \tilde{p}_{g,f} A_y \frac{k_{s,f} k_{rg,f}}{\mu_{g,f}} \left( \frac{\partial P_{g,f}}{\partial y} - \frac{1}{144 g_c} \rho_{g,f} \frac{\partial G}{\partial y} \right) + \phi_j S_{g,f} A_y D_{eff} \frac{\partial}{\partial y} \left( y_{i,f} \tilde{p}_{g,f} \right)
$$

$$
\frac{\partial}{\partial z}\left\{ x_k f \tilde{p}_{o,f} \frac{k_{s,k} k_{ro,f}}{\mu_{o,f}} \left( \frac{\partial P_{o,f}}{\partial z} - \frac{1}{144 g_c} \rho_{o,f} \frac{\partial G}{\partial z} \right) \right\} \Delta z + y_{i,f} \tilde{p}_{g,f} A_z \frac{k_{s,f} k_{rg,f}}{\mu_{g,f}} \left( \frac{\partial P_{g,f}}{\partial z} - \frac{1}{144 g_c} \rho_{g,f} \frac{\partial G}{\partial z} \right) + \phi_j S_{g,f} A_z D_{eff} \frac{\partial}{\partial z} \left( y_{i,f} \tilde{p}_{g,f} \right)
$$

$$
+ M_{i,f} + \Gamma_{i,f} + \Lambda_{i,f} = \frac{1}{5.615} \frac{\partial}{\partial t} \left( V_{j,f} \phi_j S_{g,f} x_j f \tilde{p}_{o,f} + V_{j,f} \phi_j S_{g,f} y_{j,f} \tilde{p}_{g,f} \right)
$$

(6.14)

where the source terms $\Gamma_{i,f}$ and $\Lambda_{i,f}$ are molar exchange rate of component $i$ between natural fracture and matrix domain and between natural fracture and hydraulic fracture domain, respectively.

In matrix domain, additional source term for gas adsorbed or released is introduced in addition to the mass exchange terms between domains. Governing flow equation in matrix system can be written as follows.
\[
\frac{\partial}{\partial x}\left( x_{i,M} \hat{P}_{o,M} A_x \frac{k_{v,M}}{\mu_{o,M}} \left( \frac{\partial P_{o,M}}{\partial x} - \frac{1}{144} g_c \rho_{o,M} \frac{\partial G}{\partial x} \right) \Delta x \right) + y_{i,M} \hat{P}_{g,M} A_x \frac{k_{v,M}}{\mu_{g,M}} \left( \frac{\partial P_{g,M}}{\partial y} - \frac{1}{144} g_c \rho_{g,M} \frac{\partial G}{\partial y} \right) \Delta y + y_{i,M} \hat{P}_{g,M} A_x \frac{k_{v,M}}{\mu_{g,M}} \left( \frac{\partial P_{g,M}}{\partial z} - \frac{1}{144} g_c \rho_{g,M} \frac{\partial G}{\partial z} \right) \Delta z + M_{i,M} + M_{i,sp}^* + \Gamma_{i,M} + M_{i,M} = \frac{V_b}{5.615} \frac{\partial}{\partial t} \left( \phi_M S_{o,M} x_{i,M} \hat{P}_{o,M} + \phi_M S_{g,M} y_{i,M} \hat{P}_{g,M} \right)
\]

where \( M_{i,sp}^* \), \( \Gamma_{i,M} \), and \( M_{i,M} \) represent gas adsorbed/release of component \( i \) from matrix surface, molar exchange rate of component \( i \) between matrix and natural fracture domain and between matrix and hydraulic fracture domain via NNC, respectively. The adsorption term \( M_{i,sp}^* \) can be determined from Eqs. (6.16) and (6.17).

\[
M_{i,sp}^* = -\frac{1}{5.615} \frac{V_{a,i}^{n+1} - V_{a,i}^n}{\Delta t}
\]

\[
V_{a,i}^{n+1} = V_{a,i}^n \exp \left( -\frac{\Delta t}{\tau} \right) + V_{a,i}^n \left[ 1 - \exp \left( -\frac{\Delta t}{\tau} \right) \right]
\]

In Eq. (6.17), \( V_{a,i}^{n+1} \) and \( V_{a,i}^n \) are the amount of gas adsorbed and adsorption capacity of the gas component \( i \) at time step \( n+1 \) in \( lbmol \), respectively. The pseudo-steady state sorption time constant \( \tau \) represents the time delay for adsorbed gas to transport through the micropores in matrix. The adsorption model follows the equilibrium sorption model proposed by Manik (2002).
The governing flow equation for hydraulic fracture is similar to the equation for natural fracture with slight modifications. Flow in hydraulic fractures is two dimensional and has its own coordinate system aligned to the hydraulic fracture dimensions (i.e., length and width). Let \( u \)- and \( v \)- be the directions aligned with the hydraulic fracture length and width, respectively. The governing flow equation for hydraulic fracture domain can be derived as follows.

\[
\frac{\partial}{\partial u} \left[ x_{i,F} \tilde{P}_{o,F} A_u k_{u,F} k_{m,F} \left( \frac{\partial P_{o,F}}{\partial u} - \frac{1}{144} \frac{g}{\rho_{o,F}} \frac{\partial G}{\partial u} \right) \right] + y_{i,F} \tilde{P}_{g,F} A_u k_{u,F} k_{rg,F} \left( \frac{\partial P_{g,F}}{\partial u} - \frac{1}{144} \frac{g}{\rho_{g,F}} \frac{\partial G}{\partial u} \right) + \phi_x S_{g,F} A u \frac{\partial}{\partial u} \left( y_{i,F} \tilde{P}_{g,F} \right) \Delta u
\]

\[
+ \frac{\partial}{\partial v} \left[ x_{i,F} \tilde{P}_{o,F} A_v k_{v,F} k_{m,F} \left( \frac{\partial P_{o,F}}{\partial v} - \frac{1}{144} \frac{g}{\rho_{o,F}} \frac{\partial G}{\partial v} \right) \right] + y_{i,F} \tilde{P}_{g,F} A_v k_{v,F} k_{rg,F} \left( \frac{\partial P_{g,F}}{\partial v} - \frac{1}{144} \frac{g}{\rho_{g,F}} \frac{\partial G}{\partial v} \right) + \phi_y S_{g,F} A D_{eff} \frac{\partial}{\partial v} \left( y_{i,F} \tilde{P}_{g,F} \right) \Delta v
\]

\[
+ M_{i,F} + M_{i,F} + \Lambda_{i,F} = \frac{1}{5.615} \frac{\partial}{\partial t} \left( V_{i,F} \phi \tilde{S}_{o,F} x_{i,F} \tilde{P}_{o,F} + V_{i,F} \phi \tilde{S}_{g,F} y_{i,F} \tilde{P}_{g,F} \right)
\]

(6.18)

The source terms \( M_{i,F} \) and \( \Lambda_{i,F} \) are molar exchange rate of component \( i \) between hydraulic fracture and matrix domain and between hydraulic fracture and natural fracture domain, respectively.

Similarly, the governing flow equation for water component in natural fracture domain is shown in Eq. (6.19).

\[
\frac{\partial}{\partial x} \left( A k_{x,F} k_{m,F} \left( \frac{\partial P_{x,F}}{\partial x} - \frac{1}{144} \frac{g}{\rho_{x,F}} \frac{\partial G}{\partial x} \right) \right) \Delta x + \frac{\partial}{\partial y} \left( A k_{y,F} k_{m,F} \left( \frac{\partial P_{y,F}}{\partial y} - \frac{1}{144} \frac{g}{\rho_{y,F}} \frac{\partial G}{\partial y} \right) \right) \Delta y
\]

\[
+ \frac{\partial}{\partial z} \left( A k_{z,F} k_{m,F} \left( \frac{\partial P_{z,F}}{\partial z} - \frac{1}{144} \frac{g}{\rho_{z,F}} \frac{\partial G}{\partial z} \right) \right) \Delta z + q_{w,f} + \Gamma_{w,f} + \Lambda_{w,f} = \frac{V_{w,F}}{5.615} \frac{\partial}{\partial t} \left( \phi \tilde{S}_{w,F} \right)
\]

(6.19)
The terms $q_{w,f}^{sc}$, $\Gamma_{w,f}$, and $\Lambda_{w,f}$ refer to source/sink for well, mass exchange of water component between natural fracture and matrix domains and between natural fracture and hydraulic fracture domains, respectively.

Adsorption is ignored in water flow in matrix domain. Thus, the water governing flow equation in matrix system is can be written in Eq. (6.20).

$$\frac{\partial}{\partial x} \left( \frac{A_{k_{n,m}} k_{w,m}}{\mu_{w,M} B_{w,M}} \left( \frac{\partial P_{w,M}}{\partial x} - \frac{1}{144} \frac{g}{\rho_{w,M}} \frac{\partial G}{\partial x} \right) \right) \Delta x + \frac{\partial}{\partial y} \left( \frac{A_{k_{n,m}} k_{w,m}}{\mu_{w,M} B_{w,M}} \left( \frac{\partial P_{w,M}}{\partial y} - \frac{1}{144} \frac{g}{\rho_{w,M}} \frac{\partial G}{\partial y} \right) \right) \Delta y + \frac{\partial}{\partial z} \left( \frac{A_{k_{n,m}} k_{w,m}}{\mu_{w,M} B_{w,M}} \left( \frac{\partial P_{w,M}}{\partial z} - \frac{1}{144} \frac{g}{\rho_{w,M}} \frac{\partial G}{\partial z} \right) \right) \Delta z + q_{w,m}^{sc} + M_{w,m} + \Gamma_{w,m} = \frac{V_b}{5.615 / \Delta t} \left( \frac{\phi_m S_{w,m}}{B_{w,m}} \right) \tag{6.20}$$

where $M_{w,m}$ and $\Gamma_{w,m}$ the mass exchange of water component between matrix and hydraulic fracture domains via NNC source term and mass exchange of water component between matrix and natural fracture, respectively. Since mass is assumed to flow from/to matrix to/from natural fractures, the source term $\Gamma_{w,m}$ for mass exchange between the two domains is equal in magnitude but opposite in sign as shown in Eq. (6.21).

$$\Gamma_{w,m} = -\Gamma_{w,f} \tag{6.21}$$

The governing flow equation for water component in hydraulic fracture is written similarly to that is written for hydrocarbon components.

$$\frac{\partial}{\partial x} \left( \frac{A_{k_{n,f}} k_{w,F}}{\mu_{w,F} B_{w,F}} \left( \frac{\partial P_{w,F}}{\partial x} - \frac{1}{144} \frac{g}{\rho_{w,F}} \frac{\partial G}{\partial x} \right) \right) \Delta x + \frac{\partial}{\partial y} \left( \frac{A_{k_{n,f}} k_{w,F}}{\mu_{w,F} B_{w,F}} \left( \frac{\partial P_{w,F}}{\partial y} - \frac{1}{144} \frac{g}{\rho_{w,F}} \frac{\partial G}{\partial y} \right) \right) \Delta y + q_{w,F}^{sc} + M_{w,f} + \Lambda_{w,f} = \frac{V_b}{5.615 / \Delta t} \left( \frac{\phi_f S_{w,f}}{B_{w,F}} \right) \tag{6.22}$$

where the parameters $q_{w,f}^{sc}$, $M_{w,f}$, and $\Lambda_{w,f}$ are well source/sink term, volumetric exchange rate of water component between hydraulic fracture and matrix domains and between hydraulic fracture and natural fracture domains via NNC, respectively.
6.3.1 Calculation of Inter-porosity Transmissibility

Mass exchange rates between porosity domains are described in this section. For $n$ porosity pairs, the total number of possible pairs is $\frac{n(n-1)}{2}$. Thus, in our triple-porosity model, a total of three inter-porosity transmissibility pairs are discussed.

6.3.1.1 Matrix-Natural Fracture Transmissibility

For a matrix and natural fracture porosity pair, the transmissibility is assumed to follow the Warren and Root (1963) dual-continuum formulation. The fluid transport is assumed to be under pseudo-steady state. Molar exchange rate between matrix and natural fracture can be calculated from Eq. (6.23).

$$\Gamma_{i,M} = \sigma V_{b,i,M} \frac{k_{M}k_{ro,M}}{\mu_{o,M}} (P_{o,M} - P_{o,f}) + \sigma V_{b,y,i,M} \frac{k_{M}k_{tg,M}}{\mu_{g,M}} (P_{g,M} - P_{g,f})$$

$$+ \sigma V_{b,y,i,M} \frac{K_{g,s}}{5.615} (\tilde{P}_{g,M} - \tilde{P}_{g,f}) \quad (6.23)$$

$$\Gamma_{i,f} = -\Gamma_{i,M} \quad (6.24)$$

Flow of water component in matrix system is driven mainly by pressure gradient. The volumetric exchange rate between matrix and natural fracture can be calculated as follows:

$$\Gamma_{w,M} = \sigma V_{b} \frac{k_{rw,M}}{\mu_{w,M}B_{w,M}} (P_{w,M} - P_{w,f}) \quad (6.25)$$

$$\Gamma_{w,f} = -\Gamma_{w,M} \quad (6.26)$$

The parameter $\sigma$ is a shape factor in units of $mD/ft^2$. Two different formulations for shape factors are available in PennComp and are shown in Eq. (6.27) and Eq. (6.28).
Warren and Root (1963):

\[
\sigma = \frac{20}{3} k \left( \frac{1}{L_x} + \frac{1}{L_y} + \frac{1}{L_z} \right)^2 \tag{6.27}
\]

and Kazemi (1976):

\[
\sigma = 4 \left( \frac{k_x}{L_x^2} + \frac{k_y}{L_y^2} + \frac{k_z}{L_z^2} \right) \tag{6.28}
\]

It should be noted that fluid transport between matrix and natural fracture depends only on matrix permeability. Diffusion from matrix to natural fracture only occurs in the gas phase.

### 6.3.1.2 Matrix-Hydraulic Fracture Transmissibility

Molar exchange rate between hydraulic fracture and matrix domains can be calculated from Eq. (6.29).

\[
M_{i,F} = \sum_{m=1}^{N_{mf}} A_{m}^{MF} \sum_{j=1}^{N_{mf}} \frac{k_{m}^{MF} k_{nj}^{MF}}{\mu_{j}} \left[ \frac{(P_j - \frac{1}{144} \frac{g}{\rho_j} G) - (P_j - \frac{1}{144} \frac{g}{\rho_j} G)_m}{d_{m}^{MF}} \right] + \phi S_{i}^{MF} \frac{D_{ef} A_{m}^{MF}}{5.615 d_{m}^{MF}} \left( y_{i} \tilde{\rho}_s - y_{i} \tilde{\rho}_s^{MF} \right) \tag{6.29}
\]

\[
M_{i,M} = -M_{i,F} \tag{6.30}
\]

Volumetric exchange rate of water between hydraulic fracture and matrix domains can be calculated from Eq. (6.31).

\[
M_{w,F} = \sum_{m=1}^{N_{mf}} A_{m}^{MF} \frac{k_{m}^{MF} k_{w}^{MF}}{\mu_{w} B_{w}} \left[ \frac{(P_w - \frac{1}{144} \frac{g}{\rho_w} G) - (P_w - \frac{1}{144} \frac{g}{\rho_w} G)_m}{d_{m}^{MF}} \right] \tag{6.31}
\]

\[
M_{w,M} = -M_{w,F} \tag{6.32}
\]
The area $A_{m}^{MF}$ is the area that fracture intersects the matrix block and is based on fracture orientation. It is assumed that transport occurs via Darcy flow only.

### 6.3.1.3 Natural Fracture-Hydraulic Fracture Transmissibility

Molar exchange rate between natural and hydraulic fractures can be calculated from Eq. (6.33).

$$\Lambda_{i,f} = \sum_{m=1}^{N_{p}} \left( A_{m}^{F} \sum_{j=1}^{N_{r}} k_{m}^{F} k_{rj} \left( \frac{p_{j} - \frac{1}{144} g \rho_{j} G}{d_{m}^{F}} - \frac{p_{j} - \frac{1}{144} g \rho_{j} G}{d_{m}^{F}} \right) \right) + \phi S_{i}^{F} \frac{D_{ef} A_{m}^{F}}{5.615 d_{m}^{F}} \left( y_{i} \tilde{G}_{s} - y_{i} \tilde{G}_{s}^{F} \right)$$

(6.33)

$$\Lambda_{i,F} = -\Lambda_{i,f}$$

(6.34)

Volumetric exchange rate of water between natural fracture and hydraulic fracture domains can be calculated from Eq. (6.35).

$$\Lambda_{w,f} = \sum_{m=1}^{N_{p}} \left( A_{m}^{F} k_{m}^{F} k_{rw} \left( \frac{p_{w} - \frac{1}{144} g \rho_{w} G}{d_{m}^{F}} - \frac{p_{w} - \frac{1}{144} g \rho_{w} G}{d_{m}^{F}} \right) \right)$$

(6.35)

$$\Lambda_{w,F} = -\Lambda_{w,f}$$

(6.36)

The area $A_{m}^{IF}$ is an effective area open to flow between natural fracture and hydraulic fracture and is calculated from Eq. (6.37).

$$A_{m}^{IF} = \alpha_{IF} \cdot A_{m}^{MF}$$

(6.37)

where $\alpha_{IF}$ is natural fracture-hydraulic fracture intersecting coefficient and is specified by the user. The default value for intersecting coefficient is equal to natural fracture porosity ($\phi_{f}$).
Using this default value, it is assumed that an effective area can be represented by natural fracture porosity, which is a pore space that is available to hold fluid and intersect with hydraulic fractures. The average normal distance between natural fracture and hydraulic fracture segment \( d_{mF} \) is assumed to be equal to the distance between matrix and hydraulic fracture.

### 6.4 Highlights of the Chapter

In this chapter, the implementations of effect of capillary pressure on phase behaviors and embedded discrete fracture model are discussed. The formulation of the triple-porosity model and the calculation of inter-porosity transmissibility are presented. These topics can be summarized as follows:

- The modified negative flash calculation is implemented in the simulator to account for capillary pressure. The role of the modified negative flash is to determine the number of phase and fluid properties. Macleod and Sugden correlation is used to calculate gas-oil interfacial tension.

- The data structure for the EDFM and different types of non-neighboring connections are discussed. Fractures that intersect the well are assumed to be perpendicular to the well bore. Each well-fracture intersection is treated as an additional perforation of the well. Peaceman’s well model is used to calculate the production/injection from/to the fracture segment.

- The three porosity types in the triple-porosity model are matrix, natural fracture, and hydraulic fracture. The matrix and natural fracture co-exist in the grid block, and the presence of discrete fracture serves as the third porosity type. Flow in the triple-porosity model is fully coupled and occurs simultaneously in all porosity types.
The inter-porosity transmissibility between matrix and natural fracture follows Warren and Root (1963) dual-continuum model where a shape factor is used to model the shape of the matrix block. Source terms similar to Peaceman’s well model are used to handle flows between matrix and hydraulic fracture and between natural fracture and hydraulic fracture. The area open to flow and average normal distance between matrix and hydraulic fracture are directly calculated from the geometry of the discrete fracture that intersects the grid block. The intersecting coefficient is introduced to represent an effective area open to flow between natural fracture and hydraulic fracture.
Chapter 7

Model Validation

In this chapter, the compositional model is validated against commercial simulator for single-porosity model, dual-porosity, single-permeability model, dual-porosity, dual-permeability model, and single-porosity model with local grid refinement. It should be noted that in dual-porosity model of the commercial reservoir simulator, the matrix porosity doesn’t communicate with well directly. This means, hydrocarbon from matrix must flow to natural fracture before it can flow to the well. Capillary pressure between phases is ignored in all validation cases. Two different fluids are used in the validations shown in Table 7-1 and Table 7-2. Rock-fluid properties are shown in Figure 7-1.

Table 7-1: Compositional data for 6-component fluid for validation tests

<table>
<thead>
<tr>
<th>Component</th>
<th>Mole Fraction</th>
<th>Critical Pressure (psia)</th>
<th>Critical Temperature (oR)</th>
<th>Acentric Factor</th>
<th>Molecular Weight (lb/lbmol)</th>
<th>Critical Volume (ft³/lbmol)</th>
<th>Parachor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.36</td>
<td>667.20</td>
<td>343.68</td>
<td>0.008</td>
<td>16.04</td>
<td>1.58</td>
<td>77.0</td>
</tr>
<tr>
<td>C₂</td>
<td>0.15</td>
<td>708.35</td>
<td>550.32</td>
<td>0.098</td>
<td>30.07</td>
<td>2.37</td>
<td>108.0</td>
</tr>
<tr>
<td>C₃</td>
<td>0.10</td>
<td>615.76</td>
<td>666.24</td>
<td>0.152</td>
<td>44.10</td>
<td>3.25</td>
<td>150.3</td>
</tr>
<tr>
<td>NC₅</td>
<td>0.19</td>
<td>489.38</td>
<td>845.88</td>
<td>0.251</td>
<td>72.15</td>
<td>4.87</td>
<td>231.5</td>
</tr>
<tr>
<td>NC₁₀</td>
<td>0.10</td>
<td>305.68</td>
<td>1,112.28</td>
<td>0.490</td>
<td>142.29</td>
<td>9.66</td>
<td>433.5</td>
</tr>
<tr>
<td>NC₁₆</td>
<td>0.10</td>
<td>205.74</td>
<td>1,291.20</td>
<td>0.742</td>
<td>226.45</td>
<td>15.31</td>
<td>676.9</td>
</tr>
</tbody>
</table>

Table 7-2: Compositional data for 2-component fluid for validation tests

<table>
<thead>
<tr>
<th>Component</th>
<th>Mole Fraction</th>
<th>Critical Pressure (psia)</th>
<th>Critical Temperature (oR)</th>
<th>Acentric Factor</th>
<th>Molecular Weight (lb/lbmol)</th>
<th>Critical Volume (ft³/lbmol)</th>
<th>Parachor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.36</td>
<td>667.20</td>
<td>343.68</td>
<td>0.008</td>
<td>16.04</td>
<td>1.58</td>
<td>77.0</td>
</tr>
<tr>
<td>NC₁₆</td>
<td>0.10</td>
<td>205.74</td>
<td>1,291.20</td>
<td>0.742</td>
<td>226.45</td>
<td>15.31</td>
<td>676.9</td>
</tr>
</tbody>
</table>
7.1 Validation of Single-porosity, Single-permeability Model

In the validation of single-porosity, single-permeability model, three development scenarios will be demonstrated and compared with a commercial reservoir simulator: primary depletion, water injection, and gas injection. From all the validation runs, our in-house reservoir simulator matches rates, bottom-hole pressures, and well block pressures exactly.

7.1.1 Primary Depletion

For validation of primary depletion, the reservoir model is shown in Figure 7-2. The reservoir model is three dimensional. One vertical well is located at the center of the reservoir and is perforated only at the top layer.
Table 7-3: Input data for validation test for primary depletion in single-porosity model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir dimensions</td>
<td>1,500 × 1,500 × 75</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>75</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>4,000</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>200</td>
<td>ºF</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Layer 1 (top)</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Layer 2 (middle)</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Layer 3 (bottom)</td>
<td>0.9</td>
<td>fraction</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.3</td>
<td>fraction</td>
</tr>
<tr>
<td>Porosity</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Permeability</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x-direction</td>
<td>100</td>
<td>mD</td>
</tr>
<tr>
<td>y-direction</td>
<td>100</td>
<td>mD</td>
</tr>
<tr>
<td>z-direction</td>
<td>10</td>
<td>mD</td>
</tr>
<tr>
<td>Well location (x,y,z)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Well-1: Producer</td>
<td>Top-layer</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>center (8,8,1)</td>
<td>-</td>
</tr>
<tr>
<td>Well specification:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Constant bottom-hole pressure</td>
<td>500</td>
<td>psia</td>
</tr>
</tbody>
</table>

Figure 7-2: Reservoir model for validation of primary depletion
Figure 7-3: Validation of primary depletion in single-porosity model – oil production rate comparison

Figure 7-4: Validation of primary depletion in single-porosity model – gas production rate comparison
Figure 7-5: Validation of primary depletion in single-porosity model – water production rate comparison

Figure 7-6: Validation of primary depletion in single-porosity model – well block pressure comparison
7.1.2 Water Injection

For validation case of water injection, we used a two-dimensional reservoir with 3 wells as shown in Figure 7-7. The reservoir fluid properties are shown in Table 7-1.

Table 7-4: Input data for validation test for water injection in single-porosity model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir dimensions</td>
<td>$2,215 \times 1,275 \times 100$</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>4,000</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>200</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Permeability</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x-direction</td>
<td>20-100</td>
<td>$mD$</td>
</tr>
<tr>
<td>y-direction</td>
<td>20-100</td>
<td>$mD$</td>
</tr>
<tr>
<td>z-direction</td>
<td>100</td>
<td>$mD$</td>
</tr>
<tr>
<td>Well location (x,y,z)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Well-1: Producer</td>
<td>(25,3,1)</td>
<td>-</td>
</tr>
<tr>
<td>Well-2: Producer</td>
<td>(5,15,1)</td>
<td>-</td>
</tr>
<tr>
<td>Well-3: Injector</td>
<td>(40,25,1)</td>
<td>-</td>
</tr>
<tr>
<td>Well specification:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Well-1: Constant bottom-hole pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Well-2: Constant bottom-hole pressure</td>
<td>800</td>
<td>psia</td>
</tr>
<tr>
<td>Well-3: Constant water injection rate</td>
<td>300</td>
<td>STB/day</td>
</tr>
</tbody>
</table>

Figure 7-7: Reservoir model for validation of water injection
Figure 7-8 to Figure 7-11 show production rates and well block pressures comparisons for Well-1 between our model and the commercial reservoir simulator. Figure 7-12 to Figure 7-15 show production rates and well block pressures for Well-2 between our model and the commercial reservoir simulator. In the case of Well-3, the well is injecting water at constant rate of 300 STB/day. The well block and well bottom-hole pressures are compared in Figure 7-16 and Figure 7-17.

Figure 7-8: Validation of water injection in single-porosity model – Well-1 oil production rate comparison
Figure 7-9: Validation of water injection in single-porosity model – Well-1 gas production rate comparison

Figure 7-10: Validation of water injection in single-porosity model – Well-1 water production rate comparison
Figure 7-11: Validation of water injection in single-porosity model – Well-1 producer well block pressure comparison

Figure 7-12: Validation of water injection in single-porosity model – Well-2 oil production rate comparison
Figure 7-13: Validation of water injection in single-porosity model – Well-2 gas production rate comparison

Figure 7-14: Validation of water injection in single-porosity model – Well-2 water production rate comparison
Figure 7-15: Validation of water injection in single-porosity model – Well-2 producer well block pressure comparison

Figure 7-16: Validation of water injection in single-porosity model – Well-3 injector well block pressure comparison
For validation of gas injection, two cases with similar reservoir setting will be demonstrated. The first case is gas injection under constant injection rate. The second case is gas injection under constant bottom-hole pressure. In both cases, Peng-Robinson (1976) equation of state is used. The input data is shown in Table 7-5.
Table 7-5: Input data for validation test for gas injection in single-porosity model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir dimensions</td>
<td>1,500 × 1,500 × 75</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>75</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>4,000</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>200</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Layer 1 (top)</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Layer 2 (middle)</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Layer 3 (bottom)</td>
<td>0.9</td>
<td>fraction</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.3</td>
<td>fraction</td>
</tr>
<tr>
<td>Permeability</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x-direction</td>
<td>100</td>
<td>mD</td>
</tr>
<tr>
<td>y-direction</td>
<td>100</td>
<td>mD</td>
</tr>
<tr>
<td>z-direction</td>
<td>10</td>
<td>mD</td>
</tr>
<tr>
<td>Well location (x,y,z)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Well-1: Producer</td>
<td>Top-layer</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>top-left corner (15,15,1)</td>
<td>-</td>
</tr>
<tr>
<td>Well-2: Injector</td>
<td>Middle-layer</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>bottom-right corner (1,1,2)</td>
<td>-</td>
</tr>
<tr>
<td>Well specification:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Well-1: Constant bottom-hole pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Well-2 (Case 1): Constant surface injection rate</td>
<td>3,000</td>
<td>Mscf/day</td>
</tr>
<tr>
<td>Well-2 (Case 2): Constant bottom-hole pressure</td>
<td>4,000</td>
<td>psia</td>
</tr>
</tbody>
</table>

The reservoir model is shown in Figure 7-18. The reservoir is three-dimensional modeled with a 15×15×3 grid. The bottom layer is saturated with water and residual oil. The initial reservoir pressure is 4,000 psia. A vertical injector is located at the bottom left corner perforated at the middle layer. A vertical producer is located at the top right corner perforated at the top layer. The compositional data is shown in Table 7-1. In Case 1, pure methane is injected at constant surface volumetric rate of 3,000 Mscf/day. In Case 2, methane is injected under constant bottom-hole pressure of 4,000 psia, which is equal to the initial reservoir pressure. In both cases, the injection starts immediately, and the well injects pure methane (CH₄). The producer is producing under constant bottom-hole pressure of 500 psia. Miscibility is formed near the injection well.
Figure 7-18: Reservoir model for validation of gas injection

7.1.3.1 Case 1 – Constant Surface Volumetric Injection Rate

Figure 7-19: Case 1 – validation of gas injection under constant injection rate in single-porosity model – oil production rate comparison
Figure 7-20: Case 1 – validation of gas injection under constant injection rate in single-porosity model – gas production rate comparison

Figure 7-21: Case 1 – validation of gas injection under constant injection rate in single-porosity model – water production rate comparison
Figure 7-22: Case 1 – validation of gas injection under constant injection rate in single-porosity model – producer well block pressure comparison

Figure 7-23: Validation of gas injection under constant injection rate in single-porosity model – injector well block pressure comparison
Figure 7-24: Validation of gas injection under constant injection rate in single-porosity model – gas injection rate at reservoir condition comparison

Figure 7-25: Validation of gas injection under constant injection rate in single-porosity model – injector bottom-hole pressure comparison
7.1.3.2 Constant Bottom-hole Injection Pressure

Figure 7-26: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – oil production rate comparison

Figure 7-27: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – gas production rate comparison
Figure 7-28: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – water production rate comparison

Figure 7-29: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – producer well block pressure comparison
Figure 7-30: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – gas injection rate at surface condition comparison

Figure 7-31: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – gas injection rate at reservoir condition comparison
Figure 7-32: Case 2 – validation of gas injection under constant injection pressure in single-porosity model – injector well block pressure comparison

7.2 Validation of Dual-porosity, Single-permeability Model

This validation case uses compositional data as shown in Table 7-1. The top view of the two-dimensional reservoir model is shown in Figure 7-33.
Table 7-6: Input data for validation test for dual-porosity, single-permeability model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir dimensions</td>
<td>$3,000 \times 2,000$</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>4,000</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation, matrix</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Initial water saturation, fracture</td>
<td>0.25</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.3</td>
<td>fraction</td>
</tr>
<tr>
<td>Fracture porosity</td>
<td>0.05</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.05</td>
<td>mD</td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>1</td>
<td>mD</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Well location (x,y,z)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Well-1</td>
<td>Top left (5,5,1)</td>
<td>-</td>
</tr>
<tr>
<td>Well-2</td>
<td>Bottom right (25,15,1)</td>
<td>-</td>
</tr>
<tr>
<td>Well specification:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Well-1: Constant bottom-hole pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Well-2: Constant bottom-hole pressure</td>
<td>800</td>
<td>psia</td>
</tr>
</tbody>
</table>

The production rate and well block pressure comparison for Well-1 and Well-2 are shown in Figure 7-34 to Figure 7-41.

![Figure 7-34: DPSK validation – Well-1 oil production rate comparison](image-url)
Figure 7-35: DPSK validation – Well-1 gas production rate comparison

Figure 7-36: DPSK validation – Well-1 water production rate comparison
Figure 7-37: DPSK validation – Well-1 well block pressure comparison

Figure 7-38: DPSK validation – Well-2 oil production rate comparison
Figure 7-39: DPSK validation – Well-2 gas production rate comparison

Figure 7-40: DPSK validation – Well-2 water production rate comparison
7.3 Validation of Dual-porosity, Dual-permeability Model

In this validation case, PennComp’s DPDK option is validated against CMG’s DPDK option. The reservoir model and properties are exactly the same as the validation for DPSK model. The model is shown in Figure 7-33. The reservoir properties are shown in Figure 7-19. Note that in the case of DPDK, flow between matrix blocks is allowed. However, matrix blocks do not communicate with the well directly. From Figure 7-42 to Figure 7-49, the oil, gas, water rates and well block pressure comparisons are in perfect agreement with the commercial software.
Figure 7-42: DPDK validation – Well-1 oil production rate comparison

Figure 7-43: DPDK validation – Well-1 gas production rate comparison
Figure 7-44: DPDK validation – Well-1 water production rate comparison

Figure 7-45: DPDK validation – Well-1 well block pressure comparison
Figure 7-46: DPDK validation – Well-2 oil production rate comparison

Figure 7-47: DPDK validation – Well-2 gas production rate comparison
Figure 7-48: DPDK validation – Well-2 water production rate comparison

Figure 7-49: DPDK validation – Well-2 well block pressure comparison
7.4 Validation of Embedded Discrete Fracture Model

To validate the embedded discrete fracture model, local grid refinement is used to create fractures and validated against the in-house model where fractures are simulated using EDFM. Production comparisons from both models are then compared. A comparison of production from a hydraulically fractured horizontal well in tight rock with no flow boundaries at the outer edges is made for model validation. The reservoir parameters are shown in Table 7-7. The fluid used in this validation is shown in Table 7-2. The model assumes zero capillary pressure.

Table 7-7: Input data for validation test for embedded discrete fracture model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>90% NC$_{16}$ – 10% C$_1$</td>
<td></td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>1,100 × 1,100</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>4,000</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>160</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.11</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.1</td>
<td>fraction</td>
</tr>
<tr>
<td>Fracture porosity</td>
<td>1</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.05</td>
<td>mD</td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Fracture width</td>
<td>0.05</td>
<td>ft</td>
</tr>
<tr>
<td>Well location (x,y,z)</td>
<td>Center (7,7,1)</td>
<td></td>
</tr>
<tr>
<td>Well specification:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Constant bottom-hole pressure</td>
<td>500</td>
<td>psia</td>
</tr>
</tbody>
</table>

The reservoir model is shown in Figure 7-50 where the red line represents the discrete fracture. In this case, a 100-feet long horizontal well is placed at the center of a closed reservoir with one discrete fracture intersecting the well.
The results from three different fracture modeling techniques are compared: the in-house simulator with EDFM, the in-house simulator with a fine-grid model, and the commercial simulator with LGR. Oil, gas, and water production rates are shown in Figure 7-51 to Figure 7-53. Blue, red, and green curves show the production from the fine-grid model, EDFM, and LGR, respectively. Production rates from the three different fracture modeling techniques are in excellent agreement.
Figure 7-51: EDFM validation – oil production rate comparison

Figure 7-52: EDFM validation – gas production rate comparison
Figure 7-53: EDFM validation – water production rate comparison

7.5 Highlights of the Chapter

In this chapter, we demonstrated that the developed in-house reservoir simulator agrees well to the simulations from commercial software for various simplified cases. In the following chapters, simulations of hydraulically fractured tight rocks and shales with capillary pressure on phase behavior and flow will be demonstrated using the proposed triple-porosity model.
Chapter 8

Simulation of Multi-mechanistic Triple-porosity Triple-permeability Compositional Model

This chapter discusses simulations of the proposed triple-porosity, triple-permeability model (TPTK). In the TPTK model, the grid block contains two porosity types: matrix and natural fracture. Hydraulic fractures are modeled discretely using the EDFM, and the discrete fractures serve as the third porosity type (i.e., the grid block that contains discrete fracture has three porosity types). With the TPTK model, the reservoir properties can be assigned accordingly to the porosity type. Consequently, the model can potentially give more accurate results compared to single-porosity and dual-porosity models. The simulation results from the proposed TPTK model are compared with the single-porosity model coupled with EDFM and the dual-porosity, dual-permeability model with grid refinement. Finally, a parametric study of the proposed model is shown in the last section. Water is the wetting phase in simulation runs in this chapter.

8.1 Comparison with the single-porosity model coupled with EDFM

In naturally fractured reservoirs, the formation contains two vastly different types of porosities: matrix and natural fracture. Matrix has high fluid storativity of hydrocarbons compared to that of natural fractures but has low fluid transmissibility. Conversely, natural fracture systems have low storage capacity but serves as relatively high-permeability channels for hydrocarbons to flow to the wellbore. Recall that in the single-porosity model coupled with the EDFM, grid blocks in the model represent a formation that consists of both matrix and natural
fractures while discrete fractures modeled by EDFM represent hydraulic fractures. From this point onward, the single-porosity model coupled with EDFM will be referred as EDFM. On the other hand, the TPTK model enables us to use respective reservoir properties corresponding to the porosity types in the reservoir without having to perform averaging techniques on the properties and assign one “representative” value to the grid block as is done in EDFM. This is because the grid block in the TPTK model contains up to three porosity types (e.g., matrix, natural fracture, and hydraulic fracture).

The main parameters of interest in comparing the two models are porosity and permeability. In the EDFM, total porosity assigned to the grid block is equal to the sum of matrix porosity and natural fracture porosity. Porosity-weighted permeability, natural fracture permeability as an upper-bound value, and matrix permeability as a lower-bound value are assigned for permeability in the EDFM. Eq. (8.1) shows the calculation of porosity-weighted permeability.

\[
    k_{\text{ave}} = \frac{\phi_M k_M + \phi_f k_f}{\phi_M + \phi_f}
\]  

(8.1)

Three different EDFM runs are simulated for comparison with the TPTK model. In the TPTK model, matrix porosity and permeability are assigned to the matrix domain. Similarly, natural fracture porosity and permeability are assigned to the natural fracture domain. For comparison of the TPTK model with EDFM, we run the models for 1 year. Bakken oil is used in the study. The reservoir parameters are shown in Table 8-1. The total contact area between discrete fracture and grid blocks is 390,000 $ft^2$. Rock-fluid properties are shown in Figure 9-1 and Figure 9-2. In all cases, the total hydrocarbon in-place is conserved.
Table 8-1: Parameters for comparison of EDFM with TPTK model

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td></td>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td></td>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td></td>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td></td>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td></td>
<td><strong>EDFM</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Porosity</td>
<td>0.07</td>
<td>fraction</td>
</tr>
<tr>
<td></td>
<td>Upper-bound permeability</td>
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<td>mD</td>
</tr>
<tr>
<td></td>
<td>Porosity-weighted permeability</td>
<td>0.0723</td>
<td>mD</td>
</tr>
<tr>
<td></td>
<td>Lower-bound permeability</td>
<td>0.001</td>
<td>mD</td>
</tr>
<tr>
<td></td>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td></td>
<td>Fracture width</td>
<td>0.05</td>
<td>ft</td>
</tr>
<tr>
<td></td>
<td><strong>TPTK</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td></td>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td></td>
<td>Matrix permeability</td>
<td>0.001</td>
<td>mD</td>
</tr>
<tr>
<td></td>
<td>Natural fracture permeability</td>
<td>0.5</td>
<td>mD</td>
</tr>
<tr>
<td></td>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td></td>
<td>Fracture width</td>
<td>0.05</td>
<td>ft</td>
</tr>
</tbody>
</table>

Figure 8-1: Three-stage hydraulically fractured reservoir model for study of the TPTK model. Each grid block contains matrix and natural fracture.

Figure 8-2 shows oil production rate comparison between the single-porosity model with EDFM and the TPTK model. The production rates from all EDFM runs are drastically different. The EDFM case with porosity-weighted permeability initially gives production profile along the...
same line as the TPTK model. However, the production from the two models behaves differently after approximately 60 days. The production from the EDFM-AVE declines smoothly. Conversely, the rate from the TPTK model declines quickly until approximately 30 days. The rate then steadily declines until the end of the simulation. This reflects the dual-continuum nature of the TPTK model (i.e., in dual-continuum model, production initially comes from the natural fracture and later from matrix).

The rate from the EDFM case with lower-bound permeability falls rapidly within the first day of production because hydrocarbons stored in the discrete fracture is produced. Gas forms in the fractures and is also produced immediately leaving only heavy hydrocarbon components in the fractures. However, the ultra-low permeability of 0.001 $mD$ prevents the hydrocarbons stored in grid blocks to flow quickly to the discrete fractures. Once oil flows to the discrete fracture, the oil production rate begins to climb as shown by green curve in Figure 8-2. The system becomes more stabilized as can be seen from the gradual decline of oil rate.

![Figure 8-2: Oil production rate comparison between EDFM and TPTK model](image-url)
Figure 8-3 shows cumulative oil production from three EDFM cases and the TPTK mode. The cumulative oil production from lower-, upper-, and average-EDFM are 32,781 STB, 494,383 STB, and 248,889 STB, respectively, after one year of production. The cumulative production for the TPTK model after one year of production is 302,845 STB. The cumulative production from the TPTK model is 21.68% higher as compared to the EDFM run with porosity-weighted permeability.

Figure 8-3: Cumulative oil production comparison between EDFM and TPTK model

Figure 8-4 shows the pressure distribution for the EDFM-AVE and TPTK models. It can be seen that with the TPTK model, the reservoir is drained more effectively as natural fracture serves as a secondary flow channel other than hydraulic fractures. Based on the comparison, we can see the importance of characterizing the reservoir with multiple-porosity types.
8.2 Comparison with Dual-porosity Models

To compare with dual-porosity models, we start by comparing the DPSK and DPDK models. From Figure 8-5, the productions between both models are almost identical owing to the ultra-low permeability. Therefore, the proposed TPTK model is compared against only the DPDK model here.
To compare DPDK with TPTK, a fine-grid model is used for hydraulic fractures in the DPDK model. Hydraulic fracture permeability is assigned to the fine grid blocks that represent hydraulic fractures. The width of the fracture grid block is 0.05 ft which is equal to the width of the discrete fracture. The TPTK model remains the same as the previous comparison with EDFM (Figure 8-1). The grid for the TPTK model is 25×25×1. The grid blocks that host hydraulic fracture for both DPDK and TPTK models are shown in Figure 8-6. The productions from the TPTK and DPDK models are compared. Table 8-2 shows the reservoir parameters for the comparison of the TPTK model against the DPDK model.

Figure 8-5: Oil production rate comparison between DPDK and DPSK models
Figure 8-6: Grid block that hosts a segment of hydraulic fracture. (a) Grid refinement is used to represent discrete fracture in the DPDK model; (b) Discrete fracture is embedded in the grid block.

Table 8-2: Parameters for comparison of DPDK model with TPTK model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.001</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.5</td>
<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Fracture width</td>
<td>0.05</td>
<td>ft</td>
</tr>
</tbody>
</table>

Relative permeability for the matrix is the same as shown in Figure 9-1. However, to preserve the flow characteristics in the natural fracture domain of the DPDK model, straight-line relative permeability curves (with zero residual saturations and end-points equal to one) for the natural fracture porosity of the DPDK model and TPTK model are used. Capillary pressure is ignored in this case. Both the TPTK and DPDK models have the same exact initial hydrocarbon- and water-in-place. Again, oil production rates and pressure distributions at the end of the simulations between the DPDK and TPTK models are shown in Figure 8-7 and Figure 8-8, respectively.
Figure 8-7: Oil production rate comparison between the DPDK and TPTK models

From Figure 8-7, the oil production rates from the DPDK model is significantly higher compared to the rate from TPTK. This is mainly due to the natural fracture-hydraulic fracture transmissibility assumption used in the TPTK model. In the TPTK model, by default, the
intersecting area that is open to flow between natural fractures and hydraulic fractures is determined from an effective intersecting area, which is a porosity-weighted of the intersecting area between a matrix block and hydraulic fracture (see Eq. (6.37)). Conversely, in the case of the DPDK model, a fine grid is used to represent hydraulic fractures. The intersecting area between a natural fracture and hydraulic fracture is essentially the height multiplied by length of the grid block. In other words, the intersecting area between natural fracture and hydraulic fracture in the TPTK model is only 1% of the intersecting area in the DPDK model. In the case of the TPTK model, flow from matrix to hydraulic fracture is considered in addition to flow between natural fractures and hydraulic fractures. Conversely, in the DPDK model, fluid flows from matrix to natural fracture before it enters the hydraulic fracture blocks. For this reason, the TPTK model should obtain a higher production rate compared to the DPDK model. However, since the transmissibility between natural fracture and hydraulic fracture in the TPTK model is only 1% of that is used in the DPDK model, the additional communication is negligible here.

To confirm that the effective area between natural fracture and hydraulic fracture plays a vital role in the prediction of oil and gas in the TPTK model, another run using the TPTK model is made assuming hydraulic fractures fully intersects natural fractures (i.e., the intersecting coefficient $\alpha_{fF}$ of 1). This gives an effective intersecting area equal to the matrix-hydraulic fracture area of intersection. Physically, this is likely the case that hydraulic fracture generally opens up natural fractures. Figure 8-9 shows the production comparison between the TPTK model with an intersecting coefficient of 1 and the DPDK model. The production rates between the two models are in perfect agreement. Thus, the TPTK model simplifies to the DPDK model when a fine grid is used to model the discrete fracture.
The comparisons seen in this section highlight the importance of correctly identifying the transmissibility between different porosity types. A more study of the natural fracture-hydraulic fracture transmissibility will be demonstrated in the next section.

8.3 Parametric Study of the Triple-porosity Model

In this section, three main components of the developed TPTK model are studied. The first component is multi-mechanistic flow where both diffusive and convective flows are considered in the simulation. Production is compared for different values of diffusion coefficients. The second component is the transmissibility between the natural fracture and hydraulic fracture. Variation of an effective intersecting area ($A_{in}^{RF}$) is compared with the default...
value of effective intersecting area \( A_{MF}^{F} = \phi_f \cdot A_{m}^{MF} \). Finally, simulations of the fully coupled TPTK model are shown to compare with the TPTK model with sequential flow assumption.

### 8.3.1 Multi-mechanistic Flow

In this section, multi-mechanistic flow using the TPTK model is demonstrated. Recall the fluid transport from matrix to hydraulic fracture through NNC (Eq. (6.29)). Only Darcy flow is considered in the formulation. However, in tight formation such as shales, diffusion is the primary mechanism for flow from matrix blocks to fractures. In dual-continuum systems, gas flows from matrix blocks to natural fractures following a multi-mechanistic flow. It is assumed here that diffusion is governed by Fick’s law and occurs only in the gas phase. Only diffusion in gas phase is considered because diffusion coefficient of a compound is typically 10,000 times as great in gas as in liquid (Haynes, 2014). To demonstrate the importance of considering diffusion in tight formations, we focus on changes in cumulative production of oil and gas when diffusion is considered. Figure 8-10 shows the reservoir model considered. The reservoir properties are shown in Table 8-3. The simulation is run for 30 years because of the ultra-tight system (i.e., \( k_m = 100 \, nD \)).
Table 8-3: Input Data for Study of Multi-mechanistic Flow of the TPTK model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>Bakken oil</td>
<td>-</td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
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<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.01</td>
<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>0 – 20</td>
<td>ft/day</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 8-10: Three-stage hydraulically fractured reservoir with fracture network

Table 8-4 shows the impact of diffusion coefficient on cumulative production of oil and gas after 30 years of production. From the table, as diffusion coefficient increases, the oil production decreases while gas production increases. The increase in cumulative gas production is from the diffused gas components from the matrix to natural and hydraulic fractures. The
impact of diffusion on primary recovery is insignificant unless the value of diffusion coefficient is unrealistically high (i.e., effective diffusion coefficient of 20). This may be due to the fact that the reservoir is hydraulically fractured. Therefore, the flow from fractures, which is dominated by Darcy flow, mainly contributes to the overall production rather than diffusion. After 30 years of production, the majority of the reservoir is still above bubble point pressure, and therefore, the effect of diffusion is insignificant. Nevertheless, it should be noted that the effect of diffusion may be more dominant during injection of gas for EOR.

Table 8-4: Oil and gas production comparison showing the effect of diffusion on recovery

<table>
<thead>
<tr>
<th>Effective Diffusion Coefficient</th>
<th>Cumulative Oil Production (STB)</th>
<th>Cumulative Gas Production (Mscf)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1E-6</td>
<td>333,816</td>
<td>403,585</td>
</tr>
<tr>
<td>1E-1</td>
<td>333,744</td>
<td>404,115</td>
</tr>
<tr>
<td>20</td>
<td>320,581</td>
<td>478,540</td>
</tr>
</tbody>
</table>

8.3.2 Natural Fracture-Hydraulic Fracture Intersecting Coefficient

From earlier comparisons with the DPDK model, the importance of the transmissibility between the two porosity types (i.e. natural fracture and hydraulic fracture) was briefly discussed. In this section, the intersecting coefficient ($\alpha_{ff}$) will be explored in more detail. We vary the intersecting coefficient for natural fracture-hydraulic fracture from $\phi_f$ (default value) to 1 to study the production response from the simulation. The reservoir model is shown in Figure 8-1. The reservoir parameters are shown in Table 8-5.
Table 8-5: Input data for study of natural fracture-hydraulic fracture intersecting coefficient of the TPTK model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
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<tbody>
<tr>
<td>Reservoir fluid</td>
<td>Bakken oil</td>
<td>-</td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
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<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.001</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.5</td>
<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 8-11 and Figure 8-12 show oil production rate and cumulative oil production profiles for three different intersecting coefficients. The rate and cumulative production are drastically different when coefficient changes from 0.01 to 0.1. Recall oil production rate comparison between the TPTK model and the DPDK model with fine grid to represent hydraulic fracture (Figure 8-9). For an orthogonal fracture intersecting a grid block, the intersecting area used in the transmissibility calculation is essentially the height multiplied by the width of the grid block. As the coefficient increases to one, the production profiles collapse to that predicted by the DPDK model with grid refinement.
Figure 8-11: Oil production rate profiles for parametric study on the natural fracture-hydraulic fracture communication coefficient of 0.01, 0.1, and 1

Figure 8-12: Cumulative oil production profiles for parametric study on the natural fracture-hydraulic fracture communication coefficient of 0.01, 0.1, and 1
Using the case with a coefficient of 0.01 as a base (default value), the cumulative oil productions from the runs with coefficients of 0.1 and 1 are 20.97% and 29.15% higher, respectively. Cumulative oil production for different values of coefficients is shown in Table 8-6. As the intersecting coefficient increases to 1, the increase due to increasing in intersecting area diminishes.

Table 8-6: Comparison of cumulative oil production from natural fracture-hydraulic fracture communication coefficient ranging from 0.01 to 1

<table>
<thead>
<tr>
<th>Natural fracture-hydraulic fracture communication coefficient</th>
<th>Cumulative Oil Production (STB)</th>
<th>% Increase in Cumulative Oil Production from Base Case</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>505,917</td>
<td>(base case)</td>
</tr>
<tr>
<td>0.1</td>
<td>612,027</td>
<td>20.97</td>
</tr>
<tr>
<td>0.2</td>
<td>631,927</td>
<td>24.91</td>
</tr>
<tr>
<td>0.4</td>
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</tr>
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<td>0.8</td>
<td>651,824</td>
<td>28.84</td>
</tr>
<tr>
<td>1</td>
<td>653,417</td>
<td>29.15</td>
</tr>
</tbody>
</table>

8.3.3 Fully Coupled Triple-porosity Model

Many multi-porosity models assume a sequential flow from matrix to natural fracture and, finally, to hydraulic fracture. In addition, some multi-porosity models decouple flow within certain porosity types (e.g., flow between matrix blocks). In the proposed TPTK model, flows in different porosity types are fully coupled without making the sequential flow assumption and without decoupling flow within a porosity type. The major differences in the fully couple flow model are the transports between matrix and hydraulic fracture and between matrix blocks. The intersecting coefficient for natural and hydraulic fracture communication is kept at the default value (i.e., coefficient is equal to natural fracture porosity). In this section, comparisons between fully coupled and sequential flow models, both using the TPTK, are demonstrated. The same model as in the previous case (Figure 8-1) is used but with different reservoir fluids: simple two-
component fluid, Bakken oil, and Eagle Ford oil. The simulation is run for 10 years for the case of two-component fluid and 1 year for Bakken and Eagle Ford oils.

Table 8-7: Input data for production analysis of the TPTK model using the two-component fluid

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
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<td>Reservoir dimensions</td>
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</tr>
<tr>
<td>Formation thickness</td>
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<td>ft</td>
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<tr>
<td>Initial reservoir pressure</td>
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<td>psia</td>
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<tr>
<td>Initial reservoir temperature</td>
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<td>°F</td>
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<tr>
<td>Initial water saturation</td>
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<td>Matrix porosity</td>
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<td>fraction</td>
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<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
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<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
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<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
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<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
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<td>-</td>
</tr>
</tbody>
</table>

Figure 8-13 and Figure 8-14 show oil production rates and cumulative oil productions between the fully coupled and sequential flow models, respectively. After 1 year of production, the cumulative production from the fully coupled model is approximately 16.32% higher compared to that from the sequential flow model. Rates from both models approach to the same rate toward the end of the simulation. During this period, contact between matrix and hydraulic fractures provides additional transmissibility for oil to flow to the wellbore and increase the production rate. At 10 years, the fully coupled model predicts 7.66% greater cumulative oil production than sequential flow.
Figure 8-13: Oil production rate comparison between fully coupled and sequential flow models for two-component fluid in three-stage hydraulically fractured reservoir

Figure 8-14: Cumulative oil production comparison between fully coupled and sequential flow models for two-component fluid in three-stage hydraulically fractured reservoir
In the second case, Bakken oil and representative reservoir properties are shown in Table 8-8. Similarly, oil production rate and cumulative oil production are compared.

**Table 8-8: Input data for production analysis of the TPTK model using Bakken oil**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>Bakken oil</td>
<td>-</td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.0001</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.01</td>
<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>

Simulation results are shown in Figure 8-15 and Figure 8-16. From the log-log oil production rate in Figure 8-15, the rates from both models are essentially equal until approximately 1 day of production. The high production rate at the beginning of the simulation is due to production from the hydraulic fractures only. The first deflection point at roughly 0.001 days occurs when pressure in the hydraulic fracture segments (that intersect the well) falls below bubble-point pressure. The second deflection point at approximately 0.1 day occurs because the gas saturation in the hydraulic fractures increases above the critical gas saturation of 0.2, the minimum gas saturation at which gas begins to flow. As the reservoir approaches 1 day, we begin to drain from matrix blocks. At the end of 1 year of production, cumulative oil production is 16.41% higher when fully coupled model is used. As the production continues, we can expect the higher production rate from the fully coupled model to decline as can be seen in the case of two-component fluid (Figure 8-13).
Figure 8-15: Oil production rate comparison between fully coupled and sequential flow models for Bakken oil in three-stage hydraulically fractured reservoir.

Figure 8-16: Cumulative oil production comparison between fully coupled and sequential flow models for Bakken oil in three-stage hydraulically fractured reservoir.
In the third case, production from Eagle Ford shale is analyzed where the Eagle Ford representative reservoir properties are used (Table 8-9). The reservoir model remains the same as the previous cases.

**Table 8-9: Input data for production analysis of the TPTK model using Eagle Ford oil**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>Eagle Ford oil</td>
<td>-</td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>237</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.3</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.11</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.0001</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.005</td>
<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>

Simulation results are shown in Figure 8-17 and Figure 8-18. A similar production profile is observed where the rate drops significantly after 1 day of simulation. With the fully coupled model, the cumulative oil production rate is 31.87% higher than the sequential flow model indicating the importance of using a fully coupled flow model.
Figure 8-17: Oil production rate comparison between fully coupled and sequential flow models for Eagle Ford oil in three-stage hydraulically fractured reservoir

Figure 8-18: Cumulative oil production comparison between fully coupled and sequential flow models for Eagle Ford oil in three-stage hydraulically fractured reservoir
In the last case, we increase contact area between matrix and hydraulic fractures by introducing branch fractures as shown in Figure 8-10. The main branch of the fracture has a permeability of 8,000 $mD$ while the fracture network, assumed opened by hydraulic fracturing, has a permeability of 5,000 $mD$. Only Bakken oil is considered in this case. Figure 8-19 and Figure 8-20 show the oil production rate and cumulative oil production comparison between fully coupled model and sequential flow model, respectively. The fully coupled model gives 33.22% cumulative oil production higher compared to the model with sequential flow assumption.

Figure 8-19: Oil production rates of fully coupled and sequential flow models for Bakken oil in three-stage hydraulically fractured reservoir with fracture network
In summary, ignoring the fluid transport between or within certain porosity types and assuming sequential flow in hydraulically fractured shale reservoir may lead to an underestimation of the production from shale oil reservoirs. In the fully coupled model, the transport between matrix and hydraulic fracture contributes primarily to the increase in oil production. In contrast, the contribution of the flow between matrix blocks to the increase in oil production is relatively small because production mainly comes from the hydraulically fractured zone.

8.4 Rate Transient Analysis of the Triple-porosity Model

The TPTK model is simplified by using a two-component fluid: NC$_{16}$ 90% and C$_1$ 10%. The reservoir model is the same as previous case where three hydraulic fractures are evenly...
spaced along the horizontal well (Figure 8-1). Ranges of reservoir parameters are shown in Table 8-10. In this study, both matrix and natural fracture domains share the same rock-fluid properties. However, rock-fluid properties for hydraulic fracture assume straight-line relative permeability curves.

Table 8-10: Input data for rate transient analysis of the TPTK model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>90% NC_{16} – 10% C_{1}</td>
<td>-</td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.001</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.5</td>
<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 8-21 shows rate transient response from the production at various values of natural fracture permeability. When the natural fracture permeability is high (1 mD), production rate is maintained above 1,000 STB/day for up to 100 days. This is because the natural fractures provide a channel for hydrocarbon to flow to the wellbore. It also helps draining fluid from the matrix. The production rate then falls rapidly by the end of the simulation at 1,000 days. However, we see a clear deflection when the natural fracture permeability is low (0.001 mD). This indicates that the production at the beginning came mainly from the hydraulically fractured zone. With the tight matrix permeability and low natural fracture permeability, the relatively low production rate is maintained for a longer period of time.
Figure 8-21: Log-log plot of oil production rate for natural fracture permeability ranging from $0.001 \text{ mD}$ to $1 \text{ mD}$ and a fixed matrix permeability of $100 \text{ nD}$

A similar analysis is performed to study the effect of matrix permeability. The log-log plot analysis of the oil production rate is shown in Figure 8-22. As the matrix permeability becomes extremely low ($10 \text{ nD}$), the production rates reach a low value after the hydrocarbons stored in the hydraulically fractured area are depleted.
In this section, the transient production rate behaviors from the fully coupled triple-porosity model were shown and discussed. The recovery from these tight formations depends strongly on the natural fracture permeability. Based on the comparison of the fully coupled TPTK model, the contacting area between hydraulic fractures and the formation is essential to successfully produce hydrocarbons from tight formations.

8.5 Highlights of the Chapter

In this chapter, simulations of the multi-mechanistic, triple-porosity, triple-permeability model are demonstrated. The TPTK model allows us to assign reservoir properties corresponding to the porosity type. The fully coupled flow between all porosity types captures better the physics of flow in hydraulically fractured unconventional reservoirs. For these reasons, the model can
potentially give more accurate results compared to existing models. The following is the summary of the simulation results:

- The TPTK model is compared with the single-porosity model coupled with EDFM and dual-porosity, dual-permeability model with grid refinement to represent fractures.
  - Productions from three different values of permeability in the EDFM are compared with that from the TPTK. The TPTK gives cumulative production 21.68% higher than the EDFM with porosity-weighted average value of permeability indicating that the single-porosity model may not be sufficient to capture heterogeneity of matrix and natural fractures.
  - The behavior of the TPTK is similar to that of the DPDK when the intersecting coefficient is equal to one, which is equal to the intersecting area between the fine grid blocks representing the discrete fractures and the adjacent grid blocks in the DPDK. The productions from the two models are in perfect agreement.

- The effect of diffusion in the hydraulically fractured shale oil reservoir is insignificant. This is because the formation is hydraulically fractured and filled with oil. Diffusion doesn’t come into the picture until a large amount of gas forms in the reservoir. In addition, Darcy flow is the dominating mechanism in high-permeability hydraulic fractures and transport between matrix blocks and hydraulic fractures.

- The importance of accurate estimation of effective area for natural and hydraulic fractures transmissibility is highlighted. Cumulative oil productions from the runs with intersecting coefficients of 0.1 and 1 are 20.97% and 29.15% higher than the run with default coefficient of 0.01, respectively.

- Productions from the fully coupled and sequential flow TPTK models are demonstrated. The additional transmissibility between matrix and hydraulic fractures in the fully coupled model results in a higher cumulative oil production up to 31.87%.
Chapter 9

Effect of Capillary Pressure on Phase Behavior

In this chapter, the effect of capillary on phase behavior is investigated. First, the effect on original oil- and gas-in-place is demonstrated. Simulation for a single-porosity reservoir incorporating the effect of capillary pressure on phase behavior is shown. The cumulative oil production at various initial reservoir pressures is compared. Simulations of hydraulically fractured shale reservoirs incorporating the effect of capillary pressure on phase behavior are shown using the EDFM and the TPTK models. Capillary pressure on flow is considered in all simulation runs. Thus, the term “with/without capillary pressure” refers to the capillary pressure on phase behavior. Two main fluids are used: Bakken and Eagle Ford oils, and the compositional data are shown in Table 9-1 to Table 9-4. Water is assumed to be the wetting phase.

Table 9-1: Compositional data for Bakken oil (Nojabaei et al., 2013)

<table>
<thead>
<tr>
<th>Component</th>
<th>Mole Fraction</th>
<th>Critical Pressure (psia)</th>
<th>Critical Temperature (°R)</th>
<th>Acentric Factor</th>
<th>Molecular Weight (lb/lbmol)</th>
<th>Critical Volume (ft³/lbmol)</th>
<th>Parachor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>0.36736</td>
<td>655.02</td>
<td>355.336</td>
<td>0.0102</td>
<td>16.5350</td>
<td>1.58</td>
<td>74.8</td>
</tr>
<tr>
<td>C₂</td>
<td>0.14885</td>
<td>721.99</td>
<td>549.969</td>
<td>0.1028</td>
<td>30.4330</td>
<td>2.34</td>
<td>107.7</td>
</tr>
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<td>C₃</td>
<td>0.09334</td>
<td>615.76</td>
<td>665.970</td>
<td>0.1520</td>
<td>44.0970</td>
<td>3.25</td>
<td>151.9</td>
</tr>
<tr>
<td>C₄</td>
<td>0.05751</td>
<td>546.46</td>
<td>759.208</td>
<td>0.1894</td>
<td>58.1240</td>
<td>4.11</td>
<td>189.6</td>
</tr>
<tr>
<td>C₅-C₆</td>
<td>0.06406</td>
<td>461.29</td>
<td>875.479</td>
<td>0.2684</td>
<td>78.2950</td>
<td>5.39</td>
<td>250.2</td>
</tr>
<tr>
<td>C₇-C₁₂</td>
<td>0.15854</td>
<td>363.34</td>
<td>1,053.250</td>
<td>0.4291</td>
<td>120.5620</td>
<td>8.81</td>
<td>350.2</td>
</tr>
<tr>
<td>C₁₃-C₂₁</td>
<td>0.07330</td>
<td>249.61</td>
<td>1,332.095</td>
<td>0.7203</td>
<td>220.7160</td>
<td>15.19</td>
<td>590.0</td>
</tr>
<tr>
<td>C₂₂-C₈₀</td>
<td>0.03704</td>
<td>190.12</td>
<td>1,844.491</td>
<td>1.0159</td>
<td>443.5180</td>
<td>36.00</td>
<td>1,216.8</td>
</tr>
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</table>
Table 9-2: Binary interaction parameters for Bakken oil (Nojabaei et al., 2013)

<table>
<thead>
<tr>
<th></th>
<th>C_1</th>
<th>C_2</th>
<th>C_3</th>
<th>C_4</th>
<th>C_5-C_6</th>
<th>C_7-C_12</th>
<th>C_13-C_21</th>
<th>C_22-C_80</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_1</td>
<td>0.00050</td>
<td>0.0035</td>
<td>0.0035</td>
<td>0.0037</td>
<td>0.0033</td>
<td>0.0033</td>
<td>0.0033</td>
<td>0.0033</td>
</tr>
<tr>
<td>C_2</td>
<td>0.00050</td>
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<td>0.0031</td>
<td>0.0031</td>
<td>0.0031</td>
<td>0.0026</td>
<td>0.0026</td>
<td>0.0026</td>
</tr>
<tr>
<td>C_3</td>
<td>0.0035</td>
<td>0.0031</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>C_4</td>
<td>0.0035</td>
<td>0.0031</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>C_5-C_6</td>
<td>0.0037</td>
<td>0.0031</td>
<td>0</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>C_7-C_12</td>
<td>0.0033</td>
<td>0.0026</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>C_13-C_21</td>
<td>0.0033</td>
<td>0.0026</td>
<td>0</td>
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<td>0</td>
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</tr>
<tr>
<td>C_22-C_80</td>
<td>0.0033</td>
<td>0.0026</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

Parachor for Eagle Ford oil is computed from Fanchi (1990) correlation.

Table 9-3: Compositional data for Eagle Ford oil (Orangi et al., 2011)

<table>
<thead>
<tr>
<th>Component</th>
<th>Mole Fraction</th>
<th>Critical Pressure (psia)</th>
<th>Critical Temperature (°R)</th>
<th>Acentric Factor</th>
<th>Molecular Weight (lb/lbmol)</th>
<th>Critical Volume (ft^3/lbmol)</th>
<th>Parachor^1</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_1</td>
<td>0.31231</td>
<td>673.1</td>
<td>343.3</td>
<td>0.0130</td>
<td>16.04</td>
<td>1.5658</td>
<td>71.50</td>
</tr>
<tr>
<td>N_2</td>
<td>0.00073</td>
<td>492.3</td>
<td>227.2</td>
<td>0.0400</td>
<td>28.01</td>
<td>1.4256</td>
<td>43.55</td>
</tr>
<tr>
<td>C_2</td>
<td>0.04314</td>
<td>708.4</td>
<td>549.8</td>
<td>0.0986</td>
<td>30.07</td>
<td>2.3556</td>
<td>113.93</td>
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<td>C_3</td>
<td>0.04148</td>
<td>617.4</td>
<td>665.8</td>
<td>0.1524</td>
<td>44.10</td>
<td>3.2294</td>
<td>151.28</td>
</tr>
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<td>547.6</td>
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<td>1.5126</td>
<td>78.92</td>
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<tr>
<td>IC_4</td>
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<td>529.1</td>
<td>734.6</td>
<td>0.1848</td>
<td>58.12</td>
<td>4.2127</td>
<td>183.14</td>
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<td>NC_4</td>
<td>0.03382</td>
<td>550.7</td>
<td>765.4</td>
<td>0.2010</td>
<td>58.12</td>
<td>4.1072</td>
<td>191.38</td>
</tr>
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<td>IC_5</td>
<td>0.01805</td>
<td>483.5</td>
<td>828.7</td>
<td>0.2223</td>
<td>72.15</td>
<td>4.9015</td>
<td>224.09</td>
</tr>
<tr>
<td>NC_5</td>
<td>0.02141</td>
<td>489.5</td>
<td>845.6</td>
<td>0.2539</td>
<td>72.15</td>
<td>5.0232</td>
<td>232.06</td>
</tr>
<tr>
<td>NC_6</td>
<td>0.04623</td>
<td>439.7</td>
<td>914.2</td>
<td>0.3007</td>
<td>86.18</td>
<td>5.9782</td>
<td>273.53</td>
</tr>
<tr>
<td>C_7+</td>
<td>0.16297</td>
<td>402.8</td>
<td>1,060.5</td>
<td>0.3739</td>
<td>114.40</td>
<td>7.4093</td>
<td>368.51</td>
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<td>C_11+</td>
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<td>0.5260</td>
<td>166.60</td>
<td>10.682</td>
<td>534.48</td>
</tr>
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<td>C_15+</td>
<td>0.10044</td>
<td>241.4</td>
<td>1,368.4</td>
<td>0.6979</td>
<td>230.10</td>
<td>14.739</td>
<td>743.97</td>
</tr>
<tr>
<td>C_20+</td>
<td>0.07306</td>
<td>151.1</td>
<td>1,614.2</td>
<td>1.0456</td>
<td>409.20</td>
<td>26.745</td>
<td>1,390.13</td>
</tr>
</tbody>
</table>

^1 Parachor for Eagle Ford oil is computed from Fanchi (1990) correlation.
Table 9-4: Binary interaction parameters for Eagle Ford oil (Orangi et al., 2011)

<table>
<thead>
<tr>
<th></th>
<th>C_1</th>
<th>N_2</th>
<th>C_2</th>
<th>C_3</th>
<th>CO_2</th>
<th>IC_4</th>
<th>NC_4</th>
<th>IC_5</th>
<th>NC_5</th>
<th>NC_6</th>
<th>C_7+</th>
<th>C_11+</th>
<th>C_15+</th>
<th>C_20+</th>
</tr>
</thead>
<tbody>
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<td>0.036</td>
<td>0</td>
<td>0</td>
<td>0.1</td>
<td>0</td>
<td>0</td>
<td>0</td>
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9.1 Effect of Capillary Pressure on Original Oil and Gas in Place and Cumulative Production

In this section, we study the importance of incorporating capillary pressure in the estimations of OOIP using Bakken and Eagle Ford crude.

9.1.1 Bakken Oil

Reservoir parameters for the simulations with Bakken oil are shown in Table 9-5. The Bakken fluid properties and binary interaction parameters are reproduced and shown in Table 9-1 and Table 9-2, respectively (Nojabaei et al., 2013). Relative permeability data is in Figure 9-1.

Table 9-5: Parameters for study of importance of capillary pressure on original oil-in-place (Bakken)

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<tr>
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Figure 9-1: Relative permeability for Bakken formation

Figure 9-2: Capillary pressure for Bakken formation

Figure 9-3 shows the phase envelope for Bakken oil, where the red and blue curves are the bubble-point curves with and without considering the effect of capillary pressure on phase behavior, respectively. The full phase envelope is also shown in Figure 9-3 with the red circle indicating the enlarged region. Three points of interest are marked by A, B, and C at the Bakken reservoir temperature. Point A is a pressure where both cases with and without capillary pressure are above bubble-point pressure, while Point B is above the bubble point with capillary pressure included, but not without. Point C coincides to a pressure below bubble point independent of the inclusion of capillary pressure.
Figure 9-4 shows the OOIP corresponding to various initial reservoir pressures ranging from 2,000 to 3,500 psia, which are above and below the various bubble points. From initial reservoir pressure of 3,500 psia to approximately 2,850 psia, the reservoir is a single-phase oil with and without capillary pressure. Therefore, incremental OOIP due to capillary pressure in this pressure range is zero as shown by the green curve in Figure 9-4. As the pressure approaches the bubble point for no capillary pressure as shown by the yellow-highlighted section (initial reservoir pressure between 2,750 - 2,870 psia), the initial reservoir fluid remains single-phase oil for the case with capillary pressure, but two phases for the case without the effect of capillary pressure on phase behavior (see point B in Figure 9-3 for example). When capillary pressure is not considered, gas forms at B and the oil phase that forms has a different composition and density than when capillary pressure is included. The OOIP increases by approximately 1.2% in this window when capillary pressure is included since the fluid remains single phase there. At pressures below 2,750 psia, both cases with and without capillary pressure are in the two-phase
region (see point C in Figure 9-3 for example). The increase in OOIP is up to 4.1% as initial reservoir pressure decreases to 2,000 psia. The increase in OOIP is due to the suppression of bubble-point pressure, which consequently alters the fluid properties inside the phase envelope. The increase in OOIP is obtained because the oil saturation is larger when capillary pressure is included in flash calculations.

Simulations are made for various initial reservoir pressures at the constant reservoir temperature of 240 °F (see Table 9-5). These simulations are for a closed square reservoir with a production well at the center. No discrete fractures exist in the simulations, but permeability enhancement of 1 mD is used. The grid for the model is 35×35×1. Figure 9-5 shows the cumulative oil production after 1.0 year of simulation. Cumulative oil production increases approximately 11-13% until the initial reservoir pressure approaches the bubble-point pressure. The lower the initial pressure in the two-phase region, the greater the % increase in cumulative oil production with capillary pressure compared to without. The percentage increases because a larger region of the reservoir becomes two-phase with gas and stays there longer compared to the case with larger initial reservoir pressure. This results in greater impact of capillary pressure inside the two-phase region. At a smaller initial reservoir pressure of 2,000 psia, the increase in recovery with capillary pressure taken into account in the flash calculation is up to 38.2%. Thus, reservoirs with an initial pressure close to the bubble-point pressure observed in standard PVT reports (no confined effect) will likely show significantly greater impact of capillary pressure on recovery than those that are at initial pressures substantially greater than bubble point.
Figure 9-4: Effect of capillary pressure on OOIP estimation for Bakken oil at reservoir temperature of 240 °F

Figure 9-5: Effect of capillary pressure on cumulative oil production after 1 year for Bakken oil at reservoir temperature of 240 °F
The case with initial reservoir pressure of 3,500 \( psia \) is selected to simulate for 10 years of production. Oil production rates and cumulative oil production are shown in Figure 9-6. Oil production rates stabilize after approximately 3 years. The incremental recovery due to the effect of capillary pressure on phase behavior is approximately 9.6%. The average reservoir pressures at the end of the simulation for the case with and without capillary pressure effects on phase behavior are 2,618 and 2,731 \( psia \), respectively.

![Figure 9-6: Cumulative oil production after 10 years of production for initial reservoir pressure of 3,500 \( psia \) for Bakken oil](image)

9.1.2 Eagle Ford Oil

A similar study is done for Eagle Ford oil. We compare the original oil-in-place as a function of initial reservoir pressure with the effect of capillary pressure on phase behavior included. Simulations are run for 1 year, and cumulative production is compared. The reservoir parameters for the simulation with Eagle Ford oil are shown in Table 9-6. The Eagle Ford fluid
properties and binary interaction parameters are shown in Table 9-3 and Table 9-4, respectively (Orangi et al., 2011). Relative permeability data is in Figure 9-7.

Table 9-6: Parameters for study of importance of capillary pressure on original oil-in-place (Eagle Ford)

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<th>Unit</th>
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<td>psia</td>
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<td>Constant bottom-hole pressure</td>
<td>500</td>
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Figure 9-7: Relative permeability for Eagle Ford formation (Agboada and Ahamadi, 2013)

Figure 9-8: Capillary pressure for Eagle Ford formation
The phase behavior for the Eagle Ford oil is examined similarly to Bakken, where the key reservoir parameters are shown in Table 9-6. Fluid properties and binary interaction parameters of the Eagle Ford crude are given in Table 9-3 and Table 9-4, respectively (Orangi et al., 2011), where the parachors are calculated from the Fanchi (1990) correlation. The relative permeability data used are shown in Table 9-7 (Agboada and Ahmadi, 2013). The capillary pressure data is obtained by normalizing and scaling capillary pressure data from the Bakken formation (Figure 9-8).

Figure 9-9 shows the phase diagram with the effect of capillary pressure on phase behavior included and where there was no modification of the IFT (green curve). The figure also show the case with capillary pressure, but with IFT multiplied by three (red curve). The blue curve shows the phase envelope without capillary pressure. The different multipliers of IFT shown in the phase envelope highlight the uncertainty of IFT on the effect of capillary pressure and the importance of an accurate estimation of IFT from the laboratory. From this fluid description, the effect of capillary pressure on bubble-point suppression is substantial for the Eagle Ford. At an initial reservoir temperature of 237 °F, points A, B, and C mark the pressure regions similar to those identified for the Bakken. That is, B lies below the bubble-point pressure with no confinement, but above the bubble-point pressure with capillary pressure included. Point C lies below all calculated bubble points.
The original oil-in-place corresponding to various initial reservoir pressures and reservoir temperature of 237 °F are shown in Figure 9-10. For initial reservoir pressures above 2,050 psia (region corresponding to point A in Figure 9-9), the reservoir is single-phase liquid with and without capillary pressure effect on phase behavior. Therefore, the increase in OOIP due to capillary pressure is zero. For reservoir pressures between 1,180 and 2,050 psia (yellow highlighted region), the reservoir is single-phase oil when capillary pressure is included, while two-phase when it is not. The increase in OOIP due to capillary pressure is up to 29% in this region. As initial reservoir pressure decreases below 1,180 psia, both cases are in the two-phase region, but the OOIP increases by nearly 46.3% at an initial reservoir pressure of 900 psia. The impact on OOIP is substantially greater than in the Bakken for this fluid characterization.
Figure 9-10: Effect of capillary pressure on OOIP estimation for Eagle Ford oil at reservoir temperature of 237 °F

Figure 9-11 shows the cumulative oil production corresponding to various initial reservoir pressures after 1.0 year of production. For an initial reservoir pressure of 3,000 psia, the increase in cumulative oil production is approximately 7.2-12.4% when capillary pressure is considered. As initial reservoir pressure decreases, however, the importance of capillary pressure becomes more significant. Increases in cumulative oil production of 23.4% to 154% are found at initial reservoir pressures of 1,900 and 1,500 psia, respectively. This large increase in cumulative oil production in the Eagle Ford is mainly the result of bubble-point suppression and the greater OOIP (oil saturations) at lower pressures. Larger oil saturations increase oil relative permeability as well.
Figure 9-11: Effect of capillary pressure on cumulative oil production after 1 year for Eagle Ford oil at reservoir temperature of 237 °F

Figure 9-12 shows the oil production rate and cumulative oil production comparisons with and without the effect of capillary pressure on phase behavior. The cases where original IFT from the Macleod and Sugden correlation and IFT multiplied by three are also shown for comparison. When capillary pressure on phase behavior is not considered, IFT only impacts the flow of gas and oil through the capillary pressure curves, and the impact on production is insignificant. Each observable drop in oil production rate in Figure 9-12 is caused by gas appearance and gas saturation increases above the critical gas saturation of 0.05 (assumed here). After 10 years of production, the case with 3×IFT (capillary pressure on phase behavior included) remains single-phase oil as shown in the purple curve. The increases in cumulative oil production due to capillary pressure are approximately 5.6% and 13.2% for the case of 1×IFT and 3×IFT, respectively. When the IFT multiplier is increased from one to three, the cumulative oil production for the case of 3×IFT is found to be 7.1% higher compared to that of 1×IFT. This highlights the importance of obtaining an accurate IFT.
Figure 9-12: Cumulative oil production after 10 years of production for initial reservoir pressure of 3,000 psia for Eagle Ford oil

9.2 Handling of Large Capillary Pressure in the Well Model

In most reservoir simulators, oil phase pressure \( (P_o) \) is used as the principal unknown and reference phase pressure. Gas phase pressure \( (P_g) \) and water phase pressure \( (P_w) \) are updated at the end of the iteration using capillary pressure relationships. For a water-wet system, water is the wetting phase, and oil phase is the intermediate phase. In such a system, large capillary pressure may cause unphysical production behavior (i.e., for a well with bottom-hole pressure specification, \( P_o \) and \( P_g \) may remain above bottom-hole pressure, but \( P_w \) can decrease below bottom-hole pressure due to capillary pressure). If time-step sizes and grid block sizes are too large, the effect becomes more severe. The computer model will assume counter-current flow for the water phase. The counter-current flow means flows of phases do not go in the same direction.
due to capillary pressure. In the well, capillary pressure leads to an unphysical injection of water into the reservoir while producing oil and gas from the same perforation. This is inconsistent as oil, gas, and water must flow co-currently from the well block to the well for a producer and vice versa for an injector. This effect is insignificant in conventional reservoirs with low capillary pressure, but it can be significant in tight systems with large pressure gradients.

In this section, discussion of common methods to alleviate this challenge with large capillary pressure in tight rocks and shales is presented. We simulate production from a 1,005-foot long 1-D reservoir with a producer located at the middle of the reservoir using various grid block sizes. The thickness and width of the reservoir are 5 feet. Half of the reservoir model is shown in Figure 9-13. The production well produces under constant bottom-hole pressure of 500 psia. The initial reservoir water saturation is 30% to allow for a small flow of water since $S_{\text{water}} = 0.1$. Bakken oil is used. Relative permeability and capillary pressure data are shown in Figure 9-1 and Figure 9-2. Production is simulated for 1 year using a fixed time-step size of 1 day.

![Figure 9-13: Half of the reservoir model for study of impact of large capillary pressure near the wellbore](image)

9.2.1 Use of Small Grid Block Size

The use of smaller grid block size to better capture capillary pressure near the wellbore can alleviate the challenge with counter-current flow. To study the large capillary pressure near the wellbore, we simulate production from the reservoir model shown in Figure 9-13 using four different grid block sizes, 5, 10, 15, 25 and 50 ft. The height and width of the reservoir are kept at 5 ft.
Figure 9-14 shows the water phase pressure with time in the well block for five different grid resolutions. The impact of large oil-water capillary pressure is less significant for smaller grid blocks as smaller grid blocks capture better the high pressure gradients near the well. The water phase pressure approaches the well bottom-hole pressure after approximately 30 days for all grid block sizes. The counter-current flow caused by large capillary pressure diminishes very quickly (i.e., roughly after 2 days) with small grid block size of 5 ft but takes a longer period of time (i.e., approximately 30 days) for larger grid block size of 50 ft.

![Graph showing water phase pressure over time for different grid block sizes](image)

**Figure 9-14: Water phase pressure in the well grid block for 5-ft, 10-ft, 15-ft, 25-ft, and 5-ft grid block sizes as a function of time**

Figure 9-15 shows the water phase pressure over the distance of 500 ft from the well at the end of the simulation (i.e., after 365 days of production). Using a finer grid resolution and smaller time steps could remediate this numerical problem but requires more computational time. When a smaller grid block size is used, water phase pressure is captured better, and the area impacted by water phase pressure falling below bottom-hole pressure is smaller. The counter-
current flow occurs up to 120-foot distance from the well when small grid block size is used but up to 150-ft distance from the well when large grid block size is used.

![Graph showing water phase pressure in the well grid block for different grid block sizes after 365 days of production.](image)

**Figure 9-15:** Water phase pressure in the well grid block for 5-ft, 10-ft, 15-ft, 25-ft, and 50-ft grid block sizes after 365 days of production

Figure 9-16 shows phase pressure over 500-ft length from the well at the end of the simulation for the model with grid block size of 5 ft. Again, oil and gas phase pressures are still above the well bottom-hole pressure while water phase pressure falls below bottom-hole pressure and causes counter-current flow. The unintentional injection of wetting phase becomes less significant when small grid block size and small time-step sizes are used. However, the injected wetting phase maintains the reservoir pressure and may impact the solutions. One numerical technique to handle the challenge is to shut-in the production of the phase that the phase pressure falls below the specified bottom-hole pressure.
Figure 9-16: Different phase pressures in the well grid block for 5-ft grid block sizes at the end of the simulation

9.2.2 Ignoring Capillary Pressure in the Well Model

Relative permeability and capillary pressure are usually introduced to the well model originally developed by Peaceman (1982). In the previous section, we discuss the issue of large capillary pressure in the well model (i.e., counter-current flow and injection of water phase in the producing well). Assuming that pressure gradients for each phase are equal in the well model (i.e., capillary pressure in the well model is zero) can avoid the problem with large capillary pressure altogether. Therefore, all phase pressures converge to one value and is equal to the reference phase pressure. Even though capillary pressure is essentially zero at the sandface, this assumption is not accurate in reservoir simulation because the reservoir is discretized into grid blocks, which have certain grid block size, and capillary pressures between phases in the grid block are not zero. For this reason, the method ignores the physics of the flow by ignoring the
capillary pressure in the well model. However, zero capillary pressure in the well model is commonly assumed in commercial reservoir simulator (CMG 2012). In this approach, regardless of phase, only oil phase pressure (or reference phase pressure) is used in the computation of production/injection source term regardless of phase as shown in Eqs. (8.2) and (8.3).

\[ q_{ij} = -\omega_{ij} \rho_j \frac{2\pi k_{ave} h}{\ln \left( \frac{r_e}{r_w + S} \right) \mu_j} \left( P_o - P_{wf} \right) \quad \text{where } j = o, g \] 

Alternatively, instead of assuming zero capillary pressure in all phases in the well model, one can assume zero oil-water capillary pressure in a water-wet system. If water is at irreducible water saturation, this is an acceptance assumption. With this assumption, \( P_o \) and \( P_w \) are equal everywhere because zero oil-water capillary pressure is assumed. The gas-oil capillary pressure is considered in the well model, but the water-oil capillary pressure is ignored. This approach is similar to assuming zero capillary pressure in the well model as previously discussed. This approach may be more accurate as compared to the earlier approach in the case of immobile water because the assumption of zero capillary pressure in the well model is neglected only for the water phase.

We simulate production from a tight reservoir shown in Figure 9-13 to demonstrate the three different assumptions on phase pressures in the well model:

1. well model that considers capillary pressure for all phases,
2. well model that considers capillary pressure for all phases, but oil-water capillary pressure is assumed to be zero everywhere,
3. well model that assumes zero capillary pressure in all phases.
Figure 9-17 to Figure 9-19 show phase pressures over half of the reservoir. The well is located at a distance of zero feet. Oil and gas phase pressures remain above bottom-hole pressure for all three assumptions. In Figure 9-19, when capillary pressure is considered in the well model (blue curve), the water phase pressure drops below well bottom-hole pressure due to capillary pressure. This creates the aforementioned counter-current flow and injection of water into the well block. On the other hand, when oil-water capillary pressure is ignored for the entire reservoir (red curve), water phase pressure remains above the well bottom-hole pressure. The most noticeable effect of capillary pressure in the well model is seen when capillary pressure is completely ignored in the well model (green curve). When water phase pressure is calculated, it falls below atmospheric pressure and becomes negative.

![Graph showing oil phase pressure in the well grid block for different well models after 365 days of production](image)

**Figure 9-17:** Oil phase pressure in the well grid block for different well models after 365 days of production
Figure 9-18: Gas phase pressure in the well grid block for different well models after 365 days of production

Figure 9-19: Water phase pressure in the well grid block for different well models after 365 days of production
Figure 9-20 to Figure 9-22 show the oil, gas, and water productions for the 1-D reservoir using the three assumptions. When capillary pressure is considered in the well model, production from the reservoir is lower resulting in a higher reservoir pressure at the end of the simulation compared to the runs using the other two assumptions. Capillary pressure creates counter-current flow in the water phase, and water is numerically injected into the production well. When capillary pressure is ignored, the production of water phase continues because oil phase pressure is used in the water phase production calculation. There’s no counter-current flow with this well model (i.e., oil, gas, and water pressures are above bottom-hole pressure). We can observe similar production profile when zero oil-water capillary pressure is assumed.

Figure 9-20: Oil production comparison with and without consideration of capillary pressure in the wellbore model
Figure 9-21: Gas production comparison with and without consideration of capillary pressure in the wellbore model

Figure 9-22: Water production comparison with and without consideration of capillary pressure in the wellbore model
9.2.3 Use Wetting Phase Pressure as Reference Phase

In most reservoir simulators, an intermediate phase pressure or oil phase pressure is used as reference phase. In the case of a water wet system, water phase pressure is smaller than oil phase pressure because the water phase occupies the largest pores. This can lead to a counter-current flow as was discussed in the previous subsections. In such a case, using water phase pressure as a reference phase and assigning water phase pressure to it (instead of oil phase pressure) during the reservoir initialization could avoid this issue because water phase pressure will always be the smallest value. Care should be taken because phase pressure is also used in phase behavior calculation. The problem becomes more complicated when the capillary pressure on phase behavior is considered in phase behavior calculation. This will change the solutions entirely.

9.3 Simulation of EDFM Incorporating the Effect of Capillary Pressure

In the study of EDFM incorporating the effect of capillary pressure on phase behavior in the fractured reservoir modeled by EDFM, it is assumed that there’s no capillary pressure in the hydraulic fracture (EDFM) and therefore, no effect of capillary pressure on phase behavior in hydraulic fractures. The relative permeability in the hydraulic fractures assumes straight-line curves. Three simulation cases are demonstrated:

Case 1: Three-stage hydraulically fractured reservoir

Case 2: Three-stage hydraulically fractured reservoir with branch fractures

Case 3: Fractured well with fracture network

The reservoir parameters are shown in Table 9-7.
Table 9-7: Parameters for simulation studies of EDFM incorporating the effect of capillary pressure using Bakken oil

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<tr>
<th>Parameters</th>
<th>Value</th>
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</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Fracture porosity</td>
<td>1</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.05</td>
<td>mD</td>
</tr>
<tr>
<td>Fracture permeability:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Case 1: Three main fractures</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Case 2: Main fractures</td>
<td>8,000</td>
<td>mD</td>
</tr>
<tr>
<td>Branch fractures</td>
<td>5,000</td>
<td>mD</td>
</tr>
<tr>
<td>Case 3: All fractures</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Fracture width</td>
<td>0.05</td>
<td>ft</td>
</tr>
</tbody>
</table>

The reservoir to be studied for the remaining of this chapter is initially at irreducible water saturation. From the previous study, at irreducible water saturation, water phase flow is negligible, and oil-water capillary pressure is ignored in our subsequent simulations. However, gas-oil capillary pressure in flow is still considered the simulation studies. The impact of oil-water capillary pressure is likely very important, however, for identifying the impact of fracking fluid on subsequent hydrocarbon production.

9.3.1 Grid Convergence

First, we demonstrate grid convergence of the solutions for the reservoir model shown in Figure 9-23. The figure shows the base grid of the two-dimensional reservoir modeled with a 25×25×1 grid. The base model is coarsened and refined, and the results are compared to the base case. The coarsened model has 7×9×1 grid. In the refined model, each grid block that hosts a well and/or fracture segment is refined by a factor of three in both $x$- and $y$-direction. The refined model has 51×51×1 grid. Figure 9-24 and Figure 9-25 show the oil production rate and cumulative oil production for three different refinements (coarse, base, and 3× refine). The oil
production rates and cumulative oil productions from the base and 3x refine are in good agreement. The simulation studies that follow use the base case grid shown in Figure 9-23.

![Reservoir model for simulation study of fractured reservoir](image1)

**Figure 9-23:** Reservoir model for simulation study of fractured reservoir

![Grid convergence – oil production rate for coarse, base, and 3x refinement](image2)

**Figure 9-24:** Grid convergence – oil production rate for coarse, base, and 3x refinement
9.3.2 Three-stage Hydraulically Fractured Reservoir

The first case is production from a multi-stage hydraulically fractured horizontal well (see Figure 9-23). The horizontal well is 1,300-feet long, where the well grid blocks are in yellow. Three stages of hydraulic fracturing are evenly spaced as shown by the red lines. The total contact area between discrete fracture and grid blocks is 870,828 ft$^2$. The open-hole horizontal well is at a constant bottom-hole pressure of 500 psia. It is assumed that pressure drops along the horizontal well are small.

Figure 9-26 shows the pressure distribution after 30, 90, 180, and 365 days of production. After 30 days, the area between hydraulic fractures remains at higher pressure. The pressure of the grid blocks that host a discrete fracture decreases quickly and propagates away from the
fracture. Figure 9-27 and Figure 9-28 show oil and gas production rates and cumulative oil and
gas production for the cases with and without capillary pressure effect on phase behavior at one
year. Hydrocarbons are produced quickly at the beginning of the simulation and decline rapidly to
reach a stabilized rate. At the end of the simulation, the cumulative oil production when capillary
pressure is considered is 5.2% higher compared the case when capillary pressure is not
considered. That is, the effect of capillary pressure is to give a somewhat higher stabilized rate.

Figure 9-26: Case 1 – Pressure distribution after 30, 90, 180, and 365 days
Figure 9-27: Case 1 – oil production rate and cumulative oil production

Figure 9-28: Case 1 – gas production rate and cumulative gas production
Table 9-8 shows cumulative oil production comparison for the model with Bakken oil and Eagle Ford oil for different initial reservoir pressure. The effect of capillary pressure on phase behavior is more dominant as initial reservoir pressure decreases. The cumulative oil production increases due to capillary pressure on Bakken oil is up to 28.1% as initial reservoir pressure decreases to 2,500 $psia$. Similarly, as initial reservoir pressure on Eagle Ford formation decreases to 2,000 $psia$, the increase due to capillary pressure on phase behavior is up to 21.8%.

**Table 9-8: Comparison of cumulative oil production at various initial reservoir pressures for Bakken oil and Eagle Ford oil**

<table>
<thead>
<tr>
<th>Bakken</th>
<th>Cumulative Oil Production (STB)</th>
<th>Initial Reservoir Pressure</th>
<th>Without Pc</th>
<th>Pc</th>
<th>% Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>5,500</td>
<td>195,605</td>
<td>205,841</td>
<td>5.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2,800</td>
<td>111,857</td>
<td>128,130</td>
<td>14.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2,500</td>
<td>74,918</td>
<td>96,001</td>
<td>28.1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Eagle Ford</th>
<th>Cumulative Oil Production (STB)</th>
<th>Initial Reservoir Pressure</th>
<th>Without Pc</th>
<th>Pc</th>
<th>% Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>3,000</td>
<td>315,149</td>
<td>344,055</td>
<td>9.2%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2,500</td>
<td>275,742</td>
<td>302,856</td>
<td>9.8%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2,000</td>
<td>213,319</td>
<td>259,885</td>
<td>21.8%</td>
</tr>
</tbody>
</table>

**9.3.3 Three-stage Hydraulically Fracture Reservoir with Branch Fractures**

In this case, three-stage hydraulic fracturing creates a fracture network as shown in Figure 8-10. The reservoir properties and rock-fluid data are the same as the previous case. Fractures in this case contact more area. The total contact area between discrete fracture and grid blocks is 870,828 $ft^2$ as compared to 390,000 $ft^2$ in Case 1. The hydraulic fracture permeability of the main fracture is reduced to 8,000 $mD$ as compared to 10,000 $mD$ in the previous case to reflect lower energy and proppants concentrating on the main fractures. The branch fractures have
permeability of 5,000 \text{ mD}. Figure 9-29 shows the pressure distribution in the reservoir after 30, 90, 180, and 365 days.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure929.png}
\caption{Case 2 – Pressure distribution after 30, 90, 180, and 365 days}
\end{figure}

Figure 9-30 and Figure 9-31 show production rates and cumulative production for oil and gas, respectively. The increase in cumulative oil production due to capillary pressure is 5.2%. The percentage increase is approximately the same as the previous case. However, the cumulative recovery of oil and gas is higher in this case because the fractures contact more area. In Case 2, the cumulative oil production when capillary pressure is not considered is 245,981 \text{ STB} (26.36\% higher than Case 1).
Figure 9-30: Case 2 – oil production rate and cumulative oil production

Figure 9-31: Case 2 – gas production rate and cumulative gas production
9.3.4 Fractured Well with Fracture Network

In the last example case, a well is placed at the center of the reservoir. The well is intersected by a fracture network as shown by red lines in Figure 9-32. The reservoir parameters are the same as for Case 1 (see Table 9-7). The well is put on production under constant bottom-hole pressure of 500 psia. The total contact area between discrete fractures and grid blocks is 591,543 ft².

Figure 9-32: Reservoir model for case 3

Figure 9-33 shows the pressure distribution after 30, 90, 180, and 365 days. Pressure drops quickly along the discrete fractures and propagates outward. The fracture network serves as a main conduit for hydrocarbons to flow to the wellbore. Figure 9-34 and Figure 9-35 show the oil and gas production rates and cumulative productions. Production rates are shown by solid lines; cumulative production is shown with dashed lines. When capillary pressure impacts phase behavior, fluid properties change causing the oil production rate to remain slightly higher
compared to the case without capillary pressure. After 1 year of production, the cumulative oil production increases by approximately 3.5% compared to the case without the effect of capillary pressure. The increase due to capillary pressure is smaller compared to the previous two cases because the production is limited by the length of the horizontal well, even though the contact area is higher. Only a small portion of the reservoir falls below bubble point.

Figure 9-33: Case 3 – Pressure distribution after 30, 90, 180, and 365 days
Figure 9-34: Case 3 – oil production rate and cumulative oil production

Figure 9-35: Case 3 – gas production rate and cumulative gas production
9.4 Simulation of Dual-porosity Model Incorporating the Effect of Capillary Pressure

Dual-porosity, dual-permeability model with stimulated reservoir volume is used in the study of the effect of capillary pressure on phase behavior. In the DPDK model, the reservoir is split into two porosity domains: matrix and natural fracture. Stimulated reservoir volume model, where natural fracture permeability around the well is enhanced by hydraulic fracturing, is used to represent hydraulically fractured zone around the horizontal well. Table 9-9 shows the reservoir properties for the study of the effect of capillary pressure on phase behavior on the DPDK model. The initial condition of the reservoir is above bubble-point pressure. Stimulated natural fracture permeability is shown in Figure 9-36.

Table 9-9: Input data for simulation of the DPDK model incorporating the effect of capillary pressure on phase behavior

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>Bakken oil</td>
<td>-</td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.0001</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.05</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>25</td>
<td>ft</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>
Figure 9-36: Natural fracture permeability of the DPDK model

Figure 9-37 and Figure 9-38 show oil production rates and cumulative oil production when capillary pressure on phase behavior is considered in both matrix and natural fracture. It can be seen that production rate from the case with capillary pressure is higher over the simulation duration. At the end of 1 year, the cumulative oil production from the case with capillary pressure is 6.84% higher.
Figure 9-37: Oil production rate comparison at initial reservoir pressure of 5,500 psia for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior in both matrix and natural fracture.

Figure 9-38: Cumulative oil production comparison at initial reservoir pressure of 5,500 psia for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior in both matrix and natural fracture.
Capillary pressure in natural fracture is generally small as pore radius may be very large compared to matrix. Therefore, another simulation of the DPDK model is done where capillary pressure on phase behavior is considered only in the matrix. A conventional flash calculation is used in the natural fracture. The cumulative oil production comparison is shown in Figure 9-39.

![Figure 9-39: Cumulative oil production comparison at initial reservoir pressure of 5,500 psia for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior only in the matrix](image)

Oil production rates increase owing to capillary pressure becomes insignificant when capillary pressure is considered in the matrix only. The cumulative oil production with capillary pressure only in the matrix is almost identical to the case without capillary pressure on both matrix and natural fracture. Recall that the effect of capillary pressure causes bubble-point suppression. More light components remain in the oil phase compared to the system with the unsuppressed bubble-point pressure. This results in a swelling of the oil phase and reduction in viscosity and density. This behavior occurs only in the matrix. When oil flows from the matrix which is a confined system to the natural fracture which is unconfined system, the light components, which are in oil
phase in the suppressed system, become unsuppressed and split to gas phase. Therefore, the increase in cumulative oil production is not observed in this case. Transport from suppressed to unsuppressed system reduces the positive impact of capillary pressure on phase behavior.

Figure 9-40 shows cumulative oil productions from the same reservoir model but with initial reservoir pressure of 3,000 \( psia \). The increase in cumulative oil production due to capillary pressure is 10.97%. Compared to the previous case with initial reservoir pressure of 5,500 \( psia \), the increase in cumulative oil production due to capillary pressure is higher at lower initial reservoir pressure. However, no impact of capillary pressure on cumulative oil production is observed when capillary pressure is incorporated only in the matrix. Hydrocarbons flow from confined system to unconfined system. The unsuppressed light components in natural fracture forms gas phase and flow to the well.

![Figure 9-40: Cumulative oil production comparison at initial reservoir pressure of 3,000 \( psia \) for simulation of DPDK model incorporating the effect of capillary pressure on phase behavior only in the matrix](image)
9.5 Simulation of Triple-porosity Model Incorporating the Effect of Capillary Pressure

The effect of capillary pressure on phase behavior is simulated using the TPTK model. Bakken oil is used in the cases of this section. The reservoir properties are shown in Table 9-10 for Bakken formation. In this study, flow between and within porosity types are fully coupled. The formation is ultra-tight with the matrix permeability in the nano-Darcy range. Comparison is made for three scenarios: no capillary pressure, capillary pressure only in the matrix, capillary pressure in both matrix and natural fracture. Note that zero capillary pressure in hydraulic fracture is assumed in all studies of the TPTK model. The initial reservoir pressure of the reservoir is above saturation pressure. The simulation is run for 5 years.

Table 9-10: Input data for simulation of the TPTK model incorporating the effect of capillary pressure on phase behavior for Bakken oil

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>Bakken oil</td>
<td>-</td>
</tr>
<tr>
<td>Reservoir dimensions</td>
<td>2,500 × 2,500</td>
<td>ft</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>5,500</td>
<td>psia</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>240</td>
<td>°F</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.18</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.06</td>
<td>fraction</td>
</tr>
<tr>
<td>Natural fracture porosity</td>
<td>0.01</td>
<td>fraction</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.0001</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.01</td>
<td>mD</td>
</tr>
<tr>
<td>Hydraulic fracture permeability</td>
<td>10,000</td>
<td>mD</td>
</tr>
<tr>
<td>Natural fracture spacing</td>
<td>5</td>
<td>ft</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.25</td>
<td>ft</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>500</td>
<td>psia</td>
</tr>
<tr>
<td>Skin factor</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>

9.5.1 TPTK Model without Enhanced Fracture Permeability Due to Hydraulic Fracturing

Comparison of oil production rates and cumulative oil production are shown in Figure 9-41 and Figure 9-42, respectively. Due to ultra-tight formation, oil production rate is less than 100 STB/day for the entire 10-year production period. With capillary pressure on both matrix...
blocks and natural fractures, the cumulative oil production is 83,787 STB/day which is 2.46% higher compared to the case without capillary pressure. The increase in oil production due to bubble-point suppression from capillary pressure is small because the formation is ultra-tight and initial condition is far from the two-phase zone. The increase will be more pronounced as the reservoir pressure stays longer in the two-phase zone.

Interestingly, cumulative oil production when capillary pressure is considered only in the matrix gives a negative effect on production. Light components in oil phase that were in the confined matrix enter the gas phase when the fluid enters the natural fractures and hydraulic fractures, which are unconfined systems. Oil phase in these fractures does not swell. Instead, gas formation in the fractures is observed earlier because light components in oil are transported to the fractures. Presence of gas in fractures impedes the flow of oil and results in a lower cumulative oil production compared to the case without capillary pressure. This behavior is similar to the study of the effect of capillary pressure in the DPDK. From Figure 9-43, gas production from the case with capillary pressure only in the matrix is also less because gas formation is delayed by bubble-point suppression. Additionally, although gas is present in fractures and matrix, the gas saturations in all porosities are still below critical gas saturation ($S_{gc} = 0.3$). Thus, gas does not flow and contribute to the production.
Figure 9-41: Oil production rate comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture.

Figure 9-42: Cumulative oil production comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture.
9.5.2 Simulation of Three-stage Hydraulically Fractured Reservoir with Fracture Network using TPTK

In this study, three-stage hydraulic fracturing creates a fracture network similar to the model shown in Figure 8-10. However, this time the reservoir is modeled using the TPTK model. In the model, hydraulic fracturing opens up natural fractures, which can be represented by an increase in natural fracture permeability in the grid blocks that host discrete fractures. The natural fracture permeability is shown in Figure 9-44. Matrix permeability in these matrix blocks remains unchanged. Two cases are shown in the study using different sets of relative permeability:

Case 1: Straight-line relative permeability curves are used only in hydraulic fracture

Case 2: Straight-line relative permeability curves are used in both natural and hydraulic fractures
The model is run for 1,500 days. The oil production rate and cumulative oil production are shown in Figure 9-45 and Figure 9-46, respectively.

*Figure 9-44: Natural fracture permeability of the TPTK model*
Figure 9-45: Case 1 – Oil production rate comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture.

Figure 9-46: Case 1 – Cumulative oil production comparison for simulation of the TPTK model incorporating the effect of capillary pressure on phase behavior in matrix and/or natural fracture.
As expected, the case where capillary pressure is considered in both matrix and natural fracture gives the highest cumulative oil production. This is approximately 4.76% higher compared to the case without capillary pressure. In this case, the fracture network aids in the production of oil and gas to the well by increasing the contact area.

Figure 9-47 and Figure 9-48 show oil production rate and cumulative oil production when capillary pressure is considered. The straight-line relative permeability curves are used in natural and hydraulic fractures. Production profiles whether capillary pressure is considered or not are on top of each other indicating that the effect of capillary pressure is insignificant in this case.

Figure 9-47: Case 2 – Oil production rate comparison for simulation of TPTK model incorporating the effect of capillary pressure on phase behavior in matrix
Figure 9-48: Case 2 – Cumulative oil production comparison for simulation of the TPTK model incorporating the effect of capillary pressure on phase behavior in matrix

9.6 Highlights of the Chapter

In this chapter, the impact of capillary pressure on original oil-in-place estimation and cumulative oil production is investigated using Bakken and Eagle Ford fluids. The effect of capillary pressure on phase behavior is studied using the single-porosity, dual-porosity, and TPTK models. EDFM is used to model hydraulic fractures in the reservoir. Natural fracture permeability is assumed to open up due to hydraulic fracturing. This results in an increase in natural fracture permeability. The following is the summary of the simulation results:

- Capillary pressure suppresses bubble-point and alters fluid properties. As initial reservoir pressure decreases, the impact of capillary pressure on phase behavior becomes more significant. The study of impact of capillary pressure on simple model reveals:
- Original oil-in-place estimations increase up to 4.1% for Bakken oil and 46.3% for Eagle Ford oil as initial reservoir pressure decreases.
- Cumulative oil production increases up to 46.3% for Bakken formation and 154% for Eagle Ford formation at low initial reservoir pressure.

- Large capillary pressure creates a challenge in the well model. In a water-wet system where intermediate phase pressure is used as a reference phase, large capillary pressure can cause counter-current flow of the wetting phase. Three methods that can be used to overcome this challenge are as follows:
  - Use of small grid block and time-step sizes can alleviate the impact of capillary pressure on simulation results because small grid block and time-step sizes capture better the high pressure gradients near the well.
  - Assuming equal phase gradient in the well model (i.e., no capillary pressure in the well model) can avoid the pressure of wetting phase falling below bottom-hole pressure. This approach is used in commercial reservoir simulators. However, when wetting phase pressure is calculated from the capillary pressure relationship, the wetting phase pressure may fall below bottom-hole pressure.
  - Use of wetting phase pressure as reference phase can avoid the challenge altogether because wetting phase pressure is always the smallest value.

- Grid sensitivity analysis is performed to determine the optimum number of grid blocks in the studies where EDFM is used to model fractures. The grid block size of 100×100 ft is used in all simulations.

- Contact area between fractures and the formations play a crucial role in an estimation of ultimate recovery. The case with branch fractures contacts formation approximately 1.2 times higher compared to the case with three main fractures, and the cumulative oil production is 26.36% higher.
Simulation of EDFM incorporating the effect of capillary pressure shows that as initial reservoir pressure decreases, the cumulative oil productions increase by 5.2 - 28.1% for Bakken oil and 9.2 – 21.8% for Eagle Ford oil.

Study of effect of capillary pressure in natural fractures of the DPDK and TPTK models shows that as hydrocarbons flow from confined matrix system to unconfined natural fracture system, the suppressed light components become unsuppressed and form gas phase. This results in a negligible increase in cumulative oil production due to capillary pressure. Increase in cumulative oil production is observable when capillary pressure is considered in both matrix and natural fractures.

- In the DPDK, stimulated reservoir volume is used to represent hydraulically fractured reservoir where natural fracture permeability is enhanced by the stimulation. Simulation shows that an increase in cumulative oil production due to capillary pressure is observed only when phase behavior of hydrocarbons in both matrix and natural fractures are under capillary effect, and the increase is 6.84%.

- In the TPTK, the increase due to capillary pressure is 4.76% when both matrix and natural fractures are under the effect of capillary pressure. When capillary pressure is incorporated only in the matrix, the impact of capillary pressure on phase behavior can be positive or negative on cumulative oil production. This depends on reservoir properties.
Chapter 10

Summary and Conclusions

Compositional reservoir simulation plays a vital role in the development of conventional and unconventional reservoirs. Two major building blocks of compositional simulation are phase behavior and fluid transport computation. The oil and gas reserves and flow of reservoir fluids are strongly dependent on phase behavior. In conventional reservoirs, capillary pressure is relatively small and is ignored in phase behavior calculations. However, large capillary pressure values are encountered in tight formations such as tight-rocks and shales and therefore should not be ignored in phase equilibria calculations. Ignoring the effects of capillary pressure on phase behavior can lead to an inaccurate estimation of original oil- and gas-in-place as well as the recovery performance. In spite of this, the effect of capillary pressure on phase behavior in reservoirs with natural and discrete fractures (hydraulic fractures) has not been incorporated in compositional simulation. Furthermore, accurate capturing of the heterogeneity and flow behavior in different porosity domains is utmost important to the prediction of oil and gas recovery in shales. Multi-porosity simulation has been developed to overcome this challenge. Unfortunately, the most current compositional reservoir simulators assume sequential flow from one porosity type to another. In many multi-porosity models, flows between different porosity types are not fully coupled (i.e., flow within a porosity type or between a certain porosity pair is ignored), and in some model, flow is fully coupled using a simplified transmissibility function. An enhanced matrix permeability on the grid block that hosts short-scale fractures is commonly used to eliminate natural fractures and simplify the model.
In this study, we have developed a new fully implicit compositional model for unconventional reservoirs. The model uses natural variables following Coats (1980) formulation. The simulator is capable of modeling up to three porosity types: matrix, natural fracture, and hydraulic fracture. The developed model has several advantages over other existing models. The fully coupled triple-porosity model allows us to better accurately capture fluid flow through heterogeneous porous mediums in unconventional reservoirs that other models can’t. Reservoir properties of matrix, natural fractures, and hydraulic fractures can be assigned to the corresponding porosity types. No assumption of sequential flow is made in this model. These porosity types are fully coupled; i.e., all communications between and within porosity types are allowed. Communication between matrix and natural fracture is handled by dual-continuum concept. In addition, modeling of discrete fractures can be computationally extensive for field simulation. EDFM is used to effectively and efficiently capture heterogeneity of the fracture and flow dynamics of the hydraulic fractures without using LGR or a fine-grid model. Our developed model can potentially capture the proper physics and heterogeneity of the actual fractured reservoir. Simulation results show that the method can be effectively used to model hydraulically fractured tight rock and shales. Various production scenarios using Bakken oil in hydraulically fractured reservoirs were demonstrated.

A modified negative-flash algorithm was implemented into the simulator to account for the effect of capillary pressure on phase behavior. In the modified negative flash, the corresponding phase pressure is used in the calculation of the phase fugacity. The iterative procedure continues until the equilibrium criterion is achieved. At convergence, fluid properties (compressibility factor, molecular weight, density, and viscosity) are calculated and used fluid transport computation. The modified negative flash is also used to determine the number of phases in equilibrium. If vapor mole fraction \( V \) falls out of range 0 and 1, a single-phase condition is assumed.
In the simulations, representative reservoir properties are used. Unless otherwise stated, the initial reservoir pressure is 5,500 psia for the Bakken and Eagle Ford. The following observations and conclusions are drawn from the study:

- The developed TPTK model enables use of accurate reservoir properties corresponding to the porosity types and allows for fully coupled flow. Assigning incorrect reservoir properties may lead to an incorrect prediction of oil and gas production. Assuming sequential flow and decoupling flow between and within porosity types may lead to an underestimation of cumulative oil production by up to 16.41% for Bakken oil and 31.87% for Eagle Ford oil.

- Intersecting coefficient (area fraction) for natural fracture and hydraulic fracture communication play a vital roles in the modeling of triple-porosity model. Comparison with the DPDK model gives a perfect agreement when intersecting coefficient of one is used model. However, the use of fine grid to represent fractures in the DPDK model is limited by the orientation of fractures and efficiency of the simulation time. More grid refinement is needed for non-orthogonal fractures;

- Original oil-in-place and cumulative oil production as a function of initial reservoir pressure were analyzed for the impact of capillary pressure for Bakken and Eagle Ford oils. The impact of capillary pressure depends on reservoir pressure rather than presence of fractures:
  - The bubble-point suppression in Bakken oil is roughly 120 psia at reservoir temperature of 240 °F. The estimation of OOIP increases by up to 4.1% in the case of Bakken oil as initial reservoir pressure decreases to 2,000 psia. In the case of Eagle Ford oil, the bubble-point suppression is approximately 900 psia, and OOIP increase can be up to 46.3% depending on initial reservoir pressure;
Cumulative oil production as a function of initial reservoir pressure shows that as reservoir pressure becomes lower, the effect of capillary pressure on phase behavior becomes more significant. The increase in cumulative oil production from Bakken ranges from 9 - 38.2%. In the case of Eagle Ford shale, an increase in cumulative production of 7.2 - 154% is observed;

- After 10 years of simulation of Bakken oil production, the results show higher cumulative oil production due to capillary pressure by 9.6%. For the case of Eagle Ford oil, two different values of IFT were used (1× and 3×) owing to its uncertainty. The increases in cumulative oil production after 10 years of simulation are 5.6% and 13.2% for the case of 1×IFT and 3×IFT, respectively. Therefore, an accurate determination of IFT from laboratory experiments is crucial to the accuracy of the simulation when capillary pressure is considered as the Macleod and Sugden correlation may incorrectly estimate the IFT and consequently capillary pressure;

- Grid refinement can be used to remediate the impact of large oil-water capillary pressure in the well block for the water-wet system. Alternatively, assuming equal phase gradient in the well model, ignoring oil-water capillary pressure, and using wetting phase pressure as a principal unknown may be a solution to the counter-current flow in the well model;

- Simulation of hydraulically fractured reservoirs with a fracture network gives higher cumulative oil production compared to the reservoir without fracture network as fractures contact more area of the tight formation. Recovery from these tight formations depends strongly on the natural fracture permeability, and based on the comparison of the fully coupled TPTK model, the contacting area between hydraulic fractures and the formation is essential to successfully develop hydrocarbon from tight formations;

- Capillary pressure effect may take place only in specific porosity types in both DPDK and TPTK models. The positive impact of the bubble-point suppression, which results in
an increase in oil production, may not be observed as is seen in single-porosity simulations. This is because as hydrocarbons flow from confined matrix system to unconfined natural fracture system, the suppressed light components become unsuppressed and form gas phase. This results in a negligible increase in cumulative oil production due to capillary pressure. However, an increase in cumulative oil production is observed when capillary pressure is considered in both matrix and natural fractures.

The developed multi-mechanistic, triple-porosity, triple-permeability model gives insight on the flow behavior in hydraulically fractured tight rock and shale reservoirs and a more accurate prediction of oil production from shale oil reservoirs as it captures more physics of the flow in tight formations.

The recommendations for future research are as follows:

- Study more realistic cases and history match real data using the TPTK model.
- Improve robustness of phase behavior flash calculation by incorporating automatic check for maximum capillary pressure allowable for flash calculation with capillary pressure to converge.
- Use the code to interpret a shut-in test for initial phase pressure estimation. In tight formation, capillary pressure is large, and assigning the correct phase pressure to the reservoir model is important to the recovery prediction.
- Examine the impact of gas “huff-n-puff” on recovery for various wetting conditions post fracturing (including fracturing fluid).
- Study the importance of multi-mechanistic flow during a gas injection for EOR processes. In such processes, gas is filled in the low-pressure formation and diffusion may prove to be a dominating flow mechanism.
References


Kumar et al.: “Permeability Evolution of Shale and Coal Under Differential Sorption of He, CH₄, and CO₂.” American Geophysical Union, Fall Meeting 2010.


Appendix A

Derivation of Generalized Flow Equation

A.1 Conservation Equations for a Component in a Phase

Let us consider the elemental control volume (CV) in an unspecified coordinate system shown in Figure A-1.

![Figure A-1: Arbitrary control volume in flow motion](image)

The mass (or mole) conservation equation can be written as follows:

\[
\text{(Net Flux)} + \text{(Net Source/Sink)} = \text{(Net Accumulation)}
\]

(A.1)

The first term on the left hand side can be expanded.

\[
\text{(Mass In - Mass Out)} + \text{(Net Source/Sink)} = \text{(Net Accumulation)}
\]

(A.2)

Integrating Eq. (A.2) over a control volume for component \( i \) in phase \( j \), we obtain compositional balance equation.

\[
\left( -\int_{A} \bar{n} \cdot \bar{N}_{ij} dA \right) + \left( -\int_{V_{s}} R_{ij} dV_{b} - \int_{V_{o}} r_{m,ij} dV_{b} - \int_{V_{b}} Q_{ij} dV_{b} \right) = \left( -\int_{V_{s}} \frac{\partial W_{ij}}{\partial t} dV_{b} \right)
\]

(A.3)
Note that the equation can be used for both mass and mole. If mass conservation is needed, all variables must be in term of mass (e.g., \( \rho (\text{lbm} / \text{ft}^3) \)). If the equation is written for mole conservation, all variables must be in term of mass (e.g., \( \rho (\text{lbmol} / \text{ft}^3) \)). Variables in Eq. (A.3) are described below.

- \( \bar{N}_{ij} \) is the rate of mass flux of component \( i \) in phase \( j \) per surface area. The direction of \( \bar{N}_{ij} \) is positive inward the control volume. \( \bar{N}_{ij} \) has the dimension of \( \left( \frac{\text{mass}}{\text{Surface Area} \cdot \text{time}} \right) \).
- \( R_j = \varepsilon_j r_j \) is the rate of mass generation of component \( i \) in phase \( j \) per bulk volume. \( r_j \) is the rate of mass generation of component \( i \) in phase \( j \) per phase volume per time. \( R_j \) has the dimension of \( \left( \frac{\text{mass}}{\text{V} \cdot \text{time}} \right) \).
- \( r_{m,ij} \) is the rate of mass transfer of component \( i \) within phase \( j \) per bulk volume. \( r_{m,ij} \) has the dimension of \( \left( \frac{\text{mass}}{\text{V} \cdot \text{time}} \right) \).
- \( Q_j = \varepsilon_j \rho_j c_{oj} = \phi S_j \rho_j c_{oj} \) is the concentration of component \( i \) in phase \( j \) per bulk volume. \( W_j \) has the dimension of \( \left( \frac{\text{mass}}{\text{V}} \right) \).

Divergence theorem states that the outward flux of a vector field through a closed surface is equal to the volume integral of the divergence of the region inside the surface.

\[
-\int_A \bar{n} \cdot \bar{N}_{ij} dA = -\int_V \nabla \cdot \bar{N}_{ij} dV \quad (A.4)
\]

Applying divergence theorem to \( -\int_A \bar{n} \cdot \bar{N}_{ij} dA \) term in Eq. (A.3), we obtain the “weak form” of the conservation equation shown in Eq. (A.5).
\[ \int_{V_b} \left( -\nabla \cdot \bar{N}_{ij} + R_{ij} + r_{m,ij} + Q_{ij} - \frac{\partial W_{ij}}{\partial t} \right) dV = 0 \]  

(A.5)

Eq. (A.5) is applicable for arbitrary volume.

Since bulk volume \((V_b)\) can be arbitrary in shape and size, the integrand of Eq. (A.5) must be equal to zero. For example, the integrand must be zero for arbitrary function \(y = f(x)\) and limit of integration \(L_1\) and \(L_2\) as shown below:

![Figure A-2: Example of arbitrary function showing integrand must be zero](image)

Thus, we obtain the “strong form” of the conservation equation.

\[ -\nabla \cdot \bar{N}_{ij} + R_{ij} + r_{m,ij} + Q_{ij} - \frac{\partial W_{ij}}{\partial t} = 0 \]  

(A.6)

Note that Eq. (A.6) is applicable for any point in the control volume. Each term in Eq. (A.6) will be discussed below.

\(\bar{N}_{ij}\) is the sum of advection transport and hydrodynamic dispersion.

\[ \bar{N}_{ij} = \omega_{ij} \rho_j \bar{u}_j - e_j D_{\text{eff}} \cdot \nabla \left( \omega_{ij} \rho_j \right) \]  

(A.7)

where \(\omega_{ij}\) is mass fraction of component \(i\) in phase \(j\), \(\rho_j\) is density of phase \(j\), and \(\bar{u}_j\) is Darcian velocity of component \(i\) in phase \(j\). \(D_{\text{eff}}\) is effective hydraulic conductivity or diffusion/dispersion coefficient with the unit of \(\left( \frac{L^2}{\text{time}} \right)\). The diffusion coefficient is the amount of a particular
substance that diffuses across a unit area in one second under the influence of a gradient of one unit. \( \varepsilon_j \) is the volume fraction of phase \( j \). Eq. (A.7) assumes that all components in phase \( j \) flow with volume-averaged velocity \( \bar{u}_j \) (velocity of phase \( j \)) and density of component \( i \) in phase \( j \) is equal to the density of phase \( j \) (\( \rho_{ij} = \rho_j \)). Note that \( \nabla = \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k} \) for Cartesian coordinates.

Substituting the definition of \( \bar{N}_j \), \( \bar{R}_j \), and \( \bar{W}_j \) into Eq. (A.6), we obtain the conservation equation for a component in a phase in an arbitrary control volume.

\[
-\nabla \cdot \left( \omega_j \rho_j \bar{u}_j - \varepsilon_j D_{\text{eff}} \cdot \nabla \left( \omega_j \rho_j \right) \right) + \varepsilon_j r_{ij} + r_{m,ij} + Q_{ij} = \frac{\partial}{\partial t} \left( \varepsilon_j \rho_j \omega_j \right)
\]

for \( i = 1, 2, 3, ..., N_c \) & \( j = 1, 2, 3, ..., N_p \) (A.8)

Eq. (A.8) can be written \( (N_c \cdot N_p) \) times.

### A.2 Overall Compositional Balance

By summing each term in Eq. (A.8) for each phase, we obtain a compositional balance for each component. Since the equation is written for a component, the term \( r_{m,ij} \) is removed from the equation as no transport between phases is considered.

\[
-\nabla \cdot \left( \sum_{j=1}^{N_p} \left( \omega_j \rho_j \bar{u}_j - \varepsilon_j D_{\text{eff}} \cdot \nabla \left( \omega_j \rho_j \right) \right) \right) + \sum_{j=1}^{N_p} \varepsilon_j r_{ij} + \sum_{j=1}^{N_p} Q_{ij} = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_p} \varepsilon_j \rho_j \omega_j \right)
\]

(A.9)

Separating the fluid phases from solid phase,

\[
-\nabla \cdot \left( \sum_{j=1}^{N_p} \left( \omega_j \rho_j \bar{u}_j - \phi S_j D_{\text{eff}} \cdot \nabla \left( \omega_j \rho_j \right) \right) \right) + \left( \sum_{j=1}^{N_p} \phi S_j r_{ij} + (1-\phi) r_{is} \right) + \sum_{j=1}^{N_p} Q_{ij}
\]

\[
= \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_p} \phi S_j \rho_j \omega_j + (1-\phi) \rho_s \omega_s \right)
\]

(A.10)
Recall Darcy’s law:

\[
\bar{u}_j = -\frac{k_j}{\mu_j} \nabla \Phi_j \quad \text{where} \quad \Phi_j = P_j - \frac{1}{144} \frac{g}{\rho G} 
\]

(A.11)

Substituting Eq. (A.11) into Eq. (A.10) gives

\[
-\nabla \cdot \left( \sum_{j=1}^{N_p} \left( -\omega_j \rho_j \frac{k_j}{\mu_j} \nabla \Phi_j - \phi S_j D_{eff} \cdot \nabla \left( \omega_j \rho_j \right) \right) \right) + \left( \sum_{j=1}^{N_p} \phi S_j r_{ij} + (1 - \phi) r_{is} \right) \\
+ \sum_{j=1}^{N_p} Q_{ij} = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_p} \phi S_j \rho_j \omega_j \right) + (1 - \phi) \rho_s \omega_{is}
\]

(A.12)

Since solid phase does not contribute to flow (i.e., no flow in solid phase), the solid phase is removed from future consideration.

\[
\nabla \cdot \left( \sum_{j=1}^{N_p} \left( \omega_j \rho_j \frac{k_j}{\mu_j} \nabla \Phi_j + \phi S_j D_{eff} \cdot \nabla \left( \omega_j \rho_j \right) \right) \right) + \left( \sum_{j=1}^{N_p} \phi S_j r_{ij} \right) \\
+ \sum_{j=1}^{N_p} Q_{ij} = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_p} \phi S_j \rho_j \omega_j \right)
\]

(A.13)

Note that all terms in Eq. (A.13) have the unit of \( \left( \frac{mass}{V_b \cdot time} \right) \).
A.3 Compositional Conservation Equation in Cartesian Coordinates

From Eq. (A.13), we can expand the divergent terms so it is applicable for Cartesian coordinates.

\[
\frac{\partial}{\partial x} \left( \sum_{j=1}^{N_r} \left( \sum_{j=1}^{N_S} \omega_j \rho_j \frac{k_{ij} \partial \Phi_j}{\mu_j} + \phi S_j D_{ij} \frac{\partial}{\partial x} (\omega_j \rho_j) \right) \right) + \frac{\partial}{\partial y} \left( \sum_{j=1}^{N_r} \left( \sum_{j=1}^{N_S} \omega_j \rho_j \frac{k_{ij} \partial \Phi_j}{\mu_j} + \phi S_j D_{ij} \frac{\partial}{\partial y} (\omega_j \rho_j) \right) \right) + \frac{\partial}{\partial z} \left( \sum_{j=1}^{N_r} \left( \sum_{j=1}^{N_S} \omega_j \rho_j \frac{k_{ij} \partial \Phi_j}{\mu_j} + \phi S_j D_{ij} \frac{\partial}{\partial z} (\omega_j \rho_j) \right) \right) + \sum_{j=1}^{N_r} \phi S_j r_j V_j + \sum_{j=1}^{N_r} Q_j V_j = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_r} \phi S_j \rho_j \omega_j V_j \right)
\]

(A.14)

Multiply through Eq. (A.14) by \( \Delta x \Delta y \Delta z \):

\[
\frac{\partial}{\partial x} \left( \sum_{j=1}^{N_r} \left( \sum_{j=1}^{N_S} \omega_j \rho_j A_x \frac{k_{ij} \partial \Phi_j}{\mu_j} + \phi S_j A_x D_{ij} \frac{\partial}{\partial x} (\omega_j \rho_j) \right) \right) \Delta x \\
+ \frac{\partial}{\partial y} \left( \sum_{j=1}^{N_r} \left( \sum_{j=1}^{N_S} \omega_j \rho_j A_y \frac{k_{ij} \partial \Phi_j}{\mu_j} + \phi S_j A_y D_{ij} \frac{\partial}{\partial y} (\omega_j \rho_j) \right) \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( \sum_{j=1}^{N_r} \left( \sum_{j=1}^{N_S} \omega_j \rho_j A_z \frac{k_{ij} \partial \Phi_j}{\mu_j} + \phi S_j A_z D_{ij} \frac{\partial}{\partial z} (\omega_j \rho_j) \right) \right) \Delta z \\
+ \sum_{j=1}^{N_r} \phi S_j r_j V_j + \sum_{j=1}^{N_r} Q_j V_j = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_r} \phi S_j \rho_j \omega_j V_j \right)
\]

(A.15)
Note that $\mathbf{i} \cdot \mathbf{i} = \mathbf{j} \cdot \mathbf{j} = \mathbf{k} \cdot \mathbf{k} = 1$, $\mathbf{i} \cdot \mathbf{j} = \mathbf{i} \cdot \mathbf{k} = \mathbf{j} \cdot \mathbf{k} = 0$, and the unit in each term of Eq. (A.15) is \( \text{mass} / V_b \cdot \text{time} \).

Let \( Q^*_j = Q_j V_b \) be the rate of mass production or injection in the bulk volume \( \left( \text{mass} / V_b \cdot \text{time} \right) \).

Thus, from Eq. (A.15), we obtain.

\[
\frac{\partial}{\partial x} \left( \sum_{j=1}^{N_x} \left( \omega_j \rho_j A_j \frac{k_j k_{ij}}{\mu_j} \frac{\partial \Phi_j}{\partial x} + \phi S_j A_j D_{\text{eff}} \frac{\partial}{\partial x} (\omega_j \rho_j) \right) \right) \Delta x \\
+ \frac{\partial}{\partial y} \left( \sum_{j=1}^{N_y} \left( \omega_j \rho_j A_j \frac{k_j k_{ij}}{\mu_j} \frac{\partial \Phi_j}{\partial y} + \phi S_j A_j D_{\text{eff}} \frac{\partial}{\partial y} (\omega_j \rho_j) \right) \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( \sum_{j=1}^{N_z} \left( \omega_j \rho_j A_j \frac{k_j k_{ij}}{\mu_j} \frac{\partial \Phi_j}{\partial z} + \phi S_j A_j D_{\text{eff}} \frac{\partial}{\partial z} (\omega_j \rho_j) \right) \right) \Delta z \\
+ \sum_{j=1}^{N_p} \phi S_j r_j V_b + \sum_{j=1}^{N_p} Q^*_j = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_p} \phi S_j \rho_j \omega_j V_b \right) \\
\text{(A.16)}
\]

### A.4 Inventory of Equation and Unknowns

**Unknowns:**

<table>
<thead>
<tr>
<th>Unknowns</th>
<th># of Unknowns</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P_j )</td>
<td>( N_p )</td>
</tr>
<tr>
<td>( \omega_j )</td>
<td>( N_c \times N_p )</td>
</tr>
<tr>
<td>( S_j )</td>
<td>( N_p )</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>( 2N_p + (N_c \times N_p) )</td>
</tr>
</tbody>
</table>
Equations:

<table>
<thead>
<tr>
<th>Equations</th>
<th># of Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mole Balances (Flow equations)</td>
<td>$N_c$</td>
</tr>
<tr>
<td>$\sum_{i=1}^{N_c} \omega_{ij} = 1$</td>
<td>$N_p$</td>
</tr>
<tr>
<td>$\sum_{j=1}^{N_p} S_j$</td>
<td>1</td>
</tr>
<tr>
<td>$P_{c,j}$</td>
<td>$N_p - 1$</td>
</tr>
<tr>
<td>$f_{ij} = f_{il}$ where $l = \text{ref. phase}$</td>
<td>$N_c(N_p - 1)$</td>
</tr>
<tr>
<td>Total</td>
<td>$2N_p + (N_c \times N_p)$</td>
</tr>
</tbody>
</table>

A.5 Three-phase (oil, gas, water) Flow Equations

From Eq. (A.16), it is assumed that diffusion is governed by Fick’s law.

$$
\frac{\partial}{\partial x} \left( \sum_{j=1}^{N_p} \left( \omega_j \rho_j A_{ij} \frac{k_{ij}}{\mu_j} \frac{\partial \Phi_j}{\partial x} + \omega_j \phi S_j A_{ij} D_{ij} \frac{\partial \rho_j}{\partial x} \right) \right) \Delta x \\
+ \frac{\partial}{\partial y} \left( \sum_{j=1}^{N_p} \left( \omega_j \rho_j A_{ij} \frac{k_{ij}}{\mu_j} \frac{\partial \Phi_j}{\partial y} + \omega_j \phi S_j A_{ij} D_{ij} \frac{\partial \rho_j}{\partial y} \right) \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( \sum_{j=1}^{N_p} \left( \omega_j \rho_j A_{ij} \frac{k_{ij}}{\mu_j} \frac{\partial \Phi_j}{\partial z} + \omega_j \phi S_j A_{ij} D_{ij} \frac{\partial \rho_j}{\partial z} \right) \right) \Delta z \\
+ \sum_{j=1}^{N_p} \phi S_j r_j V_b + \sum_{j=1}^{N_p} Q_{ij} = \frac{\partial}{\partial t} \left( \sum_{j=1}^{N_p} \phi S_j \rho_j \omega_j V_b \right)
$$

(A.17)

Dividing through by molecular weight of phase $j$. 

We let $x_i$ and $y_i$ be mole fraction of oil and gas phase, respectively. Subscript $j$ is replaced by $o$ and $g$ for oil and gas phase, respectively. Assume that chemical reaction is negligible ($r_j = 0$).

Eq. (A.17) can be rewritten for a two-phase hydrocarbon system in term of moles.

\[
\frac{\partial}{\partial x}\left( \sum_{j=1}^{N_x} \left( \omega_j \frac{\rho_j}{MW_j} A_x \frac{k_{kr, j}}{\mu_j} \frac{\partial \Phi_j}{\partial x} + \omega_j \phi S_j A_x D_{eff} \frac{\partial \rho_j}{\partial x} \right) \right) \Delta x
\]
\[
+ \frac{\partial}{\partial y}\left( \sum_{j=1}^{N_y} \left( \omega_j \frac{\rho_j}{MW_j} A_y \frac{k_{kr, j}}{\mu_j} \frac{\partial \Phi_j}{\partial y} + \omega_j \phi S_j A_y D_{eff} \frac{\partial \rho_j}{\partial y} \right) \right) \Delta y
\]
\[
+ \frac{\partial}{\partial z}\left( \sum_{j=1}^{N_z} \left( \omega_j \frac{\rho_j}{MW_j} A_z \frac{k_{kr, j}}{\mu_j} \frac{\partial \Phi_j}{\partial z} + \omega_j \phi S_j A_z D_{eff} \frac{\partial \rho_j}{\partial z} \right) \right) \Delta z
\]
\[\sum_{j=1}^{N_x} \phi S_j r_j V_b + \sum_{j=1}^{N_y} Q^*_o = \frac{\partial}{\partial t}\left( \sum_{j=1}^{N_y} \frac{\phi_j}{MW_j} \omega_j V_b \right) \tag{A.18} \]

Dividing through by $\frac{1}{5.615 \frac{bbl}{ft^3}}$ and expanding the potential term in Darcy law,

\[
\frac{\partial}{\partial x}\left( x_i \tilde{\rho}_o A_x \frac{k_{kr, o}}{\mu_o} \frac{\partial \Phi_o}{\partial x} \right) \Delta x
\]
\[+ \frac{\partial}{\partial y}\left( x_i \tilde{\rho}_o A_y \frac{k_{kr, o}}{\mu_o} \frac{\partial \Phi_o}{\partial y} + y_i \tilde{\rho}_g A_y \frac{k_{kr, g}}{\mu_g} \frac{\partial \Phi_g}{\partial y} + y_i \phi S_g A_y D_{eff} \frac{\partial \tilde{\rho}_g}{\partial y} \right) \Delta y
\]
\[+ \frac{\partial}{\partial z}\left( x_i \tilde{\rho}_o A_z \frac{k_{kr, o}}{\mu_o} \frac{\partial \Phi_o}{\partial z} + y_i \tilde{\rho}_g A_z \frac{k_{kr, g}}{\mu_g} \frac{\partial \Phi_g}{\partial z} + y_i \phi S_g A_z D_{eff} \frac{\partial \tilde{\rho}_g}{\partial z} \right) \Delta z
\]
\[+ M_i = \frac{V_b}{5.615 \partial t}\left( \phi S_o \tilde{\rho}_o x_i + \phi S_g \tilde{\rho}_g y_i \right) \tag{A.19} \]
Note that the well source term is replaced by $M_i$. Each term in Eq. (A.20) has the unit of $\frac{\text{lbmol} \cdot \text{bbl}}{\text{day} \cdot \text{ft}^3}$. Expanding the partial differential terms gives the final form of two-phase hydrocarbon flow equation.

$$
\frac{\partial}{\partial x} \left( x_i \tilde{\rho}_g A_x \frac{k_{kr} \partial P_w}{\mu_o} + y_i \tilde{\rho}_g A_x \frac{k_{kr} \partial P_g}{\mu_g} + y_i \phi S_g A_x D_{ef} \frac{\partial \tilde{\rho}_g}{\partial x} \right) \Delta x \\
- \frac{\partial}{\partial x} \left( \frac{1}{144 \text{gg}} \rho_o x_i \tilde{\rho}_g A_x \frac{k_{kr} \partial G}{\mu_o} + \frac{1}{144 \text{gg}} \rho_g x_i \tilde{\rho}_g A_x \frac{k_{kr} \partial G}{\mu_g} \right) \Delta x \\
+ \frac{\partial}{\partial y} \left( x_i \tilde{\rho}_g A_y \frac{k_{kr} \partial P_w}{\mu_o} + y_i \tilde{\rho}_g A_y \frac{k_{kr} \partial P_g}{\mu_g} + y_i \phi S_g A_y D_{ef} \frac{\partial \tilde{\rho}_g}{\partial y} \right) \Delta y \\
- \frac{\partial}{\partial y} \left( \frac{1}{144 \text{gg}} \rho_o x_i \tilde{\rho}_g A_y \frac{k_{kr} \partial G}{\mu_o} + \frac{1}{144 \text{gg}} \rho_g x_i \tilde{\rho}_g A_y \frac{k_{kr} \partial G}{\mu_g} \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( x_i \tilde{\rho}_g A_z \frac{k_{kr} \partial P_w}{\mu_o} + y_i \tilde{\rho}_g A_z \frac{k_{kr} \partial P_g}{\mu_g} + y_i \phi S_g A_z D_{ef} \frac{\partial \tilde{\rho}_g}{\partial z} \right) \Delta z \\
- \frac{\partial}{\partial z} \left( \frac{1}{144 \text{gg}} \rho_o x_i \tilde{\rho}_g A_z \frac{k_{kr} \partial G}{\mu_o} + \frac{1}{144 \text{gg}} \rho_g x_i \tilde{\rho}_g A_z \frac{k_{kr} \partial G}{\mu_g} \right) \Delta z \\
+ M_i = \frac{V_b}{5.615 \partial t} \left( \phi S_w \tilde{\rho}_w x_i + \phi \tilde{\rho}_g y_i \right) \tag{A.21}
$$

Similarly, the flow equation for water component can be derived in a similar manner.

$$
\frac{\partial}{\partial x} \left( A_k k_{krw} \frac{\partial P_w}{\mu_o B_w} - \frac{1}{144 \text{gg}} \rho_o \frac{\partial G}{\partial x} \right) \Delta x + \frac{\partial}{\partial y} \left( A_k k_{krw} \frac{\partial P_w}{\mu_o B_w} - \frac{1}{144 \text{gg}} \rho_o \frac{\partial G}{\partial y} \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( A_k k_{krw} \frac{\partial P_w}{\mu_o B_w} - \frac{1}{144 \text{gg}} \rho_o \frac{\partial G}{\partial z} \right) \Delta z + q''_w = \frac{V_b}{5.615 \partial t} \frac{\partial (\phi S_w)}{B_w} \tag{A.22}
$$

Expanding the partial differential terms gives the final form of water equation.

$$
\frac{\partial}{\partial x} \left( A_k k_{krw} \frac{\partial P_w}{\mu_o B_w} - \frac{1}{144 \text{gg}} \rho_o \frac{A_k k_{krw} \partial G}{\mu_o B_w} \right) \Delta x + \frac{\partial}{\partial y} \left( A_k k_{krw} \frac{\partial P_w}{\mu_o B_w} - \frac{1}{144 \text{gg}} \rho_o \frac{A_k k_{krw} \partial G}{\mu_o B_w} \right) \Delta y \\
+ \frac{\partial}{\partial z} \left( A_k k_{krw} \frac{\partial P_w}{\mu_o B_w} - \frac{1}{144 \text{gg}} \rho_o \frac{A_k k_{krw} \partial G}{\mu_o B_w} \right) \Delta z + q''_w = \frac{V_b}{5.615 \partial t} \left( \phi S_w \right) \tag{A.23}
$$
In Eq. (A.23), it is assumed that water remain in water phase (i.e., water component does not go into oil or gas phases and vice versa). The unit of each term in Eq. (A.23) is \( \frac{\text{STB}}{\text{day}} \).
Appendix B

Thermodynamic Model

Phase behavior calculation can be described by equation of state (EoS).

B.1 Stability Analysis Based on Minimization of Tangent Plane Distance

The stationary criterion based on tangent plant distance (TPD) for component $i$ can be described as follows (Michelsen, 1981):

$$\ln f_i^{\text{trial}} - \ln f_i^{\text{test}} = 0$$

(B.1)

The first and second terms on the left hand side of Eq. (B.1) are fugacities of the trial phase and testing phase, respectively. By substituting Eq. (B.1) with the definition of fugacity, we obtain Eq. (B.2).

$$\left( \ln Y_i + \ln \phi_i^{\text{trial}} \right) - \left( \ln z_i + \ln \phi_i^{\text{test}} \right) = 0$$

(B.2)

where $Y_i$, $z_i$, $\phi_i^{\text{trial}}$, and $\phi_i^{\text{test}}$ are the composition of component $i$ of the trial phase, composition of component $i$ of the testing phase, trial phase fugacity coefficient of component $i$, and testing phase fugacity coefficient of component $i$, respectively. Eq. (B.2) is the equation we are trying to minimize. Thus, the residual equation for the minimization of tangent plane distance can be written.

$$R_i = \left( \ln Y_i + \ln \phi_i^{\text{trial}} \right) - \left( \ln z_i + \ln \phi_i^{\text{test}} \right)$$

(B.3)

Taking the partial derivative with respect to the trial phase mole number of component $j$ ($Y_j$), we obtain
\[
\frac{\partial R_i}{\partial Y_j} = \left( \frac{\partial \ln Y_i}{\partial Y_j} + \frac{\partial \phi_{i,\text{trial}}}{\partial Y_j} \right) - \left( \frac{\partial \ln z_i}{\partial Y_j} + \frac{\partial \phi_{i,\text{test}}}{\partial Y_j} \right)
\]  

(B.4)

Since the overall testing compositions and its fugacity are constant during the minimization of TPD, the partial derivatives become zero. Thus, we obtain

\[
\frac{\partial R_i}{\partial Y_j} = \frac{\partial \ln Y_i}{\partial Y_j} + \frac{\partial \phi_{i,\text{trial}}}{\partial Y_j} - \frac{1}{z_i} \frac{\partial z_i}{\partial Y_j} \frac{\partial \phi_{i,\text{test}}}{\partial Y_j} = 0
\]

(B.5)

The partial derivative terms \(\frac{\partial Y_i}{\partial Y_j}\) and \(\frac{\partial \phi_{i,\text{trial}}}{\partial Y_j}\) in Eq. (B.5) is calculated analytically based on the following derivations.

\[
\frac{\partial Y_i}{\partial Y_j} = \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j 
\end{cases}
\]  

(B.6)

\[
\frac{\partial \ln \phi_{i,\text{trial}}}{\partial Y_j} = \frac{\partial Z}{\partial Y_j} \frac{B_i}{B} - \frac{(Z-1)}{B^2} \frac{\partial B}{\partial Y_j} - \frac{1}{Z-B} \left( \frac{\partial Z}{\partial Y_j} - \frac{\partial B}{\partial Y_j} \right)
\]

\[
+ \left( \frac{1}{(m_1 - m_2)B} \frac{\partial A}{\partial Y_j} - \frac{A}{(m_1 - m_2)B^2} \frac{\partial B}{\partial Y_j} \right) \left( \frac{2}{A} \sum_{k=1}^{N_c} A_{ik} y_k - \frac{B_i}{B} \right) \ln \left( \frac{Z + m_2 B}{Z + m_1 B} \right)
\]

\[
+ \frac{2}{A} \frac{\partial}{\partial Y_j} \left( \sum_{k=1}^{N_c} A_{ik} y_k \right) \left( \frac{1}{A} - \frac{B_i}{B} \right) + \frac{B_i}{B} \frac{\partial B}{\partial Y_j} \right) \frac{A}{(m_1 - m_2)B} \ln \left( \frac{Z + m_2 B}{Z + m_1 B} \right)
\]

\[
+ \frac{A}{(m_1 - m_2)B} \left( \sum_{k=1}^{N_c} A_{ik} y_k \right) \left( \frac{\partial Z}{\partial Y_j} + m_2 \frac{\partial B}{\partial Y_j} \right) - \frac{\partial Z}{\partial Y_j} + m_1 \frac{\partial B}{\partial Y_j} \right) \left( \frac{Z + m_2 B}{Z + m_1 B} \right)
\]  

(B.7)
It can be seen from Eq. (B.7) that four partial derivative terms must be calculated: \( \frac{\partial Z}{\partial Y_j} \), \( \frac{\partial A}{\partial Y_j} \), \( \frac{\partial B}{\partial Y_j} \), and \( \frac{\partial \sum_{k=1}^{N_c} A_k Y_k}{\partial Y_j} \). These terms can be calculated as follow.

\[
\frac{\partial Z}{\partial Y_j} = \frac{(B - Z) \frac{\partial A}{\partial Y_j} - \left[ (m_1 + m_2 - 1)Z^2 + 2m_1m_2BZ - (m_1 + m_2)(2B - 1)Z - A - m_1m_2 \left( 3B^2 + 2B \right) \right] \frac{\partial B}{\partial Y_j}}{3Z^2 + 2BZ(m_1 + m_2 - 1) - 2Z + A + m_1m_2B^2 - (m_1 + m_2)(B^2 + B)}
\]  \( \text{(B.8)} \)

\[
\frac{\partial A}{\partial Y_j} = \sum_{k=1}^{N_c} \left( 2 \sum_{l=1}^{N_c} \left( A_{kl} \frac{\partial y_k}{\partial Y_l} \right) \right)
\]  \( \text{(B.9)} \)

\[
\frac{\partial B}{\partial Y_j} = \sum_{k=1}^{N_c} \left( B_k \frac{\partial y_k}{\partial Y_j} \right)
\]  \( \text{(B.10)} \)

\[
\frac{\partial \sum_{k=1}^{N_c} A_k Y_k}{\partial Y_j} = \sum_{k=1}^{N_c} \left( A_k \frac{\partial y_k}{\partial Y_j} \right)
\]  \( \text{(B.11)} \)

Recall that \( y_k = \frac{Y_k}{\sum_{k=1}^{N_c} Y_k} \). Finally, the partial derivative term \( \frac{\partial y_k}{\partial Y_j} \) that appears in Eqs. (B.9), (B.10), and (B.11) can be calculated as shown below.

\[
\frac{\partial y_k}{\partial Y_j} = \frac{\delta_{kj} \sum_{l=1}^{N_c} Y_l - Y_i}{\left( \sum_{l=1}^{N_c} Y_l \right)^2}
\]  \( \text{(B.12)} \)

where \( \delta_{kj} \) is defined in Eq. (B.13).

\[
\delta_{kj} = \begin{cases} 
1 & \text{if } k = j \\
0 & \text{if } k \neq j 
\end{cases}
\]  \( \text{(B.13)} \)
B.2 Flash Calculation Based on Minimum-variable Newton-Raphson Protocol

The partial derivatives term $\frac{\partial \ln \phi_i^L}{\partial n_k^L}$ can be derived as follows:

$$
\frac{\partial \ln \phi_i^L}{\partial n_k^L} = \frac{\partial Z_l}{\partial n_k^L} B_l - \frac{(Z_l - 1) \partial B_L}{2 B_l^2} \frac{\partial B_L}{\partial n_k^L} B_l - \frac{1}{Z_l - B_L} \left( \frac{\partial Z_l}{\partial n_k^L} - \frac{\partial B_L}{\partial n_k^L} \right)
\quad + \left[ \frac{\partial A_L}{\partial n_k^L} - \frac{A_L}{(m_1 - m_2) B_L} \right] \left( 2 \sum_{k=1}^{N_c} A_{ik} x_k \right)
\quad + \frac{A_L}{(m_1 - m_2) B_L} \left( \frac{2 \sum_{k=1}^{N_c} A_{ik} x_k}{A_L} - B_l \right) \ln \left( \frac{Z_l + m_i B_L}{Z_l + m_i B_L} \right)
\quad + \frac{A_L}{(m_1 - m_2) B_L} \left( \frac{2 \sum_{k=1}^{N_c} A_{ik} x_k}{A_L} - B_l \right) \left( \frac{\partial Z_l}{\partial n_k^L} + m_2 \frac{\partial B_L}{\partial n_k^L} \frac{\partial Z_l}{\partial n_k^L} + m_1 \frac{\partial B_L}{\partial n_k^L} \right)
$$

(B.14)

The partial derivative terms in Eq. (B.14) can be calculated from the Eqs. (B.15) to (B.18).

$$
\frac{\partial Z_l}{\partial n_k^L} = \frac{(B_L - Z_L) \frac{\partial A_L}{\partial n_k^L} - \left[ (m_1 + m_2 - 1) Z_l^2 + 2m_i m_2 B_L Z_l \right]}{3Z_l^2 + 2B_L Z_l (m_1 + m_2 - 1) - 2Z_l + A_L + m_i m_2 B_L^2 - (m_1 + m_2) (B_L^2 + B_L)}
$$

(B.15)

$$
\frac{\partial A_L}{\partial n_k^L} = 2 \sum_{k=1}^{N_c} A_{ik} x_k - A_L
$$

(B.16)

$$
\frac{\partial B_L}{\partial n_k^L} = \frac{B_k - B_L}{L}
$$

(B.17)

$$
\frac{\partial \sum_{i=1}^{N_c} A_{ik} x_i}{\partial n_k^L} = \frac{A_{ik} - \sum_{j=1}^{N_c} A_{ij} x_i}{L}
$$

(B.18)
Similarly, the partial derivative term \( \frac{\partial \ln \phi^V}{\partial n^V_k} \) can be calculated using Eqs. (B.15) to (B.18), by substituting phase identification \( L \) to \( V \).

### B.3 Molecular Weight

Molecular weight of liquid and vapor phases can be calculated straightforwardly using the following equations.

\[
MW_g = \sum_{i=1}^{N_c} y_i MW_i \quad \text{and} \quad MW_v = \sum_{i=1}^{N_c} x_i MW_i
\]

(B.19)

### B.4 Density

#### B.4.1 Hydrocarbon

The density of phase \( j \) can be calculated from molecular weight and \( Z \) factor of that phase.

\[
\rho_j = \frac{P_j}{RT} \left( \frac{MW_j}{Z_j} \right)
\]

(B.20)

In attempt to improve the accuracy of the predicted density from SRK-EoS, a volume-translation technique is introduced. In addition, Jhaveri and Youngren show that the volume-translation technique can be applied to PR-EoS as well. The calculation is shown below.

\[
v_j = v_j^{EOS} - \sum_{i=1}^{N_c} \phi_j c_i
\]

(B.21)

where \( c_i \) is component-dependent volume-shift parameters. \( c_i \) can be calculated using the following equation:
\[ c_i = s_i b_i \]  \hspace{1cm} (B.22)

where \( s_i \) and \( b_i \) are proportionality constant and pure substance’s co-volume parameter of component \( i \). Once \( v_L \) and \( v_v \) are calculated, the density can be calculated as follows.

\[ \rho_j = \frac{MW_j}{v_j} \]  \hspace{1cm} (B.23)

The unit of density in Eq. (B.23) is \( \text{lbm/ft}^3 \).

### B.4.2 Water

Density of water can be calculated from Eq. (B.24).

\[ \rho_w = \rho_w^0 \left[ 1 + c_w \left( P_w - P_{w,\text{ref}} \right) \right] \]  \hspace{1cm} (B.24)

### B.5 Viscosity

The viscosity of phase \( j \) can be calculated from Lohrenz, Bray, and Clark (1964) correlation.

\[ \mu_j = \mu_j^* + \xi_m^{-1} \left[ \begin{array}{l} 0.1023 + 0.023364 \rho_r + 0.058533 \rho_r^2 \times 10^{-4} \\ -0.040758 \rho_r^3 + 0.0093324 \rho_r^4 \end{array} \right] \]  \hspace{1cm} (B.25)

where \( \mu_j, \mu_j^*, \xi_m^{-1}, \) and \( \rho_r \) are viscosity of phase \( j \) (\( \text{cp} \)), viscosity of phase \( j \) at atmospheric pressure (\( \text{cp} \)), mixture viscosity parameter (\( \text{cp}^{-1} \)), and reduced density of phase \( j \) (unitless), respectively. These coefficients can be calculated as follows.

\[ \mu_j^* = \frac{\sum_{i=1}^{N_c} \omega_i \mu_i^* \sqrt{MW_i}}{\sum_{i=1}^{N_c} \omega_i \sqrt{MW_i}} \]  \hspace{1cm} (B.26)
where \( \omega_j \), \( MW_j \), and \( \mu^*_{ij} \) are mole fraction of component \( i \) in phase \( j \), molecular weight of component \( i \) (lbm/lbmol), and viscosity of the component \( i \) at low pressure (cp), respectively.

The parameter \( \mu^*_{ij} \) can be calculated as follows:

\[
\mu^*_{ij} = \frac{34\times10^{-3}T_{ni}^{0.94}}{\xi_i} \quad \text{for} \quad T_{ni} \leq 1.5
\]

\[
\mu^*_{ij} = \frac{17.78\times10^{-5}(4.58T_{ni} - 1.67)^{0.925}}{\xi_i} \quad \text{for} \quad T_{ni} > 1.5
\]

where \( T_{ni} \) and \( \xi_i \) are reduced temperature of component \( i \) and viscosity parameter of the component \( i \).

The parameter \( \xi_i \) and \( \xi_m \) can be calculated as follows.

\[
\xi_i = \frac{5.4402T_{ci}^{1/6}}{\sqrt{MW_i P_{ci}^{2/3}}} \quad (B.29)
\]

\[
\xi_m = \frac{5.4402T_{pc}^{1/6}}{\sqrt{MW_j P_{pc}^{2/3}}} \quad (B.30)
\]

where \( T_{pc}, P_{pc}, \) and \( MW_j \) are pseudo-critical temperature (°R), pseudo-critical pressure (psia), and molecular weight of phase \( j \) (lbm/lbmol).

Finally, the calculation of reduced density of the liquid mixture (\( \rho_r \)) has been derived from Lohrentz et al. (1969).

\[
\rho_r = \frac{\rho_j}{\rho_{pc}} = \left( \frac{\rho_j}{MW_j} \right) V_{pc}
\]

where \( T_{pc}, P_{pc}, \) and \( V_{pc} \) can be defined as follow.

\[
T_{pc} = \sum_{i=1}^{N} \chi_i T_{ci}
\]

(B.32)
\[ P_{pc} = \sum_{i=1}^{N_p} \chi_i P_{ci} \quad \text{(B.33)} \]
\[ V_{pc} = \sum_{i=1}^{N_p} \chi_i V_{ci} \quad \text{(B.34)} \]

**B.6 Saturation**

Oil saturation can be obtained from vapor and liquid mole fractions. Gas saturation, for the case of two hydrocarbon phases are present, is calculated from the remaining pore space that is not occupied by water and oil. Eqs. (B.35) and (B.36) show the formula for oil and gas saturation calculations.

\[ S_o = (1 - S_w) \frac{V_o}{V_o + V_g} = (1 - S_w) \frac{f_{nl} \times \tilde{v}_o}{f_{nl} \times \tilde{v}_o + f_{ng} \times \tilde{v}_g} \quad \text{(B.35)} \]
\[ S_g = (1 - S_w - S_o) \quad \text{(B.36)} \]

**B.7 Formation Volume Factor**

Molar production rate of hydrocarbon component \( i \) (\( M_i \)) will be sent through separators and converted to volume production rate (\( \text{scf/day} \) for gas and \( \text{STB/day} \) for oil). Formation volume factor is the ratio of volume of 1 \( \text{lbmol} \) of fluid at reservoir condition to the volume of 1 \( \text{lbmol} \) of fluid at surface condition. By performing flash calculations of well stream compositions at surface condition, formation volume factor for phase \( j \) can be calculated using Eq. (B.37).

\[ B_j = \frac{\tilde{\rho}_{j,sc}}{\tilde{\rho}_j} \quad \text{(B.37)} \]
Appendix C

Analytical Differentiation

This appendix includes the analytical derivatives of conservation equations and phase equilibrium constraints.

C.1 Derivatives of Hydrocarbon Conservation Equations

C.1.1 Transport Terms

Derivatives for transport terms in two-dimensional flow are shown in this section.

C.1.1.1 Derivative with respect to $P_o$

\[
\frac{\partial (\text{Transport})}{\partial P_o} \bigg|_{t_{x}} = \left[ x_i \frac{A_k x k_{ro}}{\Delta x} \frac{\partial \tilde{P}_o}{\partial P_o} \bigg|_{t_{x}} \frac{1}{2} \left( P_o \bigg|_{t_{x+1}} - P_o \bigg|_{t_{x}} \right) + x_i \tilde{\rho}_o \frac{k_{ro}}{\mu_o} \frac{\partial}{\partial P_o} \bigg|_{t_{x}} \frac{A_k x}{\Delta x} \right] \left( P_o \bigg|_{t_{x+1}} - P_o \bigg|_{t_{x}} \right) \\
+ x_i \tilde{\rho}_o k_{ro} A_k x \frac{\partial}{\partial P_o} \bigg|_{t_{x}} \frac{1}{2} \left( P_o \bigg|_{t_{x+1}} - P_o \bigg|_{t_{x}} \right) - x_i \tilde{\rho}_o \frac{A_k x k_{ro}}{\Delta x} \mu_o \\
- \left[ x_i \frac{A_k x k_{ro}}{\Delta x} \frac{\partial \tilde{P}_o}{\partial P_o} \bigg|_{t_{x}} \frac{1}{2} \left( P_o \bigg|_{t_{x-1}} - P_o \bigg|_{t_{x}} \right) + x_i \tilde{\rho}_o \frac{k_{ro}}{\mu_o} \frac{\partial}{\partial P_o} \bigg|_{t_{x}} \frac{A_k x}{\Delta x} \right] \left( P_o \bigg|_{t_{x-1}} - P_o \bigg|_{t_{x}} \right) \\
+ x_i \tilde{\rho}_o k_{ro} A_k x \frac{\partial}{\partial P_o} \bigg|_{t_{x}} \frac{1}{2} \left( P_o \bigg|_{t_{x-1}} - P_o \bigg|_{t_{x}} \right) + x_i \tilde{\rho}_o \frac{A_k x k_{ro}}{\Delta x} \mu_o \right] + ... 
\]
\[
... + \left[ y_i \frac{A k_x}{\Delta x} \frac{\partial \tilde{\rho}_g}{\partial P_{\alpha}} \left|_{x_{1/2}} \right. \left( P_{x_{xx}} - P_{x_{xxk}} \right) + y_i \tilde{\rho}_g \frac{k_{rg}}{\mu_g} \frac{\partial}{\Delta x} \left( \frac{A k_x}{\Delta x} \right) \left|_{x_{1/2}} \right. \left( P_{x_{xx}} - P_{x_{xxk}} \right) \right] \\
+ y_i \tilde{\rho}_g \frac{k_{rg}}{\Delta x} \frac{\partial}{\partial P_{\alpha}} \left( \frac{1}{\mu_{g_{x/2}}} \right) \left( P_{x_{xx}} - P_{x_{xxk}} \right) \\
- y_i \tilde{\rho}_g \frac{k_{rg}}{\Delta x} \frac{\partial}{\partial P_{\alpha}} \left( \frac{1}{\mu_{g_{x/2}}} \right) \left( P_{x_{xxk}} - P_{x_{xx-1}} \right) + y_i \tilde{\rho}_g \frac{A k_x}{\Delta x} \frac{\partial}{\partial P_{\alpha}} \left( \frac{1}{\mu_{g_{x/2}}} \right) \left( P_{x_{xxk}} - P_{x_{xx-1}} \right) + y_i \tilde{\rho}_g \frac{A k_x}{\Delta x} \frac{\partial}{\partial P_{\alpha}} \left( \frac{1}{\mu_{g_{x/2}}} \right) \left( P_{x_{xxk}} - P_{x_{xx-1}} \right) \\
\]
\[
\left\{ \begin{array}{l}
y_i \frac{1}{144} g A^k \rho_s k_{ng} \left( \frac{\partial}{\partial P} \right)_{H \frac{1}{2}} \left( G_{k+1} - G_k \right) \\
y_i \frac{1}{144} g A^k \rho_s k_{ng} \left( \frac{\partial}{\partial P} \right)_{H \frac{1}{2}} \left( G_{k+1} - G_k \right) \\
y_i \frac{1}{144} g A^k \rho_s k_{ng} \left( \frac{\partial}{\partial P} \right)_{H \frac{1}{2}} \left( G_{k+1} - G_k \right) \\
+ y_i \rho_s k_{ng} \left( \frac{1}{144} g A^k \right) \Delta x \left( \frac{\partial}{\partial P} \right)_{H \frac{1}{2}} \left( G_{k+1} - G_k \right) \\
\end{array} \right.
\]

The derivative of the constant part of the transmissibility is shown in Eq. (C.2)

\[
\frac{\partial}{\partial P} \left( A^k \right) \left( \frac{\partial}{\partial \Delta x} \right)_{H \frac{1}{2}} = \frac{\partial}{\partial P} \left( \frac{2A_{s1}A_{s2}k_{s1}k_{s2}}{A_{s1}k_{s1}\Delta x_2 + A_{s2}k_{s2}\Delta x_1} \right) \\
= \left( \frac{2A_{s1}A_{s2}k_{s1}^2k_{s2}^2\Delta x_1}{(A_{s1}k_{s1}\Delta x_2 + A_{s2}k_{s2}\Delta x_1)^2} \right) \frac{\partial k_{s1}}{\partial P},
\]
C.1.1.2 Derivative with respect to $S_o$

$$\frac{\partial (\text{Transport})}{\partial S_{o}^{\text{it}}} = x_i A k_s \tilde{p}_o \frac{\partial k_{ro}}{\Delta x} \frac{1}{\Delta x} \left( P_{o_{it}} - P_{o_{it-1}} \right) - x_i A k_s \tilde{p}_o \frac{\partial k_{ro}}{\Delta x} \frac{1}{\Delta x} \left( P_{o_{it}} - P_{o_{it-1}} \right)$$

$$+ \left\{ \begin{array}{l} x_i \frac{g}{144} A k_s \rho_o \tilde{p}_o k_{ro} \frac{\partial k_{ro}}{\Delta x} \frac{1}{\Delta x} \left( G_{o_{it+1}} - G_{o_{it}} \right) \\ - x_i \frac{g}{144} A k_s \rho_o \tilde{p}_o k_{ro} \frac{\partial k_{ro}}{\Delta x} \frac{1}{\Delta x} \left( G_{o_{it}} - G_{o_{it-1}} \right) \end{array} \right\}$$

\hspace{1cm} (C.3)

C.1.1.3 Derivative with respect to $S_g$

$$\frac{\partial (\text{Transport})}{\partial S_{g}^{\text{it}}} = y_i A k_s \tilde{p}_g \frac{\partial k_{rg}}{\Delta x} \frac{1}{\Delta x} \left( P_{g_{it+1}} - P_{g_{it}} \right) - y_i A k_s \tilde{p}_g \frac{\partial k_{rg}}{\Delta x} \frac{1}{\Delta x} \left( P_{g_{it}} - P_{g_{it-1}} \right)$$

$$+ y_i \frac{A k_s \tilde{p}_g}{5.615 \Delta x} \frac{\partial (\phi S_g)}{\Delta x} \left( P_{g_{it}} - P_{g_{it-1}} \right)$$

$$+ \left\{ \begin{array}{l} y_i \frac{D_{off} A_s}{5.615 \Delta x} \frac{\partial (\phi S_g)}{\Delta x} \left( y_i \tilde{p}_g - y_i \tilde{p}_g \right) \\ - y_i \frac{D_{off} A_s}{5.615 \Delta x} \frac{\partial (\phi S_g)}{\Delta x} \left( y_i \tilde{p}_g - y_i \tilde{p}_g \right) \end{array} \right\}$$

\hspace{1cm} (C.4)
C.1.1.4 Derivative with respect to $x_j$

\[
\frac{\partial (\text{Transport})}{\partial x_j} = \left[ \frac{A k_s}{\Delta x} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu}\right) \left( P_{o, k+1} - P_{o, k} \right) \right] + \frac{A k_s}{\Delta x} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_{o, k+1/2}} \right) \left( P_{o, k+1} - P_{o, k} \right)
\]

\[
+ \frac{A k_s}{\Delta x} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_{o, k-1/2}} \right) \left( P_{o, k} - P_{o, k-1} \right)
\]

\[
- \frac{1}{144 g_c} \frac{A k_s}{\Delta x} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_{o, k+1/2}} \right) \left( G_{x, k+1} - G_{x, k} \right) + \frac{1}{144 g_c} \frac{A k_s}{\Delta x} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_{o, k-1/2}} \right) \left( G_{x, k} - G_{x, k-1} \right)
\]

\[
+ \frac{1}{144 g_c} \frac{A k_s}{\Delta x} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_{o, k+1/2}} \right) \left( G_{x, k+1} - G_{x, k} \right)
\]

\[
+ \frac{1}{144 g_c} \frac{A k_s}{\Delta x} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_{o, k-1/2}} \right) \left( G_{x, k} - G_{x, k-1} \right)
\]

\[
\text{(C.5)}
\]
\[
\frac{\partial (\text{Transport})}{\partial y_j} = \left[ A_k \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) + y_i A_k \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) \right] + \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) + \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) \\
- \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) + \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) \\
+ \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) + \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) \\
+ \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) + \frac{\partial \tilde{\rho}_g k_{rg}}{\partial y_j} \left( \frac{1}{\mu_g} \left( P_{g_{k+1}} - P_{g_{k}} \right) \right) \\
\right]
\]
C.1.2 Accumulation Term

C.1.2.1 Derivative with respect to $P_o$

\[
\frac{\partial (\text{Accumulation})}{\partial P_o} = \frac{\partial}{\partial P_o} \left[ \frac{V_b}{5.615 \Delta t} \left( \phi S_o x_i \tilde{P}_o + \phi S_g y_i \tilde{P}_g \right)_{t_k}^{n+1} - \left( \phi S_o x_i \tilde{P}_o + \phi S_g y_i \tilde{P}_g \right)_{t_k}^n \right]
\]

\[
= \frac{V_b}{5.615 \Delta t} \left( \phi S_o x_i \frac{\partial \tilde{P}_o}{\partial P_o} \bigg|_{t_k} + \tilde{P}_o S_o x_i \frac{\partial \phi}{\partial \tilde{P}_o} \bigg|_{t_k} + \phi S_g y_i \frac{\partial \tilde{P}_g}{\partial P_o} \bigg|_{t_k} + \tilde{P}_g S_g y_i \frac{\partial \phi}{\partial \tilde{P}_g} \bigg|_{t_k} \right)_{t_k}^{n+1}
\]

(C.7)

C.1.2.2 Derivative with respect to $S_o$

\[
\frac{\partial (\text{Accumulation})}{\partial S_o} = \frac{V_b}{5.615 \Delta t} \left( \phi \tilde{P}_o x_i \right)_{t_k}^{n+1}
\]

(C.8)

C.1.2.3 Derivative with respect to $S_g$

\[
\frac{\partial (\text{Accumulation})}{\partial S_g} = \frac{V_b}{5.615 \Delta t} \left( \phi \tilde{P}_g y_i \right)_{t_k}^{n+1}
\]

(C.9)

C.1.2.4 Derivative with respect to $x_j$

\[
\frac{\partial (\text{Accumulation})}{\partial x_j} = \frac{V_b}{5.615 \Delta t} \left( \phi S_o \tilde{P}_o \frac{\partial x_i}{\partial x_j} \bigg|_{t_k} + \phi S_g y_i \frac{\partial \tilde{P}_g}{\partial x_j} \bigg|_{t_k} \right)_{t_k}^{n+1}
\]

(C.10)
C.1.2.5 Derivative with respect to $y_j$

\[
\frac{\partial (\text{Accumulation})}{\partial y_j} = \frac{V_b}{5.615\Delta t} \left( \phi S_g \tilde{\rho}_g \frac{\partial y_j}{\partial y_j} + \phi S_g y_i \frac{\partial \tilde{\rho}_g}{\partial y_j} \right)_{x}^{n+1}
\]  

(C.11)

C.1.3 Source/Sink Term

C.1.3.1 Derivative with respect to $P_o$

\[
\frac{\partial (\text{Source})}{\partial P_o} = 
\begin{align*}
-x_i \tilde{\rho}_o \frac{k_{ro}}{\mu_o} & \left[ \frac{2\pi \tilde{k} h}{\ln \left( \frac{r_e}{r_w} + S \right)} \right] \left( P_o \bigg|_{x} - P_{wf} \right) - x_i \tilde{\rho}_o k_{ro} \frac{\partial}{\partial P_o} \left( \frac{1}{\mu_o} \right)_{x}^{\frac{1}{2}} \ln \left( \frac{r_e}{r_w} + S \right) \\
-x_i \tilde{\rho}_o \frac{2\pi \tilde{k} h}{\ln \left( \frac{r_e}{r_w} + S \right)} \left( P_o \bigg|_{x} - P_{wf} \right) - x_i \tilde{\rho}_o k_{ro} \frac{2\pi \tilde{k} h}{\ln \left( \frac{r_e}{r_w} + S \right)} \\
-y_i \tilde{\rho}_g \frac{k_{rg}}{\mu_g} & \left[ \frac{2\pi \tilde{k} h}{\ln \left( \frac{r_e}{r_w} + S \right)} \right] \left( P_o \bigg|_{x} - P_{wf} \right) - y_i \tilde{\rho}_g k_{rg} \frac{\partial}{\partial P_o} \left( \frac{1}{\mu_{g}} \right)_{x}^{\frac{1}{2}} \ln \left( \frac{r_e}{r_w} + S \right) \\
-y_i \tilde{\rho}_g \frac{2\pi \tilde{k} h}{\ln \left( \frac{r_e}{r_w} + S \right)} \left( P_o \bigg|_{x} - P_{wf} \right) - y_i \tilde{\rho}_g k_{rg} \frac{2\pi \tilde{k} h}{\ln \left( \frac{r_e}{r_w} + S \right)}
\end{align*}
\]  

(C.12)

C.1.3.2 Derivative with respect to $S_o$

\[
\frac{\partial (\text{Source})}{\partial S_o} = -x_i \tilde{\rho}_o \frac{k_{ro}}{\mu_o} \frac{2\pi \tilde{k} h}{\ln \left( \frac{r_e}{r_w} + S \right)} \left( P_o \bigg|_{x} - P_{wf} \right) 
\]  

(C.13)
C.1.3.3 Derivative with respect to $S_g$

\[
\frac{\partial (Source)}{\partial S_g |_x} = -\frac{x_i \bar{\rho}_g}{\mu_o} \frac{\partial k_{ro}}{\partial S_g |_x} \ln \left( \frac{r_c}{r_w} + S \right) (P_o |_x - P_{wf}) - \frac{2 \pi \bar{k} \bar{h}}{\mu_g} \frac{\partial k_{ro}}{\partial S_g |_x} \ln \left( \frac{r_c}{r_w} + S \right) (P_s |_x - P_{wf})
\]

C.1.3.4 Derivative with respect to $x_j$

\[
\frac{\partial (Source)}{\partial x_j |_x} = -\frac{\partial x_i |_x}{\partial x_j |_x} \frac{\partial k_{ro}}{\partial x_j |_x} \frac{2 \pi \bar{k} \bar{h}}{\mu_o} \ln \left( \frac{r_c}{r_w} + S \right) (P_o |_x - P_{wf}) - \frac{x_i \bar{\rho}_o}{\mu_o} \frac{\partial k_{ro}}{\partial x_j |_x} \frac{2 \pi \bar{k} \bar{h}}{\mu_g} \ln \left( \frac{r_c}{r_w} + S \right) (P_s |_x - P_{wf})
\]

C.1.3.5 Derivative with respect to $y_j$

\[
\frac{\partial (Source)}{\partial y_j |_x} = -\frac{\partial y_i |_x}{\partial y_j |_x} \frac{\partial k_{rg}}{\partial y_j |_x} \frac{2 \pi \bar{k} \bar{h}}{\mu_s} \ln \left( \frac{r_c}{r_w} + S \right) (P_o |_x - P_{wf}) - \frac{y_i \bar{\rho}_g}{\mu_s} \frac{\partial k_{rg}}{\partial y_j |_x} \frac{2 \pi \bar{k} \bar{h}}{\mu_g} \ln \left( \frac{r_c}{r_w} + S \right) (P_s |_x - P_{wf})
\]
C.1.3.6 Bottom-hole Pressure Specification $P_{wf}$

$$\frac{\partial \lambda_{total}}{\partial P_o} = -k_{ro} \frac{\partial \mu_o}{\partial P_o} - k_{rg} \frac{\partial \mu_g}{\partial P_o} - k_{rw} \frac{\partial \mu_w}{\partial P_o} \tag{C.17}$$

C.1.3.7 Total Reservoir Fluid Withdrawal Rate $q_t$

Total reservoir fluid withdrawal is defined as:

$$q_t = -\frac{kk_{ro}}{\mu_o} (P_o - P_{wf}) - \frac{kk_{rg}}{\mu_g} (P_g - P_{wf}) - \frac{kk_{rw}}{\mu_w} (P_w - P_{wf}) \tag{C.18}$$

Rearranging Eq. (C.18) for $P_{wf}$,

$$P_{wf} = \frac{-\frac{\Omega k_{ro}}{\mu_o} P_o + \frac{\Omega k_{rg}}{\mu_g} P_g + \frac{\Omega k_{rw}}{\mu_w} P_w + q_t}{\frac{\Omega k_{ro}}{\mu_o} + \frac{\Omega k_{rg}}{\mu_g} + \frac{\Omega k_{rw}}{\mu_w}} \tag{C.19}$$

Let $U$ and $L$ be the numerator and denominator of Eq. (C.19). Recall well source term for hydrocarbon component.

$$M_i = -x_i \tilde{\rho}_o \frac{kk_{ro}}{\mu_o} \Omega (P_o - P_{wf}) - y_i \tilde{\rho}_g \frac{kk_{rg}}{\mu_g} \Omega (P_g - P_{wf}) \tag{C.20}$$

Let $X$ be principal unknown. The derivative of hydrocarbon source term with respect to principal unknowns can be derived.

$$\frac{\partial M_i}{\partial X} = -x_i \tilde{\rho}_o \frac{kk_{ro}}{\mu_o} \frac{\partial \Omega}{\partial X} (P_o - P_{wf}) - \frac{\partial}{\partial X} \left( x_i \tilde{\rho}_o \frac{kk_{ro}}{\mu_o} \Omega \right)$$

$$- y_i \tilde{\rho}_g \frac{kk_{rg}}{\mu_g} \frac{\partial \Omega}{\partial X} (P_g - P_{wf}) - \frac{\partial}{\partial X} \left( y_i \tilde{\rho}_g \frac{kk_{rg}}{\mu_g} \Omega \right) \tag{C.21}$$
Only derivatives of $P_{of}$ with respect to principal unknowns must be calculated and they are derived as follows.

**Derivative with respect to $P_o$**

\[
\frac{\partial P_{of}}{\partial P_o} = \left( \Omega \frac{kk_{ro}}{\mu_o} P_o + \Omega \frac{kk_{rg}}{\mu_g} P_g + \Omega \frac{kk_{rw}}{\mu_w} P_w + q_i \right) - \left( \Omega \frac{kk_{ro}}{\mu_o} P_o + \Omega \frac{kk_{rg}}{\mu_g} P_g + \Omega \frac{kk_{rw}}{\mu_w} P_w + q_i \right) \cdot \frac{\partial}{\partial P_o} \left( \Omega \frac{kk_{ro}}{\mu_o} P_o + \Omega \frac{kk_{rg}}{\mu_g} P_g + \Omega \frac{kk_{rw}}{\mu_w} P_w + q_i \right) - \left( \Omega \frac{kk_{ro}}{\mu_o} + \Omega \frac{kk_{rg}}{\mu_g} + \Omega \frac{kk_{rw}}{\mu_w} \right)^2 \cdot \frac{\partial}{\partial P_o} \left( \Omega \frac{kk_{ro}}{\mu_o} + \Omega \frac{kk_{rg}}{\mu_g} + \Omega \frac{kk_{rw}}{\mu_w} \right)
\]

where

\[
\frac{\partial}{\partial P_o} \left( \Omega \frac{kk_{ro}}{\mu_o} P_o + \Omega \frac{kk_{rg}}{\mu_g} P_g + \Omega \frac{kk_{rw}}{\mu_w} P_w + q_i \right) = \Omega \frac{\partial k_{ro}}{\partial P_o} \frac{1}{\mu_o} P_o + \Omega \frac{\partial k_{rg}}{\partial P_o} \frac{1}{\mu_g} P_g + \Omega \frac{\partial k_{rw}}{\partial P_o} \frac{1}{\mu_w} P_w
\]

\[
\frac{\partial}{\partial P_o} \left( \Omega \frac{kk_{ro}}{\mu_o} + \Omega \frac{kk_{rg}}{\mu_g} + \Omega \frac{kk_{rw}}{\mu_w} \right) = \Omega \frac{\partial k_{ro}}{\partial P_o} \frac{1}{\mu_o} + \Omega \frac{\partial k_{rg}}{\partial P_o} \frac{1}{\mu_g} + \Omega \frac{\partial k_{rw}}{\partial P_o} \frac{1}{\mu_w}
\]

**Derivative with respect to $S_o$**

\[
\frac{\partial P_{of}}{\partial S_o} = \frac{L \frac{\partial U}{\partial S_o} - U \frac{\partial L}{\partial S_o}}{L^2}
\]

where

\[
\frac{\partial U}{\partial S_o} = \Omega \frac{K P_o}{\mu_o} \frac{\partial k_{ro}}{\partial S_o} + \Omega \frac{K P_g}{\mu_g} \frac{\partial k_{rg}}{\partial S_o} + \Omega \frac{K P_w}{\mu_w} \frac{\partial k_{rw}}{\partial S_o}
\]
\[ \frac{\partial L}{\partial S_a} = \Omega \frac{k}{\mu_a} \frac{\partial k_{ro}}{\partial S_a} + \Omega \frac{k}{\mu_w} \frac{\partial k_{rw}}{\partial S_a} \]  
(C.27)

Derivative with respect to \( S_g \)

\[ \frac{\partial P_{wf}}{\partial S_g} = \frac{L \frac{\partial U}{\partial S_g} - U \frac{\partial L}{\partial S_g}}{L^2} \]  
(C.28)

where

\[ \frac{\partial U}{\partial S_g} = \Omega \frac{k P_o}{\mu_o} \frac{\partial k_{ro}}{\partial S_g} + \Omega \frac{k P_g}{\mu_g} \frac{\partial k_{rg}}{\partial S_g} + \Omega \frac{k k_x}{\mu_g} \frac{\partial P}{\partial S_g} + \Omega \frac{k P_w}{\mu_w} \frac{\partial k_{rw}}{\partial S_g} + \Omega \frac{k k_w}{\mu_w} \frac{\partial P_w}{\partial S_g} \]  
(C.29)

\[ \frac{\partial L}{\partial S_g} = \Omega \frac{k}{\mu_o} \frac{\partial k_{ro}}{\partial S_g} + \Omega \frac{k}{\mu_g} \frac{\partial k_{rg}}{\partial S_g} + \Omega \frac{k}{\mu_w} \frac{\partial k_{rw}}{\partial S_g} \]  
(C.30)

Derivative with respect to \( x_i \)

\[ \frac{\partial P_{wf}}{\partial x_j} = \frac{L \Omega k_{ro} P_o \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_o} \right) - U \Omega k_{ro} \frac{\partial}{\partial x_j} \left( \frac{1}{\mu_o} \right)}{L^2} \]  
(C.31)

Derivative with respect to \( y_i \)

\[ \frac{\partial P_{wf}}{\partial y_j} = \frac{L \Omega k_{rg} P_g \frac{\partial}{\partial y_j} \left( \frac{1}{\mu_g} \right) - U \Omega k_{rg} \frac{\partial}{\partial y_j} \left( \frac{1}{\mu_g} \right)}{L^2} \]  
(C.32)

**C.1.3.8 Injection**

Derivative with respect to \( S_o \)

\[ \frac{\partial P_w}{\partial S_o} = \frac{\partial}{\partial S_o} \left( P_o - P_{con} \right) = - \frac{\partial P_{con}}{\partial S_o} \]  
(C.33)
\[
\frac{\partial k_{ro}}{\partial S_o} = \left( k_{rg} + k_{rog} \right) \frac{\partial k_{row}}{\partial S_o} + \left( k_{rg} + k_{rog} - 1 \right) \frac{\partial k_{rw}}{\partial S_o} \tag{C.34}
\]

\[
\frac{\partial \lambda_{total}}{\partial S_o} = \frac{1}{\mu_o} \frac{\partial k_{ro}}{\partial S_o} + \frac{1}{\mu_w} \frac{\partial k_{rw}}{\partial S_o} \tag{C.35}
\]

Derivative with respect to \( S_g \)

\[
\frac{\partial \lambda_{total}}{\partial S_g} = \frac{1}{\mu_o} \frac{\partial k_{ro}}{\partial S_g} + \frac{1}{\mu_g} \frac{\partial k_{rg}}{\partial S_g} + \frac{1}{\mu_w} \frac{\partial k_{rw}}{\partial S_g} \tag{C.36}
\]

Derivative with respect to \( x_i \)

\[
\frac{\partial \lambda_{total}}{\partial x_i} = -\frac{k_{ro}}{\mu_o} \frac{\partial \mu_o}{\partial x_i} \tag{C.37}
\]

Derivative with respect to \( y_i \)

\[
\frac{\partial \lambda_{total}}{\partial y_i} = -\frac{k_{rg}}{\mu_g} \frac{\partial \mu_g}{\partial y_i} \tag{C.38}
\]

C.2 Derivative of Water Conservation Equation

C.2.1 Transport Terms

C.2.1.1 Derivative with respect to \( P_o \)

\[
\left. \frac{\partial (Transport)}{\partial P_o} \right|_{kx} = \left[ \frac{\partial}{\partial P_{ox}} \left( \frac{A_{k} k_{w}}{Ax} \right) \right]_{kx+1} \frac{k_{rw}}{\mu_{w} B_{w}} \left( P_{w} \right|_{kx+1} - \left. P_{w} \right|_{kx} ) + \frac{A_{k} k_{w}}{Ax} \frac{k_{rw}}{\mu_{w} B_{w}} \left[ \frac{1}{\mu_{w} B_{w} \frac{1}{2}} \left( P_{w} \right|_{kx+1} - \left. P_{w} \right|_{kx} \right) + \ldots \right]
\]
\[
\frac{\partial}{\partial P_{o,x}} \left( A k_s \right) \frac{k_{w,x}}{\mu_B \Delta x} (P_{w,x} - P_{w,x-1}) + A k_s \frac{k_{w,x}}{\mu_B \Delta x} \frac{\partial}{\partial P_{o,x}} \left( \frac{1}{B_{w,x-1}^{1/2}} \right) (P_{w,x} - P_{w,x-1})
\]

\[
+ A k_s \frac{k_{w,x}}{\mu_B \Delta x} \frac{\partial}{\partial P_{o,x}} \left( \frac{1}{B_{w,x-1}^{1/2}} \right) (P_{w,x} - P_{w,x-1}) + A k_s \frac{k_{w,x}}{\mu_B \Delta x} \frac{\partial}{\partial P_{o,x}} \left( \frac{1}{B_{w,x-1}^{1/2}} \right) (P_{w,x} - P_{w,x-1})
\]

\[
- \left\{ \frac{1}{144 g_c} \frac{\rho_w k_{w,x}}{\mu_B \Delta x} \frac{\partial}{\partial P_{o,x}} \left( A k_s \Delta x \right) \left( G(x) - G(x-1) \right) + \frac{1}{144 g_c} \frac{A k_s k_{w,x}}{\mu_B \Delta x} \frac{\partial}{\partial P_{o,x}} \left( A k_s \Delta x \right) \left( G(x) - G(x-1) \right) \right\}
\]

\[
+ \left\{ \frac{1}{144 g_c} \frac{\rho_w k_{w,x}}{\mu_B \Delta x} \frac{\partial}{\partial P_{o,x}} \left( A k_s \Delta x \right) \left( G(x) - G(x-1) \right) + \frac{1}{144 g_c} \frac{A k_s k_{w,x}}{\mu_B \Delta x} \frac{\partial}{\partial P_{o,x}} \left( A k_s \Delta x \right) \left( G(x) - G(x-1) \right) \right\}
\]

\[
(39)
\]

### C.2.1.2 Derivative with respect to \( S_o \)

\[
\frac{\partial \text{(Transport)}}{\partial S_{o,x}} = \left[ \frac{A k_s}{\Delta x} \frac{\partial k_{w,x}}{\partial S_{o,x}} \frac{1}{\mu_B} \left( P_{w,x} - P_{w,x-1} \right) \right] - \left[ \frac{A k_s}{\Delta x} \frac{\partial k_{w,x}}{\partial S_{o,x}} \frac{1}{\mu_B} \left( P_{w,x} - P_{w,x-1} \right) \right]
\]

\[
- \left\{ \frac{1}{144 g_c} \frac{\rho_w k_{w,x}}{\mu_B \Delta x} \frac{\partial k_{w,x}}{\partial S_{o,x}} \left( G(x) - G(x-1) \right) \right\}
\]

\[
(40)
\]
C.2.1.3 Derivative with respect to $S_g$

\[
\frac{\partial (\text{Transport})}{\partial S_{g|x}} = \left[ \frac{A_{k_x}}{\Delta x} \left( \frac{1}{\mu_r B_w} \frac{\partial k_{rw|1+1}}{\partial S_{g|x}} \right) \left( P_{w|x} - P_{w|1} \right) - \frac{A_{k_x} k_{rw}}{\Delta x} \frac{\partial P_{w|1}}{\partial S_{g|x}} \right]
\]

\[
- \left[ \frac{A_{k_x}}{\Delta x} \left( \frac{1}{\mu_r B_w} \frac{\partial k_{rw|1+1}}{\partial S_{g|x}} \right) \left( P_{w|x} - P_{w|1} \right) + \frac{A_{k_x} k_{rw}}{\Delta x} \frac{\partial P_{w|1}}{\partial S_{g|x}} \right]
\]

\[
- \left\{ \frac{1}{144 \Delta x} \frac{g}{\mu_r B_w} \frac{\partial k_{rw|1+1}}{\partial S_{g|x}} \left( G_{x+1} - G_x \right) \right\} + \left\{ \frac{1}{144 \Delta x} \frac{g}{\mu_r B_w} \frac{\partial k_{rw|1+1}}{\partial S_{g|x}} \left( G_x - G_{x-1} \right) \right\} \quad (C.41)
\]

C.2.2 Accumulation Term

C.2.2.1 Derivative with respect to $P_o$

\[
\frac{\partial (\text{Accumulation})}{\partial P_{o|x}} = \frac{V_b}{5.615 \Delta t} \left[ \left( \frac{S_{w|x} \frac{\partial \phi}{\partial P_{o|x}} - \phi S_{w|x} \frac{\partial B_{w|x}}{\partial P_{o|x}}}{B_{w|x} \frac{\partial P_{o|x}}{\partial P_{o|x}}} \right) \right]^{n+1} \quad (C.42)
\]

C.2.2.2 Derivative with respect to $S_o$

\[
\frac{\partial (\text{Accumulation})}{\partial S_{o|x}} = \frac{V_b}{5.615 \Delta t} \left[ \left( \frac{-\phi}{B_{w|x}} \right) \right]^{n+1} \quad (C.43)
\]

C.2.2.3 Derivative with respect to $S_g$

\[
\frac{\partial (\text{Accumulation})}{\partial S_{g|x}} = \frac{V_b}{5.615 \Delta t} \left[ \left( \frac{-\phi}{B_{w|x}} \right) \right]^{n+1} \quad (C.44)
\]
C.2.3 Source/Sink Term

### C.2.3.1 Derivative with respect to $P_o$

\[
\frac{\partial (Source)}{\partial P_o} = -\frac{\partial k_{rw}}{\partial P_o} \left( \mu B_w \ln \left( \frac{r_c}{r_w} + S \right) \right) (P_w|_k - P_{wf}) - \frac{\partial}{\partial P_{ow}} \left( \frac{1}{\mu w} \right) B_w \ln \left( \frac{r_c}{r_w} + S \right) (P_w|_k - P_{wf})
\]

\[
+ \frac{\partial}{\partial P_{ow}} \left( \frac{1}{B_{w|k}} \right) 2\pi k_{rw} h \left( \mu B_w \ln \left( \frac{r_c}{r_w} + S \right) \right) (P_w|_k - P_{wf}) - \frac{2\pi k_{rw} h}{\mu w B_w \ln \left( \frac{r_c}{r_w} + S \right)} \frac{\partial P_{w|k}}{\partial S_{o|k}}
\]

(C.45)

### C.2.3.2 Derivative with respect to $S_o$

\[
\frac{\partial (Source)}{\partial S_o} = -\frac{\partial k_{rw}}{\partial S_o} \left( \mu B_w \ln \left( \frac{r_c}{r_w} + S \right) \right) (P_w|_k - P_{wf}) - \frac{2\pi k_{rw} h}{\mu w B_w \ln \left( \frac{r_c}{r_w} + S \right)} \frac{\partial P_{w|k}}{\partial S_{o|k}}
\]

(C.46)

### C.2.3.3 Derivative with respect to $S_g$

\[
\frac{\partial (Source)}{\partial S_g} = -\frac{\partial k_{rw}}{\partial S_g} \left( \mu B_w \ln \left( \frac{r_c}{r_w} + S \right) \right) (P_w|_k - P_{wf}) - \frac{2\pi k_{rw} h}{\mu w B_w \ln \left( \frac{r_c}{r_w} + S \right)} \frac{\partial P_{w|k}}{\partial S_{g|k}}
\]

(C.47)
C.2.3.4 Total Reservoir Fluid Withdrawal Rate \( q_t \)

\[
q_w = -\frac{kk_{rw}}{\mu_w B_w} \left( P_w - P_{wf} \right)
\]  

Let \( X \) be principal unknown. The derivative of hydrocarbon source term with respect to principal unknowns can be derived.

\[
\frac{\partial q_w}{\partial X} = -\frac{kk_{rw}}{\mu_w B_w} \frac{\partial}{\partial X} \left( P_w - P_{wf} \right) - \left( P_w - P_{wf} \right) \frac{\partial}{\partial X} \left( \frac{kk_{rw}}{\mu_w B_w} \right)
\]  

The derivatives \( \frac{\partial q_w}{\partial P_o} \), \( \frac{\partial q_w}{\partial S_o} \), \( \frac{\partial q_w}{\partial S_g} \), \( \frac{\partial q_w}{\partial X_j} \), and \( \frac{\partial q_w}{\partial y_j} \) have been derived.

C.3 Derivatives of Phase Equilibrium Constraints

C.3.1 Derivative with respect to \( P_o \)

\[
\frac{\partial R_f}{\partial P_o} = \frac{\partial \ln f_i^L}{\partial P_o} - \frac{\partial \ln f_i^V}{\partial P_o}
\]  

where
\[
\frac{\partial \ln f^L_i}{\partial p_o} = \frac{1}{P_o} + \frac{B_i}{B_L} \frac{\partial Z_L}{\partial p_o} - \frac{1}{Z_L - B_L} \left( \frac{\partial Z_L}{\partial p_o} - \frac{\partial B_L}{\partial p_o} \right) \\
+ \left( \frac{1}{(m_1 - m_2)B_L} \frac{\partial A_L}{\partial p_o} - \frac{A_L}{(m_1 - m_2)B_L} \frac{\partial B_L}{\partial p_o} \right) \left( \frac{2 \sum_{k=1}^{N_f} A_{i_k} x_{i_k}}{A_L} - \frac{B_i}{B_L} \right) \ln \left( \frac{Z_L + m_i B_L}{Z_L} \right)
\]

\[
+ \frac{A_L}{(m_1 - m_2)B_L} \left( \sum_{k=1}^{N_f} A_{i_k} x_{i_k} \right) \left( \frac{\partial Z_L}{\partial p_o} + \frac{m_i \partial B_L}{\partial p_o} - \frac{\partial Z_L}{\partial p_o} + \frac{m_i \partial B_L}{\partial p_o} \right) \left( \frac{Z_L + m_i B_L}{Z_L} \right)
\]  

(C.51)

and

\[
\frac{\partial \ln f^V_i}{\partial p_o} = \frac{1}{P_o} + \frac{B_i}{B_V} \frac{\partial Z_V}{\partial p_o} - \frac{1}{Z_V - B_V} \left( \frac{\partial Z_V}{\partial p_o} - \frac{\partial B_V}{\partial p_o} \right) \\
+ \left( \frac{1}{(m_1 - m_2)B_V} \frac{\partial A_V}{\partial p_o} - \frac{A_V}{(m_1 - m_2)B_V} \frac{\partial B_V}{\partial p_o} \right) \left( \frac{2 \sum_{k=1}^{N_f} A_{i_k} x_{i_k}}{A_V} - \frac{B_i}{B_V} \right) \ln \left( \frac{Z_V + m_i B_V}{Z_V} \right)
\]

\[
+ \frac{A_V}{(m_1 - m_2)B_V} \left( \sum_{k=1}^{N_f} A_{i_k} x_{i_k} \right) \left( \frac{\partial Z_V}{\partial p_o} + \frac{m_i \partial B_V}{\partial p_o} - \frac{\partial Z_V}{\partial p_o} + \frac{m_i \partial B_V}{\partial p_o} \right) \left( \frac{Z_V + m_i B_V}{Z_V} \right)
\]

(C.52)

C.3.2 Derivative with respect to \( x_i \)

\[
\frac{\partial R^L_{i_k}}{\partial x_j} = \frac{\partial \ln f^L_i}{\partial x_j} = \frac{\partial \ln f^L_i}{\partial x_j} + \frac{\partial \ln x_i}{\partial x_j}
\]

(C.53)

where
\[
\frac{\partial \ln x_i}{\partial x_j} = \begin{cases} 
\frac{1}{x_i} & \text{if } i = j \\
0 & \text{if } i \neq j \text{ and } i \neq N_c \\
-\frac{1}{x_i} & \text{if } i = N_c
\end{cases}
\] (C.54)

and

\[
\frac{\partial \ln \phi_L}{\partial x_j} = \frac{\partial Z_L}{\partial x_j} \frac{B_i}{B_L} - \frac{(Z_L-1) \partial B_L}{B_L} \frac{B_i}{B_L} - \frac{1}{Z_L-B_L} \left( \frac{\partial Z_L}{\partial x_j} \frac{\partial B_L}{\partial x_j} \right) \\
+ \left( \frac{2}{A_L} \frac{\partial \sum_{k=1}^{N_c} A_{ik} x_k}{\partial x_j} - \frac{2}{A_L} \frac{\partial A_i}{\partial x_j} \frac{\partial B_L}{\partial x_j} + \frac{B_i}{B_L} \frac{\partial B_L}{\partial x_j} \right) \\
+ \frac{A_i}{(m_1-m_2)B_L} \left( \frac{\partial Z_L}{\partial x_j} \frac{m_2 B_L}{Z_L + m_2 B_L} - \frac{\partial B_L}{\partial x_j} \frac{m_2}{Z_L + m_2 B_L} \right)
\] (C.55)

C.3.3 Derivative with respect to \(y_i\)

\[
\frac{\partial R_P}{\partial y_j} = -\frac{\partial \ln f^V}{\partial y_j} = -\left( \frac{\partial \ln \phi^V}{\partial y_j} + \frac{\partial \ln y_i}{\partial y_j} \right)
\] (C.56)

where
\[
\frac{\partial \ln y_i}{\partial y_j} = \frac{1}{y_i} \frac{\partial y_i}{\partial y_j}, \quad \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j \text{ and } i \neq N_C \\
-1 & \text{if } i = N_C 
\end{cases}
\] (C.57)

and

\[
\frac{\partial \ln \phi^v_i}{\partial y_j} = \frac{\partial Z_v}{\partial y_j} B_i \frac{B_i}{B_v} - \frac{(Z_v - 1) \partial B_v}{B_v} B_i - \frac{1}{Z_v - B_v} \left( \frac{\partial Z_v}{\partial y_j} - \frac{\partial B_v}{\partial y_j} \right) \\
+ \left( \frac{1}{(m_1 - m_2) B_v} \frac{\partial A_v}{\partial y_j} - \frac{A_v}{(m_1 - m_2) B_v^2} \frac{\partial B_v}{\partial y_j} \right) \left( \sum_{k=1}^{N_C} A_{ik} \frac{y_k}{A_v} \right) - \frac{B_i}{B_v} \ln \left( \frac{Z_v + m_2 B_v}{Z_v + m_1 B_v} \right) \\
+ \left( \frac{2 \frac{\partial}{\partial y_j} \sum_{k=1}^{N_C} A_{ik} y_k}{A_v} - \frac{2 \sum_{k=1}^{N_C} A_{ik} y_k}{A_v} \frac{\partial A_v}{\partial y_j} \right) + \frac{B_i}{B_v} \frac{\partial B_v}{\partial y_j} \left( \frac{A_v}{(m_1 - m_2) B_v} \right) - \frac{A_v}{(m_1 - m_2) B_v} \ln \left( \frac{Z_v + m_2 B_v}{Z_v + m_1 B_v} \right) \\
+ \frac{A_v}{(m_1 - m_2) B_v} \left( \sum_{k=1}^{N_C} A_{ik} y_k \right) \left( \frac{\partial Z_v}{\partial y_j} + m_2 \frac{\partial B_v}{\partial y_j} - \frac{\partial Z_v}{\partial y_j} + m_1 \frac{\partial B_v}{\partial y_j} \right) \right) \] (C.58)

### C.4 Derivatives of Effect of Capillary Pressure on Phase Behaviors

Recall Macleod & Sugden correlation for interfacial tension.

\[
P_{\text{cap}} = \frac{2\sigma}{\rho} = \frac{2}{\rho} \left[ \sum_{i=1}^{N_C} \chi_i \left( \tilde{\rho}_g x_i - \tilde{\rho}_h y_i \right) \right]^4 \] (C.59)

When the effect of capillary pressure is taken into phase behavior calculation, we can see that gas phase density is a function of gas phase pressure, and to obtain gas phase pressure, the capillary pressure between gas and oil phases is needed which is calculated from Eq. (C.59). Thus, an
iterative procedure is required to determine the capillary pressure. Using Newton’s method for determining \( P_{cgo} \), we obtain:

\[
P_{cgo}^{k+1} = P_{cgo}^k - \frac{f(P_{cgo}^k)}{f'(P_{cgo}^k)}
\]  

where

\[
f(P_{cgo}) = P_{cgo} - \frac{2}{r} \left[ \sum_{i=1}^{N_c} \chi_i \left( \tilde{\rho}_o x_i - \tilde{\rho}_g y_i \right) \right]^4
\]  

and

\[
f'(P_{cgo}) = 1 - \frac{8}{r} \left[ \sum_{i=1}^{N_c} \chi_i \left( \tilde{\rho}_o x_i - \tilde{\rho}_g y_i \right) \right]^3 \left( \frac{1}{Z_g RT} - \frac{P_s}{Z_g^2 RT} \right)
\]

Note that the superscript \( k \) stands for iteration level.

### C.5 Derivatives of Embedded Discrete Fracture Model

#### C.5.1 NNC Source Term for Hydrocarbon Components

Recall NNC source term for hydrocarbon components:

\[
M_{i}^{\text{nnce}} = \sum_{m=1}^{N_m} \left[ A_m^{\text{nnce}} \sum_{j=1}^{N_p} \frac{k_{mij}^{\text{nnce}}}{\mu_j} \tilde{\rho}_j \alpha_j \left( P_j - \frac{1}{144 \ g_c} \rho_j G \right) - \left( P_j - \frac{1}{144 \ g_c} \rho_j G \right) \right]_{m}^{\text{nnce}}
\]  

For a pair of NNC between matrix and fracture, Eq. (C.63) reduces to:

\[
M_{i}^{\text{nnce}} = \sum_{j=1}^{N_p} \left( \tilde{k}_{ji} \rho_j \alpha_j \frac{A^{\text{nnce}}}{d_{\text{nnce}}} \left[ \left( P_j - \frac{1}{144 \ g_c} \rho_j G \right) - \left( P_j - \frac{1}{144 \ g_c} \rho_j G \right) \right]_{M}^{\text{nnce}} \right)_{F}
\]
\[ \frac{\partial M_{i}^{\text{nnr}}}{\partial P_{o,M}} = \frac{\partial \tilde{\rho}_{o}^{k}}{\partial P_{o,M}}\frac{x_{i}}{\mu_{o}}k_{ro}^{A_{\text{nnr}}} \left[ \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{M} - \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{F} \right] \]

\[ + \frac{\partial \tilde{\rho}_{o}^{k} k_{ro}^{A_{\text{nnr}}}}{\partial P_{o,M}}\frac{x_{i}}{\mu_{o}} d_{\text{nnr}}^{A_{\text{nnr}}} \left[ \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{M} - \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{F} \right] \]

\[ + \frac{\partial}{\partial P_{o,M}} \frac{\partial}{\partial x_{i}} \frac{1}{\mu_{o}} k_{ro}^{A_{\text{nnr}}} \left( \frac{\partial}{\partial P_{o,M}} \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{M} - \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{F} \right) \]

\[ + \frac{\partial}{\partial P_{o,M}} \frac{\partial}{\partial y_{i}} \frac{1}{\mu_{o}} k_{ro}^{A_{\text{nnr}}} \left( \frac{\partial}{\partial P_{o,M}} \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{M} - \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{F} \right) \]

\[ + \frac{\partial}{\partial P_{o,M}} \frac{\partial}{\partial x_{i}} \frac{1}{\mu_{o}} k_{ro}^{A_{\text{nnr}}} \left( \frac{\partial}{\partial P_{o,M}} \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{M} - \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{F} \right) \]

\[ + \frac{\partial}{\partial P_{o,M}} \frac{\partial}{\partial y_{i}} \frac{1}{\mu_{o}} k_{ro}^{A_{\text{nnr}}} \left( \frac{\partial}{\partial P_{o,M}} \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{M} - \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{F} \right) \]

\[ (C.65) \]

\[ \frac{\partial M_{i}^{\text{nnr}}}{\partial S_{o,M}} = \frac{\partial k_{ro}^{A_{\text{nnr}}}}{\partial S_{o,M}} \frac{x_{i}}{\mu_{o}} \frac{\tilde{\rho}_{o}^{k}}{d_{\text{nnr}}^{A_{\text{nnr}}}} \left[ \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{M} - \left( P_{o} - \frac{1}{144} \frac{g}{g_{c}} \rho_{o} G \right)_{F} \right] \]

\[ (C.66) \]
C.5.1.3 Derivative with respect to $S_g$

\[
\frac{\partial M_{i}^{nnc}}{\partial S_{g,M}} = \frac{\partial k_{ro}}{\partial S_{g,M}} x_i \frac{\partial}{\partial x_i} \frac{k_{ro}}{d_{nnc}} A^{nnc} \left[ \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_M - \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_F \right] \\
+ \frac{\partial k_{rg}}{\partial S_{g,M}} y_i \frac{\partial}{\partial y_i} \frac{k_{rg}}{d_{nnc}} A^{nnc} \left[ \left( P_g - \frac{1}{144} \frac{g}{G_c} \rho_s G \right)_M - \left( P_g - \frac{1}{144} \frac{g}{G_c} \rho_s G \right)_F \right] \\
+ \frac{\partial}{\partial S_{g,M}} \frac{\partial}{\partial S_{g,M}} \left[ \left( P_g - \frac{1}{144} \frac{g}{G_c} \rho_s G \right)_M \right] \quad (C.67)
\]

C.5.1.4 Derivative with respect to $x_i$

\[
\frac{\partial M_{i}^{nnc}}{\partial x_{j,M}} = \frac{\partial x_i}{\partial x_{j,M}} \frac{\partial}{\partial x_i} \frac{k_{ro}}{d_{nnc}} A^{nnc} \left[ \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_M - \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_F \right] \\
+ \frac{\partial}{\partial x_{j,M}} \left( \frac{1}{\mu_o} \right) x_i \frac{\partial}{\partial x_i} \frac{k_{ro}}{d_{nnc}} A^{nnc} \left[ \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_M - \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_F \right] \\
+ \frac{\partial}{\partial x_{j,M}} \frac{\partial}{\partial x_{j,M}} \left( \frac{1}{\mu_o} \right) x_i \frac{\partial}{\partial x_i} \frac{k_{ro}}{d_{nnc}} A^{nnc} \left[ \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_M - \left( P_o - \frac{1}{144} \frac{g}{G_c} \rho_o G \right)_F \right] \quad (C.68)
\]
C.5.1.5 Derivative with respect to $y_i$

\[
\frac{\partial M_{i}^{\text{nnc}}}{\partial y_{j,M}} = \frac{\partial y_i}{\partial y_{j,M}} \frac{\bar{p}_g \bar{k}_rg}{\mu_g} \frac{A^{\text{nnc}}}{d^{\text{nnc}}} \left( P_g - \frac{1}{144} g \rho_g G \right)_M - \left( P_g - \frac{1}{144} g \rho_g G \right)_F
\]

\[
+ \frac{\partial \bar{p}_g}{\partial y_{j,M}} y_i \frac{\bar{k}_rg}{\mu_g} \frac{A^{\text{nnc}}}{d^{\text{nnc}}} \left( P_g - \frac{1}{144} g \rho_g G \right)_M - \left( P_g - \frac{1}{144} g \rho_g G \right)_F
\]

\[
+ \frac{\partial}{\partial y_{j,M}} \left( \frac{1}{\mu_g} \right) y_i \frac{\bar{k}_rg}{\mu_g} \frac{A^{\text{nnc}}}{d^{\text{nnc}}} \left( P_g - \frac{1}{144} g \rho_g G \right)_M - \left( P_g - \frac{1}{144} g \rho_g G \right)_F
\]

\[
+ y_i \frac{\bar{k}_rg}{\mu_g} \frac{A^{\text{nnc}}}{d^{\text{nnc}}} \left( - \frac{1}{144} g \frac{\partial \rho_g}{\partial y_{j,M}} G \right)_M
\]

(C.69)

C.5.2 NNC Source Term for Water

Recall NNC source term for water:

\[
M_w = \sum_{m=1}^{N_{\text{nc}}} A^{\text{nnc}}_m \frac{k^{\text{nnc}}_m k^{\text{nnc}}_w}{\mu_w B_w} \left[ \left( P_w - \frac{1}{144} g \rho_w G \right)_M - \left( P_w - \frac{1}{144} g \rho_w G \right)_F \right]^{\text{nnc}}
\]

(C.70)

For a pair of NNC between matrix and fracture, Eq. (C.70) reduces to:

\[
M_w = \frac{\bar{k}_{rw}}{\mu_w B_w} \frac{A^{\text{nnc}}}{d^{\text{nnc}}} \left[ \left( P_w - \frac{1}{144} g \rho_w G \right)_M - \left( P_w - \frac{1}{144} g \rho_w G \right)_F \right]
\]

(C.71)
C.5.2.1 Derivative with respect to $P_o$

\[
\frac{\partial M_w}{\partial P_{o,M}} = \frac{\partial k}{\partial P_{o,M}} \frac{k_{rw}}{\mu_w B_w} \left[ \left( P_w - \frac{1}{144} g_{c} \rho_w G \right) - \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{F} \right] + \frac{\partial}{\partial P_{o,M}} \left( \frac{1}{\mu_w} \frac{k_{rw}}{B_w} A^{nnc} \right) \left[ \left( P_w - \frac{1}{144} g_{c} \rho_w G \right) - \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{F} \right] + \frac{\partial}{\partial P_{o,M}} \left( \frac{k_{rw}}{B_w} A^{nnc} \right) \frac{\partial}{\partial P_{o,M}} \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} + \frac{\partial}{\partial P_{o,M}} \left( \frac{k_{rw}}{B_w} A^{nnc} \right) \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} \quad (C.72)
\]

C.5.2.2 Derivative with respect to $S_o$

\[
\frac{\partial M_w}{\partial S_{o,M}} = \frac{\partial k}{\partial S_{o,M}} \frac{k_{rw}}{\mu_w B_w} \left[ \left( P_w - \frac{1}{144} g_{c} \rho_w G \right) - \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{F} \right] + \frac{\partial}{\partial S_{o,M}} \left( \frac{k_{rw}}{B_w} A^{nnc} \right) \frac{\partial}{\partial S_{o,M}} \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} + \frac{\partial}{\partial S_{o,M}} \left( \frac{k_{rw}}{B_w} A^{nnc} \right) \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} \quad (C.73)
\]

C.5.2.3 Derivative with respect to $S_g$

\[
\frac{\partial M_w}{\partial S_{g,M}} = \frac{\partial k}{\partial S_{g,M}} \frac{k_{rw}}{\mu_w B_w} \left[ \left( P_w - \frac{1}{144} g_{c} \rho_w G \right) - \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{F} \right] + \frac{\partial}{\partial S_{g,M}} \left( \frac{k_{rw}}{B_w} A^{nnc} \right) \frac{\partial}{\partial S_{g,M}} \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} + \frac{\partial}{\partial S_{g,M}} \left( \frac{k_{rw}}{B_w} A^{nnc} \right) \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} \left( P_w - \frac{1}{144} g_{c} \rho_w G \right)_{M} \quad (C.74)
\]
C.5.3 Fracture-Fracture Intersection

Two discrete fracture segments numbered 1 and 2 intersect each other.

\[
\frac{\partial}{\partial P_{o,1}} \left( \frac{k_{nnc}^\text{mnc} A_{nnc}^\text{mnc}}{d_{nnc}^\text{mnc}} \right) = \frac{k_{f1} k_{f2} \omega_{f1} \omega_{f2} L_{\text{int}}}{k_{f1} \omega_{f1} d_{f2} + k_{f2} \omega_{f2} d_{f1}}
\]

(C.75)

Let \( U \) and \( L \) be the numerator and denominator in Eq. (C.75). The derivative with respect to \( P_{o,1} \) is shown in Eq. (C.76).

\[
\frac{\partial}{\partial P_{o,1}} \left( \frac{k_{nnc}^\text{mnc} A_{nnc}^\text{mnc}}{d_{nnc}^\text{mnc}} \right) = \frac{\left( L k_{f2} \omega_{f1} \omega_{f2} L_{\text{int}} - U \omega_{f1} d_{f2} \right)}{L^2} \frac{\partial k_{f1}}{\partial P_{o,1}}
\]

(C.76)

Similarly, the derivative with respect to \( P_{o,2} \) can be derived as follows:

\[
\frac{\partial}{\partial P_{o,2}} \left( \frac{k_{nnc}^\text{mnc} A_{nnc}^\text{mnc}}{d_{nnc}^\text{mnc}} \right) = \frac{\left( L k_{f1} \omega_{f1} \omega_{f2} L_{\text{int}} - U \omega_{f2} d_{f1} \right)}{L^2} \frac{\partial k_{f2}}{\partial P_{o,2}}
\]

(C.77)

C.6 Miscellaneous Derivatives

C.6.1 Permeability

\[
\frac{\partial k_{\text{ave}}}{\partial P_o} = \frac{\partial}{\partial P_o} \sqrt{k_x \cdot k_y} = \frac{1}{2 \sqrt{k_x \cdot k_y}} \frac{\partial}{\partial P_o} (k_x \cdot k_y)
\]

\[
= \frac{1}{2 \sqrt{k_x \cdot k_y}} \left( k_x \frac{\partial k_x}{\partial P_o} + k_y \frac{\partial k_y}{\partial P_o} \right)
\]

(C.78)

C.6.2 Relative Permeability

For water wet reservoir,
\[ k_{ro} = k_{rocw} \left[ \left( \frac{k_{row}}{k_{rocw}} + k_{rw} \right) \left( \frac{k_{rog}}{k_{rocw}} + k_{rg} \right) - \left( k_{rw} + k_{rg} \right) \right] \]  
(C.79)

\[ \frac{\partial k_{ro}}{\partial S_o} = k_{rocw} \left[ \left( \frac{k_{row}}{k_{rocw}} + k_{rw} \right) \left( \frac{1}{k_{rocw}} \frac{\partial k_{rog}}{\partial S_o} + \frac{\partial k_{rog}}{\partial S_g} \right) \right. \]
\[ + \left( \frac{k_{rog}}{k_{rocw}} + k_{rg} \right) \left( \frac{1}{k_{rocw}} \frac{\partial k_{row}}{\partial S_g} + \frac{\partial k_{row}}{\partial S_g} \right) \]  
(C.80)

\[ \frac{\partial k_{ro}}{\partial S_g} = k_{rocw} \left[ \left( \frac{k_{row}}{k_{rocw}} + k_{rw} \right) \frac{\partial k_{rog}}{\partial S_g} + \left( k_{rw} + k_{row} \right) \frac{1}{k_{rocw}} \frac{\partial k_{rog}}{\partial S_g} \right] \]  
(C.81)

Note that if \( k_{ro} = 0 \), the derivative is set to zero.

\[ \frac{\partial k_{ro}}{\partial S_g} = (k_{rw} + k_{row}) \frac{\partial k_{rog}}{\partial S_g} + (k_{rw} + k_{row} - 1) \frac{\partial k_{rg}}{\partial S_g} \]  
(C.82)

C.6.3 Capillary Pressure

\[ \frac{\partial P_w}{\partial S_g} = \frac{\partial}{\partial S_g} (P_o - P_{cow}) = -\frac{\partial P_{cow}}{\partial S_g} \]  
(C.83)

\[ \frac{\partial P_w}{\partial S_o} = \frac{\partial}{\partial S_o} (P_o - P_{cow}) = -\frac{\partial P_{cow}}{\partial S_o} \]  
(C.84)

\[ \frac{\partial P_g}{\partial S_g} = \frac{\partial}{\partial S_g} (P_o + P_{cgo}) = \frac{\partial P_{cgo}}{\partial S_g} \]  
(C.85)
C.6.4 Compressibility of Formation

\[
\frac{\partial \phi}{\partial P_o} = \frac{\partial}{\partial P_o} \left[ \phi^{\circ} \left( 1 + c_{f,\phi} \left( P_o - P_{ref} \right) \right) \right] = \phi^{\circ} c_{f,\phi}
\]  
(C.86)

\[
\frac{\partial k}{\partial P_o} = c_{f,k} k^{\circ} \kappa \left( 1 + c_{f,k} \left( P_o - P_{ref} \right) \right)^{k-1}
\]  
(C.87)

C.6.5 Phase Equilibrium

\[
\frac{\partial A_k}{\partial P_g} = \frac{A_k}{P_g}
\]  
(C.88)

\[
\frac{\partial B_k}{\partial P_g} = \frac{B_k}{P_g}
\]  
(C.89)

\[
\frac{\partial \rho_o}{\partial P_o} = MW_o \frac{\partial \bar{\rho}_o}{\partial P_o}
\]  
(C.90)

\[
\frac{\partial}{\partial x_j} \sum_{k=1}^{N_c} x_k \sqrt{MW_k} = \sqrt{MW_j} - \sqrt{MW_{N_c}}
\]  
(C.91)

\[
\frac{\partial}{\partial x_j} \sum_{k=1}^{N_c} x_k \mu^*_k \sqrt{MW_k} = \mu^*_j \sqrt{MW_j} - \mu^*_N \sqrt{MW_{N_c}}
\]  
(C.92)

\[
\frac{\partial \bar{P}_o}{\partial x_j} = \frac{\partial \left( \bar{P}_o \bar{v}_{pc} \right)}{\partial x_j} = \bar{P}_o \frac{\partial \bar{v}_{pc}}{\partial x_j} + \bar{v}_{pc} \frac{\partial \bar{P}_o}{\partial x_j}
\]  
(C.93)

\[
\frac{\partial}{\partial x_j} \sum_{k=1}^{N_c} x_k T_{c,k} = T_{c,j} - T_{c,N_c}
\]  
(C.94)
\[
\frac{\partial }{\partial x_j} \sum_{k=1}^{N_c} x_k P_{r,k} = P_{c,j} - P_{c,N_c}
\]  
(C.95)

\[
\frac{\partial \bar{\nabla}_{pc}}{\partial x_j} = \frac{\partial }{\partial x_j} \sum_{k=1}^{N_c} x_k \bar{\nabla}_{c,k} = \bar{\nabla}_{c,j} - \bar{\nabla}_{c,N_c}
\]  
(C.96)

\[
\frac{\partial }{\partial x_j} \sum_{k=1}^{N_c} x_k MW_k = MW_j - MW_{N_c}
\]  
(C.97)

\[
\frac{\partial x_i}{\partial x_j} = \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j \text{ & } i \neq N_c \\
-1 & \text{if } i = N_c
\end{cases}
\]  
(C.98)
Appendix D

User Guide

This appendix describes the necessary keyword inputs for PennComp and sample input files with explanations.

D.1 Model Descriptions

MODEL  

`keyword`

Selection of model based on specified keyword. Use keyword `SP` for single-porosity model, keyword `DPSK` for dual-porosity, single-permeability model, and keyword `DPDK` for dual-porosity, dual-permeability model. Default is single-porosity model.

SHAPE  

`keyword`

Constant value used in shape factor for dual-porosity option. Use keyword `WR` for Warren and Root (1963) constant of 20/3, keyword `GK` for Kazemi (1976) constant of 4.

WELLPC  

`number`

Well model for considering capillary pressure. Specify 0 for disable capillary pressure in the well, only oil phase pressure is used in well model for all phases; 1 for enable capillary pressure in the well model. Default is 1.

MTXWELL  

`number`

Matrix-well communication option for dual-porosity model. Specify 0 to disallow matrix to directly communicate with well. Fluid under this option must flow from matrix to natural fracture before it reaches the well. Specify 1 to allow matrix to communicate with well directly. Default is 0.

EOS  

`keyword`


Equation of State selection. Specify keyword PR for Peng-Robinson EoS. SRK for Soave-Relich-Kwong EoS.

**EDFM** \( number \)

Option for modeling fractures with Embedded Discrete Fracture Model. Specify 1 to enable. Require inputs in `input_DF.dat`. Default 0.

**PCPB** \( number \)

Option for modeling phase behavior with capillary pressure. Specify 1 for enable effect of capillary pressure on phase behavior, 0 for disable. Default 0.

**MHF** \( number \)

Option for coefficient for matrix-hydraulic fracture communication in TPTK model. Specify 1 for using user’s input data; 0 for using default option (intersecting area is used normally as specified). If specify 1, require input in `input_DF.dat`.

**NFHF** \( number \)

Option for coefficient for natural fracture-hydraulic fracture communication in TPTK model. Specify 1 for using user’s input data; 0 for using default option (coefficient is equal to natural fracture porosity). If specify 1, require input in `input_DF.dat`.

**D.2 Reservoir Descriptions**

**NX** \( number \)

Number of grid blocks in x-direction (number)

**NY** \( number \)

Number of grid blocks in y-direction (number)

**NZ** \( number \)

Number of grid blocks in z-direction (number)
INDEX,  \textit{keyword}

INDEX_f \textit{number ... number}

... \textit{number ... number}

Grid block index (number). If keyword \textit{CON} is specified, specify one number for all active blocks in the next line. If keyword \textit{VAR} is specified, an array of numbers must be specified in the next line for each grid block in the model.

\textbf{DX}  \textit{keyword}

\textit{number ... number}

Grid dimension in \textit{x}-direction (ft). If keyword \textit{CON} is specified, specify one number for uniform grid block size in the \textit{x}-direction in the next line. If keyword \textit{VAR} is specified, a row of numbers must be specified in the next line for each grid block along the \textit{x}-direction in the model.

\textbf{DY}  \textit{keyword}

\textit{number ... number}

Grid dimension in \textit{y}-direction (ft). If keyword \textit{CON} is specified, specify one number for uniform grid block size in the \textit{y}-direction in the next line. If keyword \textit{VAR} is specified, a row of numbers must be specified in the next line for each grid block along the \textit{y}-direction in the model.

\textbf{DX}  \textit{keyword}

\textit{number ... number}

Grid dimension in \textit{z}-direction (ft). If keyword \textit{CON} is specified, specify one number for uniform grid block size in the \textit{z}-direction in the next line. If keyword \textit{VAR} is specified, a row of numbers must be specified in the next line for each grid block along the \textit{z}-direction in the model.

\textbf{DEPTH,}  \textit{keyword}

\textbf{DEPTH_f}  \textit{number ... number}

Depth from surface to the top of the upper most layer (ft). If keyword \textit{CON} is specified, specify one number for all active blocks in the next line. The model assumes the same depth from surface to every grid block in the top layer. If keyword \textit{VAR} is specified, an array of numbers must be specified in the next line for each grid block in the top layer of the model.
POR,  \textit{keyword}

\texttt{POR\_f} \texttt{number ... number}

... 

\texttt{number ... number}

Porosity (fraction). If keyword \textit{CON} is specified, specify one number for all active blocks in the next line. If keyword \textit{VAR} is specified, an array of numbers must be specified in the next line for each grid block in the model.

\texttt{PERMX, \textit{keyword}}

\texttt{PERMX\_f} \texttt{number ... number}

... 

\texttt{number ... number}

Permeability in \textit{x}-direction (\textit{mD}). If keyword \textit{CON} is specified, specify one number for all active blocks in the next line. If keyword \textit{VAR} is specified, an array of numbers must be specified in the next line for each grid block in the model.

\texttt{PERMY, \textit{keyword}}

\texttt{PERMY\_f} \texttt{number ... number}

... 

\texttt{number ... number}

Permeability in \textit{y}-direction (\textit{mD}). If keyword \textit{CON} is specified, specify one number for all active blocks in the next line. If keyword \textit{VAR} is specified, an array of numbers must be specified in the next line for each grid block in the model.

\texttt{PERMZ, \textit{keyword}}

\texttt{PERMZ\_f} \texttt{number ... number}

... 

\texttt{number ... number}

Permeability in \textit{z}-direction (\textit{mD}). If keyword \textit{CON} is specified, specify one number for all active blocks in the next line. If keyword \textit{VAR} is specified, an array of numbers must be specified in the next line for each grid block in the model.

\texttt{DIFRAC \textit{keyword}}
number ... number

... number ... number

Dimension of matrix block in the $x$-direction ($\text{ft}$). If keyword $\text{CON}$ is specified, specify one number for all active blocks in the next line. If keyword $\text{VAR}$ is specified, an array of numbers must be specified in the next line for each grid block in the model.

**DJFRAC**

$\text{keyword}$

number ... number

...  number ... number

Dimension of matrix block in the $y$-direction ($\text{ft}$). If keyword $\text{CON}$ is specified, specify one number for all active blocks in the next line. If keyword $\text{VAR}$ is specified, an array of numbers must be specified in the next line for each grid block in the model.

**DKFRAC**

$\text{keyword}$

number ... number

...  number ... number

Dimension of matrix block in the $z$-direction ($\text{ft}$). If keyword $\text{CON}$ is specified, specify one number for all active blocks in the next line. If keyword $\text{VAR}$ is specified, an array of numbers must be specified in the next line for each grid block in the model.

**CPOR**

$\text{number}$

Compressibility of formation on porosity ($1/\text{psia}$). Default 0.

**PRPOR**

$\text{number}$

Reference pressure for compressibility of formation on porosity ($\text{psia}$). Required of $\text{CPOR}$ is specified.

**CPERM**

$\text{number}$
Compressibility of formation on permeability (1/psia)

**CFKEXP number**

Exponent for effect of compressibility on permeability (number). Required if \( CPERM \) is specified. Default is 3.

**PRPERM number**

Reference pressure for compressibility of formation on permeability (psia). Required if \( CPERM \) is specified.

**SWI, SWI_f number ... number**

...  
**number ... number**

Initial water saturation (fraction). If keyword \( CON \) is specified, specify one number for all active blocks in the next line. If keyword \( VAR \) is specified, an array of numbers must be specified in the next line for each grid block in the model.

**PRES, PRES_f number ... number**

...  
**number ... number**

Initial reservoir pressure (psia) for matrix and natural fracture. If keyword \( CON \) is specified, specify one number for all active blocks in the next line. If keyword \( VAR \) is specified, an array of numbers must be specified in the next line. The value in the array is assigned internally to each grid block in the model. For a 3-D reservoir, multiple layers of array containing pressure value must be specified.

**TRES number**

Initial reservoir temperature (°F)

---

**D.3 Well Descriptions**

The description of each well must be separated by a new line with comment **
SEPARATOR (skip to next line)

#ps  #ts
...
#ps  #ts

Pressure and temperature at each stage of the separator. Pressure is specified in psia. Temperature is specified in °F.

NW number

Number of wells

WELL name

Well name

WELLTPYE keyword

Type of well. Specify PRODUCER for producing well. Specify INJECTOR for injecting well.

OPERATE keyword1  keyword2  number

Well operating constraint. keyword1 specifies minimum (MIN) or maximum (MAX) constraint. keyword2 specifies constraint type (see below). number specifies the value for constraint specified in keyword2.

GEOMETRY keyword  #rw  #skin

Well geometry. Keyword X, Y, Z specify direction of the well. Wellbore radius rw (ft), and skin factor skin (unitless).

PERF wellname

x  y  z  OPEN  FLOW-TO  layer
...

x  y  z  OPEN  FLOW-TO  layer

Well perforation. Grid block coordinate x, y, z is specified for each line.
D.4 Rock-Fluid Properties

SWT,  (skip to next line)
SWT_f #sw  #ksw  #krow  #pcow
...
#sw  #ksw  #krow  #pcow

Water saturation table. Accept data in tabular format. Column from left to right: water saturation (fraction), water relative permeability (fraction), oil-water relative permeability (fraction), and oil-water capillary pressure (psi)

SGT,  (skip to next line)
SGT_f #sg  #krg  #krog  #pcgo
...
#sg  #krg  #krog  #pcgo

Gas saturation table. Accept data in tabular format. Column from left to right: gas saturation (fraction), gas relative permeability (fraction), oil-gas relative permeability (fraction), and gas-oil capillary pressure (psi)

PORR,  (skip to next line)
PORR_f #sg  #r
...
#sg  #r

Pore throat radius table. Accept data in tabular format. Column from left to right: gas saturation (fraction) and pore radius (nm).

D.5 Component

NC number

Number of components

NP number
Number of phases in flash calculation. Currently fixed at 2 phase hydrocarbon.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IFTW</td>
<td>Interfacial tension for water (dyne/cm). Currently disabled.</td>
</tr>
<tr>
<td>COMPNAME</td>
<td>Hydrocarbon component name</td>
</tr>
<tr>
<td>COMP</td>
<td>Hydrocarbon overall composition (fraction)</td>
</tr>
<tr>
<td>PCRIT</td>
<td>Component critical pressure (psia)</td>
</tr>
<tr>
<td>TCRIT</td>
<td>Component critical temperature (R)</td>
</tr>
<tr>
<td>VCRIT</td>
<td>Component critical volume (ft³/lbmol)</td>
</tr>
<tr>
<td>MW</td>
<td>Component molecular weight (lbmol/lbmol)</td>
</tr>
<tr>
<td>PCHOR</td>
<td>Component Parachor ( \left( \frac{\text{dyn/cm}}{\text{gmol/cm}^3} \right)^{\frac{1}{4}} )</td>
</tr>
<tr>
<td>DIFFUSION</td>
<td>Diffusion coefficient (ft²/day)</td>
</tr>
</tbody>
</table>
| VSHIFT   | }
Component volume shift (unitless)

**ADSVOL**

*number ... number*

Component Langmuir volume (scf/ton)

**ADSPRES**

*number ... number*

Component Langmuir pressure (psia)

**OMEGA**

*number ... number*

Component co-volume parameter

**OMEGB**

*number ... number*

Component attraction parameter

**BIP**

*number ... number*

...

*number ... number*

Binary interaction parameters. Accept BIP in tabular format.

**IFTMOD**

*number*

Multiplier for interfacial tension from Macleod and Sugden correlation

**WPVT**

*(skip to next line)*

#pw  #denw  #bw  #visw

...

#pw  #denw  #bw  #visw

Water PVT table. Accept data in tabular format. Column from left to right: water pressure (*psia*), density of water (*lb/ft³*), water formation volume factor (*ft³/STB*), and water viscosity (*cP*)
D.6 Numerical Control

DTMAX  \textit{number}

Maximum time step size (\textit{day}). Default is 30 days.

DTMIN  \textit{number}

Minimum time step size (\textit{day}). Default is 0.01 days.

DTFIXED  \textit{number}

Fixed time step size after the constraint is switched or at the start of the simulation (\textit{day}). Default is 0.01 days.

TFIXED  \textit{number}

Number of days to run a fixed time step size specified by DTFIXED (\textit{day}). Default is 0.

DPMAX  \textit{number}

Maximum change in pressure in each grid block. Default is 200 \textit{psia}.

DSMAX  \textit{number}

Maximum change in saturation in each grid block. Default is 0.15.

DZMAX  \textit{number}

Maximum change in composition in each grid block. Default is 0.15.

DPRES  \textit{number}

Specified desired change for pressure variable (\textit{psia}). Default value is 200 \textit{psia}.

DSAT  \textit{number}

Specified desired change for saturation variable (fraction). Default value is 0.2.

DCOMP  \textit{number}
Specified desired change for composition variable (fraction). Default value is 0.02 psia.

**DTUNE**  
*number*  
Tuning factor for automatic time step control (*number*)

**MAXITER**  
*number*  
Maximum Newton iteration for each time step (*number*)

**INNERITER**  
*number*  
Number of inner iteration for GMRES solver (*number*)

**TFINAL**  
*number*  
Final time to terminate simulation (*days*)

**D.7 Output Control**

**OUTPRN**  
*keyword* *keyword* … *keyword*  
Print output for oil pressure (*PO*), gas pressure (*PG*), water pressure (*PW*), oil saturation (*SO*), gas saturation (*SG*), water saturation (*SW*), number of phase (*NP*), oil phase composition (*XI*), gas phase composition (*YI*), overall composition (*ZI*) respectively, in the output files.

**SCNPRN**  
*keyword* *keyword* … *keyword*  
Print output for oil pressure (*PO*), gas pressure (*PG*), water pressure (*PW*), oil saturation (*SO*), gas saturation (*SG*), water saturation (*SW*), number of phase (*NP*), oil phase composition (*XI*), gas phase composition (*YI*), overall composition (*ZI*) respectively, on screen during simulation.
VITA

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- Chevron Outstanding Academic Achievement Award (2008)
- Chevron Recognizing Excellence Achievement (REACH) Scholarship (2007)
- UC Davis Engineering Dean’s Honor List (2007, 2008, 2009)
- UC Davis First Year Scholar (2007)

Selected Publications


