NUMERICAL STUDY OF CO-CURRENT WATER-DRY GAS
FLOW IN GAS GATHERING SYSTEMS

A Dissertation in
Petroleum and Natural Gas Engineering
by
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ABSTRACT

The optimum operation of the surface production system is one of the key elements needed for the successful operation of natural gas well facilities, particularly for gas stripper well facilities. Liquids, especially water, are the major culprits of excessive losses, not only in the wellbore but throughout the surface production system. Oversimplified models that consider the network system as a single phase can lead to incorrect pressure drop values because these models do not account for the condensed water along the pipes. This work will focus primarily on developing, testing, deploying and demonstrating a unique, analytical tool that is currently not available in the natural gas industry, and that will serve the primary purpose of increasing throughput capacity and improving operational reliability of natural gas gathering network infrastructures by tracking the development of a two-phase flow in the network system. The Finite Volume Method (FVM) on a staggered grid has been chosen to solve the set of four, two-fluid conservation equations for two-phase flow derived from the governing inviscid flow Euler PDE equations. Numerical solution is obtained at each control volume using the Globally Convergent Newton-Raphson technique.
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NOMENCLATURE

\( A \) = Cross sectional area of the pipe \((L^2)\)

\( A_1 \) = Cross sectional area \((L^2)\)

\( A_2 \) = Cross sectional area \((L^2)\)

\( A_3 \) = Cross sectional area \((L^2)\)

\( A_{gl} \) = Interphase area per unit volume \((L^{-1})\)

\( A_{gw} \) = Gas wetted wall area per unit volume \((L^{-1})\)

\( A_{kw} \) = Phase \(k\) wetted wall area per unit volume \((L^{-1})\)

\( A_{ww} \) = Water wetted wall area per unit volume \((L^{-1})\)

\( A_p \) = Peng-Robinson parameter \((\text{unitless})\)

\( A_{PD} \) = Passut and Danner ideal enthalpy coefficient

\((a\alpha)_i\) = Attraction parameter of component \(i\)-th of the mixture \((L^5/m-t^2)\)

\((a\alpha)_m\) = Attraction parameter for mixture \((L^5/m-t^2)\)

\( B_p \) = Peng-Robinson parameter \((\text{unitless})\)

\( B_{PD} \) = Passut and Danner ideal enthalpy coefficient

\( b_m \) = Co-volume parameter for mixture \((L^3/m)\)

\( c_{-1} \) = Coefficient for vapor pressure calculation

\( c_0 \) = Coefficient for vapor pressure calculation

\( c_1 \) = Coefficient for vapor pressure calculation

\( c_2 \) = Coefficient for vapor pressure calculation

\( c_3 \) = Coefficient for vapor pressure calculation

\( c_i \) = Mole composition of the \(i\)-th component of the mixture \((\text{unitless})\)

\( C_{PD} \) = Passut and Danner ideal enthalpy coefficient
\( d_{kh} = \) Phase k hydraulic diameter (L)

\( D = \) Pipe diameter (L)

\( D_{PD} = \) Passut and Danner ideal enthalpy coefficient

\( e = \) Specific internal energy \((L^2/t^3)\)

\( E_{PD} = \) Passut and Danner ideal enthalpy coefficient

\( f_{kw} = \) Fanning friction factor of phase k (unitless)

\( f_i = \) Interfacial friction factor

\( \vec{F}_{gg} = \) Gas gravitational force per unit volume \((m/L^2-t^2)\)

\( \vec{F}_{gw} = \) Gas wall friction force per unit volume \((m/L^2-t^2)\)

\( \vec{F}_i = \) Interfacial force per unit volume \((m/L^2-t^2)\)

\( \vec{F}_{kg} = \) Gravitational force of phase k per unit volume \((m/L^2-t^2)\)

\( \vec{F}_{kw} = \) Wall friction force of phase k per unit volume \((m/L^2-t^2)\)

\( \vec{F}_{mk} = \) Mass transfer effect force per unit volume \((m/L^2-t^2)\)

\( F_{PD} = \) Passut and Danner ideal enthalpy coefficient

\( \vec{F}_T = \) Net total force per unit volume \((m/L^2-t^2)\)

\( \vec{F}_{wg} = \) Water gravitational force per unit volume \((m/L^2-t^2)\)

\( \vec{F}_{ww} = \) Water wall friction force per unit volume \((m/L^2-t^2)\)

\( g = \) Acceleration of gravity \((L/t^2)\)

\( H_g = \) Enthalpy of gas \((L^2-t^2)\)

\( H_g^{dep} = \) Enthalpy of departure of the gas \((L^2-t^2)\)

\( H_g^{ide} = \) Ideal enthalpy of gas mixture \((L^2-t^2)\)

\( H_i^{ide} = \) Ideal enthalpy of i-th component of mixture \((L^2-t^2)\)

\( H_w = \) Enthalpy of water \((L^2-t^2)\)
\( H_k \) = Enthalpy of phase k (L^2-t^3)
\( k_{ij} \) = Peng-Robinson binary interaction coefficients (unitless)
\( k_v \) = Lee, Gonzalez and Eakin gas viscosity parameter
\( L_{gw} \) = Gas wetted perimeter (L)
\( L_{kw} \) = Phase k wetted perimeter (L)
\( L_T \) = Wetted perimeter (L)
\( L_{ww} \) = Water wetted perimeter (L)
\( \dot{M} \) = Volumetric mass transfer (m/t-L^3)
\( \dot{M}_k \) = Rate of mass transfer to phase k (m/t-L^3)
\( \dot{M}_{ki} \) = Rate of mass transfer to phase k at control volume i (m/t-L^3)
\( \dot{M}_{gi} \) = Rate of mass transfer to gas at control volume i (m/t-L^3)
\( \dot{M}_{wi} \) = Rate of mass transfer to liquid water at control volume i (m/t-L^3)
\( MW_i \) = Molecular weight of the i-th component of the mixture
\( P \) = Pressure (m/L-t^2)
\( P_v \) = Pressure vapor of water (m/L-t^2)
\( P_{ci} \) = Critical pressure of component i-th of the mixture (m/L-t^2)
\( \tilde{q} \) = Energy input vector (m/t^3)
\( \tilde{q}_k \) = Energy input of phase k vector (m/t^3)
\( Q_g \) = Gas flow rate (L^3/t)
\( Q_{gB} \) = Branch gas flow rate (L^3/t)
\( Q_{gR} \) = Run gas flow rate (L^3/t)
\( Q_w \) = Water flow rate (m/t)
\( Q_{wB} \) = Branch water flow rate (m/t)
\[ Q_{wR} = \text{Run water flow rate (m/t)} \]
\[ R = \text{Universal gas constant (L}^2/\text{T} \cdot \text{t}^2 \) 
\[ \text{Re}_k = \text{Reynolds number of phase k (unitless)} \]
\[ T = \text{Temperature (T)} \]
\[ T_{ci} = \text{Critical temperature of component i-th of the mixture (T)} \]
\[ t = \text{Time (t)} \]
\[ U = \text{Overall heat transfer coefficient (m/t}^3 \cdot \text{T)} \]
\[ \bar{V} = \text{Molar volume (L}^3/\text{m)} \]
\[ \nu = \text{Local fluid velocity (L/t)} \]
\[ \bar{v} = \text{Velocity vector (L/t)} \]
\[ \bar{v}_g = \text{Velocity vector of the gas (L/t)} \]
\[ \bar{v}_k = \text{Velocity vector of the phase k (L/t)} \]
\[ \bar{v}_w = \text{Velocity vector of the liquid water (L/t)} \]
\[ V_{Ol_i} = \text{Volume of the control volume (L}^3 \) 
\[ W = \text{Pounds of water in the gas per MMscf of gas (M/ L}^3 \) 
\[ \text{We} = \text{Weber number (unitless)} \]
\[ r_{\text{max}} = \text{Maximum droplet radius for mist flow pattern (L)} \]
\[ r_p = \text{Mean droplet radius for mist flow pattern (L)} \]
\[ W_{k_T} = \text{Rate of total work done by body and surface forces of phase k(m/L}^2 \cdot \text{t}^3 \) 
\[ W_{T} = \text{Rate of total work done by body and surface forces (m/L}^2 \cdot \text{t}^3 \) 
\[ w_i = \text{Acentric factor of component i-th of the mixture (unitless)} \]
\[ x_v = \text{Lee, Gonzalez and Eakin gas viscosity parameter} \]
\[ y_v = \text{Lee, Gonzalez and Eakin gas viscosity parameter} \]
\[ Z = \text{Compressibility factor (unitless)} \]
Greek

\( \alpha_g \) = Volumetric fraction of the gas (unitless)

\( \alpha_k \) = Volumetric fraction of the phase k (unitless)

\( \alpha_w \) = Volumetric fraction of the liquid water (unitless)

\( \Delta T \) = Temperature of ambient less CV temperature (T)

\( \Delta x \) = Length of the control volume (L)

\( \varepsilon \) = Pipe roughness (L)

\( \varepsilon_i \) = Interfacial pipe roughness (L)

\( \lambda_{gB} \) = Gas mass fraction of the branch (unitless)

\( \lambda_{gR} \) = Gas mass fraction of the run (unitless)

\( \lambda_{wB} \) = Water mass fraction of the branch (unitless)

\( \lambda_{wR} \) = Water mass fraction of the run (unitless)

\( \mu_k \) = Viscosity of the phase k (m/L-t)

\( \mu_g \) = Viscosity of gas (m/L-t)

\( \mu_w \) = Viscosity of water (m/L-t)

\( \rho \) = Density of the fluid (m/L\(^3\))

\( \rho_g \) = Density of the gas (m/L\(^3\))

\( \rho_k \) = Density of the phase k (m/L\(^3\))

\( \rho_w \) = Density of the liquid water (m/L\(^3\))

\( \theta \) = Pipe inclination angle with respect horizontal (rad)

\( \varphi \) = Pipe wetted angle in smooth stratified flow pattern (rad)

\( \sigma \) = Surface tension (m/t\(^2\))
Undoubtedly to my Lord and Almighty God, who made possible that His son presented today this work. Throughout all my life He has been my guidance and I just want to humbly be a reflection of His love, so let this work be a tribute to Him.

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CHAPTER 1

INTRODUCTION

There are several reasons that have made natural gas the fastest growing energy source in the world. It is a cleaner fuel compared to oil or coal and it is both environmentally and economically favorable within the industry, where new gas turbine power plants provide higher efficiency over coal power plants. As acknowledged by Balat (2005), natural gas use is expected to double between 1999 and 2020, playing a dominant role over the coming decade in many industrialized countries and helping to close the gap between domestic production and demand.

Natural gas pipeline transportation is the preferred method for distribution to consumers because of the low overall maintenance costs. When the construction of the pipelines is too complex or the distance is too long, this method becomes economically impractical; in this case, liquefaction of natural gas (LNG) and transportation by ship is the best alternative. A common but undesirable and inevitable reality in natural gas pipelines is the co-current flow of gas and liquid, which leads to a reduction in the deliverability of the gas because this gas-liquid phase occupies greater volume in the pipe, increases mechanical energy losses, alters composition of the gas giving a lower calorific value, and induces corrosion problems if liquid-phase water is present. Even small improvements in the accuracy of pressure drop and liquid hold-up calculations may result in a significant reduction in investment and operating costs. This liquid phase can appear at any point along the pipes as a result of heavy hydrocarbon condensation, or, in the case of water-saturated dry gas, as a result of vapor water condensation (object of study of this work).
The implementation of a two-phase flow in networks has the additional unresolved difficulty related to the poorly understood phenomenon known as "route selectivity" or "uneven split" at the network junctions. The accurate mapping of the pressure, velocities of both phases, temperature and fluid re-distribution inside the network is critical since it can reduce additional compression costs caused by the liquid phase, help to make decisions regarding water removal from the network and also affect the design of surface production equipment such as reboilers.
Pipeline network transportation is the preferred method for natural gas distribution to consumers because of the low overall maintenance costs when transportation distances are not prohibitively long. Only the U.S. has a vast pipeline network with more than 210 natural gas pipeline systems using more than 200,000 miles of interstate transmission lines and more than 1,200 compressor stations (each 50-100 miles apart) to keep the gas moving through the system [EIA, (2007)]. In 2007, 14.9 Bscf per day of natural gas pipeline capacity was added, a substantially higher increase over additions in prior years. Between 2008 and 2010 the national network pipeline capacity is expected to increase by a further 103 Bscf per day according to all current proposals [EIA, (2008)]. Figure 2.1 depicts major natural gas pipeline systems in the U.S.

Figure 2.1: U.S. natural gas pipeline and compressor station network [EIA, (2007)]
Solving for pressure drops, phases velocities and liquid holdups of these complex networks requires an explicit representation of the network structure components through a topological configuration of points and lines, also called a graph. The graph theory has its origin in the paper written in Latin by Leonhard Euler (1736) on the "Seven bridges of Königsberg". Network theory is a part of the graph theory and has applications in many disciplines such as computer science (World Wide Web), biology (gene regulatory networks), ecology (food of nutrients and energy between organizations), sociology (social networks), and network flow (analysis of traffic networks), to name a few [Bondy, (1976)].

A flow network is considered a directed graph or digraph and is defined as an ordered pair of vertices (also called nodes) and arcs (elements between two nodes). In the natural gas network analysis, the nodes are the junctions where two or more pipes (arcs) meet and supply or demand is introduced. In the same way, in circuit networks the arcs are represented by the wire making the connection, or in traffic networks those arcs represent the roads where traffic circulates. In general, a complex pipe network includes a series of pipes, parallel pipes and branching pipes, in addition to elbows, meters, pumps, and other equipment needed for the operation of the network. These pipes can be connected forming loopless or looped systems as Figure 2.2 depicts.

Figure 2.2: Loopless and looped networks
The easiest way to represent the graph of a network is through matrices, since they are easy to manipulate mathematically. The topology of any network can be described by matrices that fully represent the network graph. It is necessary to choose at least one reference or independent node [Osiadacz, (1987)]. It can be proven that the number of loops of a looped network is equal to the number of arcs (pipes) minus the number of load nodes (points where loads are placed into the network that are not reference nodes).

The interconnection of the network can be described by means of a branch-nodal incidence matrix defined as a rectangular matrix with as many rows as number of nodes and as many columns as number of pipes. The elements in the matrix can be defined as:

\[ a_{i,j} = \begin{cases} 
+1 & \text{if pipe } j \text{ enters node } i \\
-1 & \text{if pipe } j \text{ leaves node } i \\
0 & \text{if pipe } j \text{ has no connection with node } i 
\end{cases} \]  

(2.1)

The loops of the network can be described by means of a branch-loop incidence matrix defined as a rectangular matrix with as many rows as number of loops and as many columns as number of pipes. The elements in the matrix can be defined as:

\[ b_{i,j} = \begin{cases} 
+1 & \text{if pipe } j \text{ has same direction as loop } i \\
-1 & \text{if pipe } j \text{ has different direction as loop } i \\
0 & \text{if pipe } j \text{ is not in loop } i 
\end{cases} \]  

(2.2)

Storing these two matrices to fully represent the graph of the network is highly inefficient since for large networks many terms are zero (no interconnectivity with the node or the loop) so a sparse matrix is used to reduce computer storage. Osiadacz (1987) describes five different methods of loop generation widely used in the gas industry to characterize the gas networks.
2.1 Single-phase flow in networks

The single phase in the natural gas networks steady-state problem is solved when the flow rate in each pipe can be determined under some specified supply and demand patterns. Traditionally, single phase natural gas pipe networks are solved by defining a correlation between the pressure drop occurring in each pipe of the network and the flow rate through that pipe. Weymouth, Panhandle A and Panhandle B are some of the most commonly used correlations in the gas industry for this means. Then, depending on the configuration of the network, groups of pipes can be converted into an equivalent pipe, obtaining a simplified network to be solved. The network is solved very similarly to electric circuits satisfying two main premises:

a) The flow into any junction of the network equals the flow out of the junction, also known as Kirchhoff's First Law.

b) The energy loss between two junctions is independent of the path taken, also known as Kirchhoff's Second Law. In other words, a particle traveling through the network that arrives at the same initial point will have the same initial energy.

A set of non-linear equations is created and the steady-state problem is solved after solving the system of equations giving all pressures, phases velocities and liquid holdups. If all external flows to the system are known, the linear method can be used, which transforms the system of non-linear equations to a linear system [Jeppson, (1976)]. The main advantage of this method is that it does not require an initialization and it converges rather quickly. The oldest and most widely used method is the iterative-based Cross Method. To improve the slow convergence of Cross Method, the Renouard Method is also commonly used. Newton-Raphson is another iterative alternative to solve the non-linear system of equations.
2.2 Two-phase flow in pipes

Although two-phase gas-liquid flow is commonly encountered in the nuclear, chemical and petroleum industries, the fact that two different phases are flowing together represents a major challenge in solving these networks. In multiphase flow, the phase distribution is difficult to predict because of the turbulence phenomenon and the movement of the boundaries. Due to the compressibility of fluids and its deformable nature, the co-current flow of gas and liquid in a pipe is a complex process, since it may adopt a wide variety of configurations, usually called flow patterns. Many different flow patterns have been defined by various authors, and the nature of them varies with channel geometry, size, fluid physical properties, flow orientation and flow parameters. Cheng (2008) recently reviewed the developments throughout history on the study of flow patterns, compared them and stated that nearly all two-phase pressure drop correlations in the literature are purely empirical, with no reference to the flow patterns that they cover, including the leading methods such as those of Lockhart and Martinelli (1949) and Muller-Steinhagen and Heck (1986), for example. Figure 2.3 shows a schematic of flow patterns in a horizontal gas-liquid co-current flow and Figure 2.4 depicts the corresponding Baker flow pattern map, which plots gas versus liquid mass flow rates and identifies the different regions depicted in Figure 2.3.

Figure 2.3: Oil/Gas flow patterns [Cheng, (2008)]
In recent decades, the subject of two-phase flow in pipes has been an important area of research. A broad classification of those models is to divide them into homogeneous (the two-phase flow is considered as one phase with averaged transport properties) and heterogeneous (the two phases are considered separately). The Homogeneous Equilibrium Model (HEM) combines the two phases into a single phase where the fluid properties are averaged. The Drift Flux Model assumes a dependent slippage between phases depending on the flow conditions; this second model would be classified as pseudo-homogeneous. A separated model considers each phase to flow in a separated zone of the channel, while the two-fluid model considers two flowing phases. These last two models are considered heterogeneous models.

Martinelli along with Lockhart (1949) and Nelson (1948) are considered the earliest attempts of two-phase pressure drop predictions in horizontal pipes during the late ‘40s. Cheng indicates that a flaw of these models is their lack of reference to a specific flow pattern. Additional correlations came after those, but because they were empirical correlations, they were only useful when compared to conditions similar to those from which they were derived.
The Beggs and Brill (1973) correlation became one of the most widely used. Brill, Sifferman and Arirachakaran (1985) presented a work on a gas-gathering system in a major offshore oilfield in Saudi Arabia. In their work, they presented calculations for sizing the pipelines including phase behavior, pressure drop, temperature profiles, liquid volumes, flow pattern predictions, liquid flow rates and the minimum gas velocity required to continuously remove liquid from the risers. Additionally, Mukherjee and Brill (1985) presented a complete review of the tools that were presently available for two-phase flow predictions.

Taitel (1996) defines mechanistic models as those that approximate a physical phenomenon, taking into consideration the most important processes and neglecting the less important ones, which can complicate the solution of the problem and which do not considerably improve the accuracy. Taitel and Dukler (1976) was the starting point for moving from empirical correlations to two-fluid models, in part due to its current application in the nuclear industry. Barnea (1987) and Chen et al. (1997) worked towards the development of models to predict those flow patterns. Adewumi and Arastoopour (1985) presented a two-dimensional hydrodynamic analysis of gas-solid co-current flow in vertical pipes. Incorporating the liquid-vapor equilibrium equations, Vincent (1988) studied the gas-condensate two-phase flow for horizontal pipes. During this early work, isothermal conditions were considered as well as mist flow conditions. Later on, different research from Penn State improved upon those models, adding terrain variations (Mucharam, 1990), different flow pattern conditions (Boriyantoro, 1994) and solving open-network pipeline systems (Carrillo, 1999). However, the main isothermal assumption was still in place until Ayala (2001) incorporated a fifth energy balance conservation equation in order to account for the temperature dependency. He implemented the five conservation equations within a marching algorithm. The use of marching algorithms is a downside when modeling pipeline networks, since they cannot solve them. Alp (2009) conducted research on solving gas-

Bendiksen et al. (1989) presented a two-fluid model code named OLGA that employs continuity equations for gas and liquid phases and for the liquid droplets entrained in the gas, two momentum equations (one for gas and the other for liquid) and a mixture energy conservation equation. The first version of OLGA was developed in 1979 and the model has since been further developed by the Institute for Energy Technology and Scandpower. OLGA is a widely used simulation in the oil and gas industry. PIPESIM, a product of Schlumberger, incorporates most of the current industry standard multiphase flow correlations, both empirical and mechanistic to predict flow regimes, liquid hold-up and pressure drops. It incorporates two advanced mechanistic flow models: OLGA'S and TUFFP (Tulsa University Fluid Flow Projects) and it is also widely used by industry. A very interesting recent work is the one published by Munkejord et al. (2005) regarding the use of a two-fluid model in the framework of a two-dimensional multiphase Computational Fluid Dynamics (CFD) code since, as they state, little work concerning CFD pressure drop and liquid hold-up calculations in horizontal pipes has been published. In their
work they state that problems exhibiting two- and three-dimensional flow such as bends or junctions (as we encounter when solving a natural gas pipe network) are not suitable for one-dimensional approaches, so codes such as OLGA might not be suitable for solving these problems, although they have proven very reliable for the one-dimensional two-phase flow situation encountered in long pipes.

2.3 Route selectivity in two-phase networks

The phenomena that occur in the junction between pipes has been studied for many centuries. Leonardo da Vinci observed and recorded the recirculation occurring in single phase flow near the junction, as depicted in Figure 2.5. We stated previously the difficulty of modeling two-phase flow in pipes due to turbulence and the movement of boundaries. The difficulty is greatly enhanced when dealing with more complex pipe geometries and especially in those points where a drastic change in the direction of the fluids is experimented, such as the Tee junctions. It has been observed that the presence of the Tee junction causes a disturbance to the static pressure in the vicinity of the junction itself, consequently resulting in a pressure difference between the run and the branch.
The main problem when modeling a two-phase flow in networks is the route selectivity or uneven split that occurs at the junctions and where liquid and gas will split over the run and branch sides of the junction at different ratios due to the pressure difference between the run and branch, as depicted in Figure 2.6.
This unresolved problem was first described by Oranje (1973) when analyzing the route preferences of liquid condensate in the transportation of natural gas in natural gas transportation pipeline networks and constitutes the major difficulty to overcome to be able to track and map the preferential route of water and gas in the network system. He provided a purely empirical rule of thumb that is only applicable to very limited flow conditions and is dependent on the amount of gas entering the branch of a junction to predict the route preference of the liquid condensate.

A purely analytical approach for determining that pressure drop, and consequently the route preference, requires a very detailed knowledge of the two-phase flow, accounting for all the extra difficulties due to turbulence based on the geometry, something that 3D models can achieve but not 1D models. The other approach that can be taken is the use of empirical correlations but the downside of this approach is that it involves too many independent parameters. Semi-empirical models are based on the mechanical energy conservation where the pressure change is divided into reversible and irreversible being this last one calculated through the determination of loss coefficients, which are usually calculated using Gardel (1957) correlations. Saba and Lahey (1984) developed a model with a large set of semi-empirical correlations to solve the uneven split problem for homogenous flow; however, it is not applicable to stratified-wavy air-water flow. Hart and Hamersma (1991) presented an innovative study about the air-water route selectivity in horizontal T-junctions in an effort to get away from the highly empirical (and thus only applicable for very limited flow conditions) models of that time by using the Double Stream Model (DSM) and applying energy Bernoulli balance equations, showing good results for a 90° Tee-junction of low water holdup. Later on Ottens et al. (2001) studied the effect of small branch inclination (in practice most angles of inclination vary -2° to 2°) on the air-water separation in 90° Tee-junctions and compared their results to experimental data. In their work they state that even
small branch inclination angles (less than 0.5°) have a strong effect in the water-liquid flow separation. Oka et al. (2005) determined in his work the loss coefficients for tees with large area ratios and different main pipe-branch pipe angles from continuity, momentum and energy principles. One of the most recent publications regarding T-junctions is the work presented by Yang and Azzopardi (2006) where they revised different approaches throughout history to solve the uneven split problem and compared results with the Seeger et al. (1986) correlation. More recently, Costa et al. (2006) studied the edge effects on the flow characteristics in a 90° Tee-junction, concluding that rounding the corners of a sharp Tee-junction can reduce the energy losses between 10% and 20%, depending on the flow rate ratio.

As can be seen, the preferential route of gas-liquid systems depends on such variables as the inlet velocity ratios, flow patterns, physical properties of the gas and liquid, and geometry of the junction. Most of the studies carried out are based on air-water systems and are applicable only for the specific flow conditions and parameters of the study, and generally lack in applicability to other fluids and flow conditions. In this study, a two-fluid model using Euler equations applied to a Finite Volume Method (FVM) that conserves the mass and momentum equations and discretizes them is applied. Thermodynamic relations as well as the Dranchuk and Abou-Kaseem equation of state (EOS) will also be implemented. It is well known that the single-phase fully-implicit numerical scheme is unconditionally stable, but the single-pressure two-phase flow model is non-hyperbolic ill-posed formulation because of the existence of complex characteristics [Frepoli, (2003)]. Due to this fact and the high non-linearity degree of the system of equations to be solved, a Globally Convergent Method is necessary, incorporating specific convergence criteria.
CHAPTER 3

PROBLEM STATEMENT

The co-current flow of gas and liquid is a common scenario in many industries: in the nuclear industry the transport of cooling water and steam through pipes, in the petrochemical industry steam enhanced oil recovery (EOR), reboilers, and, what interests us the most, in the natural gas industry for gas-gathering systems. The presence of liquids is highly undesirable since it reduces the deliverability of the pipe and increases the costs associated with the pressure loss as well as causes corrosion problems if the liquid is water. Even if we discount the possibility of liquid hydrocarbon condensation, produced gases remain saturated with water vapor that is likely to drop out at some point along the pipe network even after all free water is removed at the well site.

Stripper wells, also called marginal wells, are defined as those producing less than 60,000 cubic feet per day (scf/day) of natural gas. The pressure drop calculated assuming single-phase flow is significantly lower than the one experienced when liquid and gas flow co-currently. These pressure losses at the surface of a stripper well gathering system can make the production go below the economic limits of operation, even for the cases where liquid dropout inside the system is low. For that reason, even small improvements in the accuracy of pressure drop and liquid hold-up calculations may result in a significant reduction of the cost of investment and operations. Although industry has not been indifferent to the problem, the lack of predictive technology to tell them precisely where and how the liquid is distributed within the system and to determine the best strategy to get rid of it is still an unsolved problem. Therefore, a technology that can map the liquid distribution in a complex network and help design strategies to maintain a
liquid-free network, decrease pressure losses and compression requirements, could translate into significant gains in performance efficiency.

To overcome the use of oversimplified single-phase models (Weymouth, Panhandle type, AGA equation) together with empirical correlations developed in order to account for the pressure drop as a consequence of the multiphase flow, this work aims at utilizing a two-fluid model together with fundamental thermodynamic and transport phenomena principles for the mapping of pressure, temperature, and fluid distribution inside dry gas (no hydrocarbon condensation) gathering networks. The route selectivity phenomenon at the network junctions is the major obstacle to overcome, since it will determine the fluids distribution along the network and define the pressures and velocities profiles. Figure 3.1 depicts a natural gas pipeline network and the water route selectivity phenomenon. This model is based on non-linear, first-order five conservation equations (two masses, two momentums and combined energy) in order to solve for the five unknowns (pressure, temperature, gas and water velocities, and liquid hold-up) and applied to a Finite Volume Method (FVM) to discretize the conservation equations and physically model the pipes and the networks.
Figure 3.1: Water route selectivity in a gas network
CHAPTER 4
DESCRIPTION OF THE MODEL

A one-dimensional steady flow for the dry gas-liquid water fractions model is composed of four conservation equations (two mass conservation and two momentum conservation equations). This work incorporates fundamental transport principles to the conservation equations so that the pressure and velocities of both phases as well as holdups can be mapped along a closed-loop pipe network. The importance of mapping where water is migrating in the network is quite high, since small amounts of liquid holdup can result in substantial additional pressure drop and, consequently, make the economics of the operation unsustainable.

4.1 The constitutive equations

By applying the second law of Newton, which states that the net force applied to a body is equal to the change in time of linear momentum, and assuming that the fluid stress is the result of the sum of a diffusing term plus a pressure term, a set of second-order Partial Differential Equations (PDEs) describing the motion of viscous fluids is obtained. This set of equations is named the Navier-Stokes equations, named after Claude-Louis Navier and George Gabriel Stokes.

A simplification of the Navier-Stokes equations can be achieved when fluid Reynolds numbers are high, whereby viscous effects and heat transfer conduction effects may be ignored (ideal fluid). As a result, the diffusive terms of the second-order Navier-Stokes equations that appear as consequence of the generalized law of Fick are cancelled and an easier first-order PDE
is derived. This set of equations is named after the Swiss mathematician Leonhard Euler who developed them in 1670 in order to directly represent momentum conservation of the fluid.

In addition to these equations, a statement of the mass conservation is needed. Mass conservation states that the mass of a closed system will remain constant. In one dimension, the governing equations are as follows:

**Mass conservation:**

\[
\frac{d\rho}{dt} + \nabla \cdot (\rho \vec{v}) = \dot{M}
\]

(4.1)

where:

- \( \rho \) = density
- \( t \) = time
- \( \vec{v} \) = velocity
- \( \dot{M} \) = Volumetric mass transfer

**Momentum conservation:**

\[
\frac{d(\rho \vec{v})}{dt} + \rho \vec{v} \nabla \cdot \vec{v} = \vec{F}_T
\]

(4.2)

where:

- \( \vec{F}_T \) = Net total force per unit volume

From this set of non-linear differential equations that represent a physical reality in a continuum medium, a set of discretized equations that approximate the solution is to be generated. Since numerical methods highly depend on the type of PDE that is being dealt with, the previous equations have to first be classified. The diffusion phenomenon has an elliptic behavior, since they act along all the space independently of the primary direction of the flux. The
convection phenomenon, which acts in the propagation direction, has a hyperbolic behavior, so it is governed primarily by the velocity field. These facts give us an idea of how the Navier-Stokes equations can be classified accordingly, depending on which phenomenon is predominantly acting.

4.2 The Finite Volume Method (FVM)

The Finite Volume Method (FVM) is applied in order to convert the continuum Euler equations into a discrete problem with a finite number of degrees of freedom. As a numerical solution, it basically consists of dividing the physical domain into imaginary, discrete subdomains that are called Control Volumes (CVs). The discretized form of the Euler equations is applied, so the conservation of fluxes through a particular CV is guaranteed, as well as the overall solution conservation. From a practical point of view, the method consists of the substitution of the integrals from the conservation equations for sums over the faces of the volume. Whenever the values of the variables are unknown, some form of interpolation is required and as a result of this, different versions of the method can be developed.

To obtain the discrete form, Euler equations are applied to the defined CVs. The volumetric fluid and flow parameters at the center of the CV are a representation of the volumetric average of those properties over the CV. Since it deals with fluxes, it can be said that it has much physical significance. The principal disadvantage is the difficulty to model irregular geometries, requiring much more effort than regular geometries.
4.3 The staggered grid

In a single-phase flow, three unknowns (pressure, temperature and velocity) are to be determined with the three conservation equations for each control volume. If the isothermal case is being considered the temperatures at each CV will remain the same, but that temperature has to be known in order to be able to calculate fluid properties by means of an EOS. It might make sense to define each group of these three unknowns at the same location of each control volume (coincidental grid). The drawback with this approach is that the non-uniform pressure field can act like a uniform pressure field in the discretized momentum conservation equation, creating wavy patterns for pressure and velocity, commonly known as the checker-board effect, as discussed by Patankar (1980). Therefore, coincidental grids are not commonly used in fluid dynamics when using FVM methods, although some attempts have been made to effectively implement a coincidental grid, as Rhie and Chow (1983) suggest, modifying the pressure term to avoid the checker-board effect.

To avoid the troublesome representation of the pressure in the discretized momentum conservation equation, Harlow and Welch (1965) proposed the use of the staggered grid for velocity values. The idea is that pressure and temperature will be evaluated at the center of one grid, but velocities will be evaluated at the center of a half CV displaced grid, or at the edges of the first defined grid. This concept makes sense physically, since evaluating the velocities at the edges of the first grid is needed in order to calculate the mass fluxes at the edges of the grid. Figure 4.1 shows the original pipe (in blue) with its grid, and the displaced or staggered mesh (in red). Mass and energy conservation equations will be evaluated at the original mesh, but momentum will be evaluated at the displaced mesh (in red). Please note that we have chosen to specify the temperature at the inlet and pressure at the outlet of the pipe.
4.4 Single-phase: Conservation equations derivation

For the case of single-phase flow, the discrete conservation equations are derived in this section using the FVM and the staggered grid previously defined. The principal unknowns are the Pressure and Velocity of the phase along the center of their respective control volumes.

4.4.1 Single-phase mass conservation

Figure 4.2 depicts the physical pipe divided into discrete, non-overlapping computational domains known as Control Volumes (CVs). At the center of the CV, the fluid and flow parameters represent the volumetric average of the CV. Above them, the mass, momentum and energy conservation principles prevail. Thus, we start with the Partial Differential Equation (PDE) that states the mass conservation applied to our CV and attempt to obtain a discretized
equation that will collapse with the PDE when the volume of our CV is infinitesimally small. Equation (4.3) represents the mass conservation PDE for a non-reactive fluid.

\[
\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k) = 0
\]  

(4.3)

where:

\( \rho_k \) = Density of the phase k

\( \mathbf{v}_k \) = Velocity of the phase k

\( t \) = Time

Integrating now over the volume to get Equation (4.4)

\[
\frac{\partial}{\partial t} \int_V \rho_k \, dV + \int_V (\nabla \cdot (\rho_k \mathbf{v}_k)) \, dV = 0
\]  

(4.4)

Applying the divergence theorem we obtain Equation (4.5) shown below. Details about the application of the divergence theorem or Gauss theorem are found in Appendix A.

\[
\frac{\partial}{\partial t} \int_V \rho_k \, dV + \oint_S (\rho_k \mathbf{v}_k) \, d\mathbf{A} = 0
\]  

(4.5)
By solving those integrals we obtain a discretized form, Equation (4.6)

\[
\frac{\partial}{\partial t} (\rho_k \ V o l_i) + (\rho_k v_k A)_{i+\frac{1}{2}} - (\rho_k v_k A)_{i-\frac{1}{2}} = 0
\]

(4.6)

where:

\[A = \text{Cross sectional area of the pipe}\]
\[Vol_i = \text{Volume of the control volume}\]
\[\rho_i = \text{Density of the control volume}\]

Observing carefully Equation (4.6) and taking into consideration the proposed staggered grid model, we immediately realize that we need values for the density at the edges of our CV. We might be tempted to use linear interpolation in order to obtain those values but in doing so, there is a potential risk of obtaining unrealistic results (e.g., negative density values). The fluid at a specific point carries with it information from its upstream state, so a weighted average of the upstream values would be a good idea. Applying this method, also known as the “upwind” method, we obtain the values of the densities at the edges of our CV as shown in Equation (4.7).

\[\rho_{i+\frac{1}{2}} = \rho_i \quad \text{and} \quad \rho_{i-\frac{1}{2}} = \rho_{i-1}\]

(4.7)

For steady state conditions, by knowing that the area of the pipe is constant and recalling the staggered grid scheme, Equation (4.8) can be rewritten as:

\[(\rho_k v_k A)_i - (\rho_k v_k A)_{i-1} = 0\]

(4.8)

It needs to be noted that when this scheme is applied to the first CV of a single pipe, \(\rho_0\) and \(\bar{V}_0\) have to be defined. Providing the volumetric flow rate at the inlet of a single pipe is equivalent to providing the initial mass flux rate \(\varpi_k\) which is equal to the expression \(\rho_0 \bar{v}_0 A_0\).
4.4.2 Single-phase momentum conservation

It should be noted that our mesh has now displaced half a CV, as we are dealing with a staggered mesh and the momentum equation is being evaluated in different CVs than the mass equations.

![Figure 4.3: Control volume for single-phase momentum conservation](image)

The change of momentum in time has to be equal to the sum of the forces acting on the system. Equation (4.9) represents the momentum conservation PDE.

\[
\frac{\partial (\rho \vec{v})}{\partial t} + \rho \vec{v} \nabla \cdot \vec{v} = \bar{F}_T
\]

(4.9)

Where \( \bar{F}_T \) = Net acting body and surface forces per unit volume. In this term, both body forces (developed without any physical contact) and surface forces (applied through an external contact area) are taken into account. The gravitational force is usually considered as the principal body force. Surface forces are those associated with the pressure gradient, which acts in the normal direction of the control volume; friction forces are those produced due to the interaction between wall and fluid flow, which act in the tangential direction to the control volume.
Accounting for these new terms, we can rearrange Equation (4.10) for a general phase $k$ as follows:

$$\frac{\partial (\rho_k \vec{v}_k)}{\partial t} + \rho_k \vec{v}_k \nabla \cdot \vec{v}_k = -\nabla P - \vec{F}_{kg} - \vec{F}_{kw}$$

(4.10)

where:

$$\vec{F}_{kg} = \text{Phase k gravitational force per unit volume}$$

$$\vec{F}_{kw} = \text{Phase k wall friction force per unit volume}$$

$P = \text{Pressure}$

Focusing on the absolute value of the parameters, and integrating over the control volume, the following expression, Equation(4.11), is obtained:

$$\frac{\partial}{\partial t} \int_V (\rho_k \vec{v}_k) \, dV + \int_V (\rho_k \vec{v}_k \nabla \cdot \vec{v}_k) \, dV = -\int_V (\nabla P + \vec{F}_{kg} + \vec{F}_{kw}) \, dV$$

(4.11)

Applying both the divergence and gradient theorems:

$$\frac{\partial}{\partial t} \int_V (\rho_k \vec{v}_k) \, dV + \oint_S (\rho_k \vec{v}_k \vec{v}_k) \, d\vec{A} = -\oint_S P \, d\vec{A} - \int_V (\vec{F}_{kg} + \vec{F}_{kw}) \, dV$$

(4.12)

And solving the integrals we obtain a discretized form of the equation:

$$\frac{\partial}{\partial t} (\rho_k \vec{v}_k \text{Vol}_{i+1}) + (\rho_k \vec{v}_k v_k A)_{i+1} - (\rho_k \vec{v}_k v_k A)_i = -(PA)_{i+1} + (PA)_i - (\vec{F}_{kg} + \vec{F}_{kw}) \text{Vol}_{i+1}$$

(4.13)

At the faces of the control volume, the values of the velocities are not known (because the staggered configuration has displaced the mesh). A cell donor scheme is again applied, and the velocities there are taken as the next available one in the direction of the flow. Taking into consideration the explained staggered grid and assuming that the area of the pipe is constant, we finally obtain Equation (4.14) considering steady state, and dividing by the volume:
\[
\frac{(\rho_k \vec{v}_k v_k)_{i+1} - (\rho_k \vec{v}_k v_k)_i + (P)_{i+1} - (P)_i}{(\Delta x)} = -(\vec{F}_{kg} + \vec{F}_{kw})_i
\]

(4.14)

It needs to be noted that this cell donor scheme for the momentum equation is equivalent to work on a coincidental grid, displacing a control volume in the direction of the flow and using the same upwind cell donor that is used for the mass conservation. To overcome the fact that densities and velocities are unknown at block i+1, zero curvature is applied. By this means, we extrapolate them from the last two known values so that we can obtain the density at that last edge of the last CV.

The calculation of the gravitational term \( \vec{F}_{kg} \) is straightforward. In single phase, the area \( A \) is the pipe cross-sectional area, but when working with two-phase, that area will be the cross-sectional area available for that phase in particular. For a general phase k and single phase, it can be calculated as follows:

\[
\vec{F}_{kg} = \rho_k g \sin \theta
\]

(4.15)

where:

\( \vec{F}_{kg} = \) Phase k gravitational force per unit volume

\( \rho_k = \) Density of phase k

\( g = \) Acceleration of gravity

\( \theta = \) Pipe inclination angle with respect horizontal

In order to calculate the friction wall term \( \vec{F}_{kw} \) we must first know the hydraulic diameter of phase k, calculated as:

\[
d_{kh} = 4 \frac{\text{Volume of phase a}}{\text{Total wall area wetted by phase a}}
\]

(4.16)

where:

\( d_{kh} = \) Phase k hydraulic diameter
It is important to note that in single-phase flow, the hydraulic diameter of the phase equals the diameter of the pipe.

After obtaining the hydraulic diameter, the Reynolds number of phase $k$ can be calculated as:

$$\text{Re}_k = \frac{\rho_k \bar{v}_k d_{kh}}{\mu_k}$$  \hspace{1cm} (4.17)

where:

- $\text{Re}_k$ = Reynolds number of phase $k$
- $\rho_k$ = Density of phase $k$
- $\bar{v}_k$ = Velocity of phase $k$
- $d_{kh}$ = Phase $k$ hydraulic diameter
- $\mu_k$ = Viscosity of phase $k$

### 4.5 Two-phase: Conservation equations derivation

In an isothermal two-phase flow system, the number of considered unknowns is increased from two to four. The model considers that both phases will have the same pressure and temperature but phases can have different velocities. The fourth unknown is the holdup or volumetric fraction of liquid.

#### 4.5.1 Two-phase gas and water mass conservation

Following the same scheme that we used for the single phase derivation, the gas mass conservation equation for a phase (gas or water) is derived starting from the PDE. It has to be
noted that an additional term is added in order to account for the mass transfer between both phases.

\[
\frac{\partial (\alpha_k \rho_k)}{\partial t} + \nabla \cdot \alpha_k \rho_k \vec{v}_k = \dot{M}_k
\]  

(4.18)

where:

\( \rho_k \) = Density of phase k  
\( \alpha_k \) = Volumetric fraction of phase k  
\( \vec{v}_k \) = Velocity of phase k  
\( t \) = Time  
\( \dot{M}_k \) = Rate of volumetric mass transfer to phase k (positive for condensation and negative for evaporation)

Following the same procedure as in single phase, we obtain an expression for a discretized form of the PDE applicable for each CV and for steady state conditions:

\[
\frac{(\rho_k \vec{v}_k \alpha_k)_i - (\rho_k \vec{v}_k \alpha_k)_{i-1}}{\Delta x} = \dot{M}_{ki}
\]  

(4.19)

where:

\( \rho_k \) = Density of phase k  
\( \alpha_k \) = Volumetric fraction of phase k  
\( \vec{v}_k \) = Velocity of phase k  
\( \dot{M}_{ki} \) = Rate of mass transfer to phase k (positive for condensation and negative for evaporation)  
\( \Delta x \) = Length of control volume
Therefore, the discretized equation can be particularized for the gas phase as follows:

\[
\frac{\left(\rho_g \bar{v}_g \alpha_g\right)_i - \left(\rho_g \bar{v}_g \alpha_g\right)_{i-1}}{\Delta x} = \dot{M}_{gi}
\]

(4.20)

where:

- \(\rho_g\) = Density of the gas
- \(\alpha_g\) = Volumetric fraction of the gas
- \(\bar{v}_g\) = Velocity of the gas
- \(\dot{M}_{gi}\) = Rate of mass transfer to gas (positive for condensation and negative for evaporation)

Equation (4.20) can be rewritten for the water liquid phase as:

\[
\frac{\left(\rho_w \bar{v}_w \alpha_w\right)_i - \left(\rho_w \bar{v}_w \alpha_w\right)_{i-1}}{\Delta x} = \dot{M}_{wi}
\]

(4.21)

where:

- \(\rho_w\) = Density of the liquid water
- \(\alpha_w\) = Volumetric fraction of the liquid water
- \(\bar{v}_w\) = Velocity of the liquid water
- \(\dot{M}_{wi}\) = Rate of mass transfer to liquid water (positive for condensation and negative for evaporation)

It must also be considered that \(\alpha_w + \alpha_g = 1\) and \(\dot{M}_{wi} = -\dot{M}_{gi}\).
4.5.2 Two-phase gas and water momentum conservation

The starting PDE for a two-phase flow is:

\[
\frac{\partial (\alpha_k \rho_k \vec{v}_k)}{\partial t} + \alpha_k \rho_k \vec{v}_k \nabla \cdot \vec{v}_k = -\alpha_k \nabla P - \alpha_k \vec{F}_{kg} - \vec{F}_{kw} + \vec{F}_i - \vec{F}_{mk}
\]

(4.22)

where:

- \(\vec{F}_i\) = Interfacial force per unit volume
- \(\vec{F}_{mk}\) = Mass transfer effect force per unit volume
- \(\vec{F}_{kg}\) = Gravitational force of phase k per unit volume
- \(\vec{F}_{kw}\) = Wall friction force of phase k per unit volume

The mass transfer effect force is several orders of magnitude smaller than the rest of the forces (Vincent, 1988), so this study does not consider the effect of this force. For the case of the gas phase, the discretized PDE is obtained after adding the additional interphase force term.

\[
\frac{\left(\alpha_g \rho_g \vec{v}_g \cdot \vec{v}_g\right)_{i+1} - \left(\alpha_g \rho_g \vec{v}_g \cdot \vec{v}_g\right)_i + \bar{\alpha}_g ((P)_{i+1} - (P)_i)}{(\Delta x)} = -\left(\alpha_g \vec{F}_{gg} + \vec{F}_{gw} - \vec{F}_i\right)_i
\]

(4.23)

where:

- \(\vec{F}_{gg}\) = Gravitational force of gas phase per unit volume
- \(\vec{F}_{gw}\) = Gas wall friction force per unit volume
- \(\bar{\alpha}_g\) = Mean average of gas holdups found at edges \(\left(\frac{(\alpha_g)_{i+1} + (\alpha_g)_i}{2}\right)\)

A similar expression can be written for the water phase as follows:

\[
\frac{\left(\alpha_w \rho_w \vec{v}_w \cdot \vec{v}_w\right)_{i+1} - \left(\alpha_w \rho_w \vec{v}_w \cdot \vec{v}_w\right)_i + \bar{\alpha}_w ((P)_{i+1} - (P)_i)}{(\Delta x)} = -\left(\alpha_w \vec{F}_{wg} + \vec{F}_{ww} + \vec{F}_i\right)_i
\]

(4.24)

where:
\[ \vec{R}_{wb} = \text{Gravitational force of water phase per unit volume} \]
\[ \vec{R}_{ww} = \text{Water wall friction force per unit volume} \]
\[ \bar{\alpha}_{wl} = \text{Mean average of liquid holdups found at edges} \left( \frac{\alpha_{wl}^{i+1} + \alpha_{wl}^{i}}{2} \right) \]

### 4.6 Finite Volume (FV) Equations and Boundary Conditions (BC) Handling

At this point the conservative differential equations have been converted to a set of discretized equations that divide the physical domain into imaginary and discrete subdomains (CVs). The system of non-linear equations is suitable to be solved as long as the number of unknowns equals the number of equations. In the case that this premise does not happen, additional equations, also called boundary conditions, must be provided. These boundaries conditions can be represented by a physical boundary (such as no flow boundary) or any kind of constraint at the inlet or outlet. Patankar (1980) proposed, under the assumption of a fully developed flow, to assure unidirectional flow, a zero curvature outflow boundary condition. The zero curvature can be written for a specific variable (velocity in our example) in terms of the second derivative as follows:

\[ 0 = \frac{\partial^2 v}{\partial x^2} \]  \hspace{1cm} (4.25)

After integrating Equation (4.25) over a CV once the following expression is found:

\[ \text{constant} = \frac{\Delta v}{\Delta x} \]  \hspace{1cm} (4.26)

Figure 4.4 depicts an example of the zero curvature application. In this particular case the velocity \( i+1 \) can be expressed as a function of the two previous velocities after applying zero curvature:
\[
\frac{v_i - v_{i-1}}{\Delta x_i} = \frac{v_{i+1} - v_i}{\Delta x_{i+1}} \quad \Rightarrow \quad v_{i+1} = \frac{\Delta x_{i+1}(v_i - v_{i-1})}{\Delta x_i} + v_i
\]

(4.27)

Figure 4.4: Zero curvature example

The zero curvature is mathematically equivalent to a linear extrapolation of the two previous values and helps to reduce the number of unknowns.

4.6.1 Straight pipe example

Depicted in Figure 4.5 is a typical two-phase flow isothermal conditions situation. For this case, 3 CVs are considered and thus 12 primary unknowns are generated, assuming \( \Box_g, \Box_w, A_1, A_2, A_3 \) and \( P_{sp1} \) are known.

Figure 4.5: Straight pipe example

In this example, gas and water flow rates are set at the inlet of the pipe (inflow BC), while the pressure \( (P_{sp1}) \) is defined at the outlet of the pipe (outflow BC). When the momentum
conservation equations are applied to the last momentum CV, it can be observed that additional
gas fractions and velocities are needed (represented with asterisks). In that case, zero curvature is
applied so those unknowns can be put as a function of the two previous ones and the number of
unknowns and equations can be balanced, thereby allowing the system to be solved.

**Gas mass balance equations for block 1-3**

\[
\begin{align*}
(\rho_g v_g \alpha_g A)_{1} - \Box_g &= 0 \\
(\rho_g v_g \alpha_g A)_{2} - (\rho_g v_g \alpha_g A)_{1} &= 0 \\
(\rho_g v_g \alpha_g A)_{3} - (\alpha_g \rho_g v_g A)_{2} &= 0
\end{align*}
\]

(4.28)

**Water mass balance equations for block 1-3**

\[
\begin{align*}
(\rho_w v_w \alpha_w A)_{1} - \Box_w &= 0 \\
(\rho_w v_w \alpha_w A)_{2} - (\rho_w v_w \alpha_w A)_{1} &= 0 \\
(\rho_w v_w \alpha_w A)_{3} - (\alpha_w \rho_w v_w A)_{2} &= 0
\end{align*}
\]

(4.29)

**Gas momentum balance equations**

\[
\begin{align*}
(\alpha_g \rho_g v_g^2)_{2} - (\alpha_g \rho_g v_g^2)_{1} + \overline{\alpha_{g'1}}((PA)_{2} - (PA)_{1}) &= -(\alpha_g \overline{F_{gg}} + \overline{F_{gw}} - \overline{F_{i1}}) \Delta x_1 \\
(\alpha_g \rho_g v_g^2)_{3} - (\alpha_g \rho_g v_g^2)_{2} + \overline{\alpha_{g'2}}((PA)_{3} - (PA)_{2}) &= -(\alpha_g \overline{F_{gg}} + \overline{F_{gw}} - \overline{F_{i2}}) \Delta x_2 \\
(\alpha_g \rho_g v_g^2)_{3} - (\alpha_g \rho_g v_g^2)_{2} + \overline{\alpha_{g'3}}((P_{sp1}A)_{3} - (PA)_{3}) &= -(\alpha_g \overline{F_{gg}} + \overline{F_{gw}} - \overline{F_{i3}}) \Delta x_3
\end{align*}
\]

(4.30)

**Water momentum balance equations**

\[
\begin{align*}
(\alpha_w \rho_w v_w^2)_{2} - (\alpha_w \rho_w v_w^2)_{1} + \overline{\alpha_{w'1}}((PA)_{2} - (PA)_{1}) &= -(\alpha_w \overline{F_{wg}} + \overline{F_{ww}} + \overline{F_{i1}}) \Delta x_1
\end{align*}
\]
\[
(\alpha_w \rho_w v_w^2)_{3} - (\alpha_w \rho_w v_w^2)_{2} + \alpha_w w^2((PA)_{3} - (PA)_{2}) = -(\alpha_w \bar{F}_{wg} + \bar{F}_{ww} + \bar{F}_{1})_2 \Delta x_2
\]

\[
(\alpha_w \rho_w v_w^*_{3} - (\alpha_w \rho_w v_w^*_{2})_3 + \alpha_w \bar{w^3}((P_{sp1}A)_{3} - (PA)_{3}) = -(\alpha_w \bar{F}_{wg} + \bar{F}_{ww} + \bar{F}_{1})_3 \Delta x_3
\]

(4.31)

Zero Curvature at pipe outlet ($\Delta x =$ uniform along the pipe)

\[
\alpha_g^* = 2\alpha_3 - \alpha_2
\]

\[
\alpha_w^* = 2\alpha_3 - \alpha_2
\]

\[
v_g^* = 2v_3 - v_2
\]

\[
v_w^* = 2v_3 - v_2
\]

\[
\bar{\alpha}_g^1 = \frac{\alpha_1 + \alpha_2}{2}
\]

(4.32)

Water fractions correlations

\[
\alpha_{w1} = 1 - \alpha_1
\]

\[
\alpha_{w2} = 1 - \alpha_2
\]

\[
\alpha_{w3} = 1 - \alpha_3
\]

(4.33)

Gas holdup averages

\[
\bar{\alpha}_g^1 = \frac{\alpha_1 + \alpha_2}{2}
\]

\[
\bar{\alpha}_g^2 = \frac{\alpha_2 + \alpha_3}{2}
\]

\[
\bar{\alpha}_g^3 = \frac{\alpha_3 + \alpha_g^*}{2}
\]

(4.34)
Water holdup averages

\[
\begin{align*}
\bar{\alpha}_{w1} &= \frac{\alpha_{w1} + \alpha_{w2}}{2} \\
\bar{\alpha}_{w2} &= \frac{\alpha_{w2} + \alpha_{w3}}{2} \\
\bar{\alpha}_{w3} &= \frac{\alpha_{w3} + \alpha_{w}}{2}
\end{align*}
\]

(4.35)

As summarized in Table 4.1, 19 equations result for 12 principal unknowns, 3 water fractions, and 4 BCs are defined. \( F_{gg}, F_{gw}, F_{wg}, F_{ww} \) and \( F_i \) are functions of the principal unknowns, as discussed in section 4.7.

<table>
<thead>
<tr>
<th>Unknowns</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P_1, P_2, P_3, )</td>
<td>3 gas mass conservation equations</td>
</tr>
<tr>
<td>( v_{g1}, v_{g2}, v_{g3}, )</td>
<td>3 water mass conservation equations</td>
</tr>
<tr>
<td>( v_{w1}, v_{w2}, v_{w3}, )</td>
<td>3 gas momentum conservation equations</td>
</tr>
<tr>
<td>( \alpha_{g1}, \alpha_{g2}, \alpha_{g3}, )</td>
<td>3 water momentum conservation equations</td>
</tr>
<tr>
<td>( \bar{\alpha}<em>{g1}, \bar{\alpha}</em>{g2}, \bar{\alpha}_{g3}, )</td>
<td>3 gas holdup averages</td>
</tr>
<tr>
<td>( \alpha_{w1}, \alpha_{w2}, \alpha_{w3}, )</td>
<td>3 water holdup averages</td>
</tr>
<tr>
<td>( \bar{\alpha}<em>{w1}, \bar{\alpha}</em>{w2}, \bar{\alpha}_{w3}, )</td>
<td></td>
</tr>
</tbody>
</table>

- 3 water holdup correlations
- 4 Zero Curvature at pipe outlet

| Total: 25 unknowns | Total: 25 Equations |

Specifications: \( Q_g, Q_w \) at inlet and \( P_{sp1} \) at outlet
Closure relationships: \( F_{gg}, F_{gw}, F_{wg}, F_{ww}, F_i \)
4.6.2 Modeling a tee network junction

A key point for solving a gas pipeline network is an accurate prediction of the phase splitting at the junction. This is neither a trivial nor a resolved task, since the effect of the fluid distribution will determine the quantity and quality of the natural gas at the points of demand. Accumulation of water at specific points of the network brings out an additional operational compression cost and can even compromise the future of the surface operations, since it can greatly impact the economics of the surface network and its production facilities. Figure 4.6 depicts a schematic of a Tee junction in which gas and water are injected at the inlet; the exact amount of gas and water that splits into the run and the branch, or the Tee junction, is unknown. The branch line is commonly found to have a $90^\circ$ angle with respect to the main line in natural gas pipe networks and that is a valid assumption for our study.

In Figure 4.6, $\lambda_{gR}$ and $\lambda_{wR}$ represents the mass fraction of gas and water running through the run of the Tee-junction with respect to the original injected at the inlet. This is:
\[ \lambda_{gR} = \frac{\dot{M}_{gR}}{\dot{M}_{gln}} ; \lambda_{wR} = \frac{\dot{M}_{wR}}{\dot{M}_{wln}} \]

(4.36)

\( \lambda_{gB} \) and \( \lambda_{wB} \) represents the mass fraction of gas and water running through the branch of the T-junction with respect to the original injected at the inlet. This is:

\[ \lambda_{gB} = \frac{\dot{M}_{gB}}{\dot{M}_{gln}} ; \lambda_{wB} = \frac{\dot{M}_{wB}}{\dot{M}_{wln}} \]

(4.37)

where:

\[ \lambda_{gR} + \lambda_{gB} = 1 ; \lambda_{wR} + \lambda_{wB} = 1 \]

(4.38)

A significant amount of research has been conducted for the determination of two-phase split for different branch angles, different fluids, pipe inclinations, nature of the junctions edges, downstream velocity ratios and initial liquid holdups. Although some empirical correlations have been developed for those specific flow conditions a more generalized approach has to be employed. The Bernoulli equation happens to be the most employed correlation used to state the mechanical energy balances to each phase at the junction. The four streams can be seen in Figure 4.7 and the Bernoulli equation can be written for each phase for an equi-potential system as follows:

![Tee figure](image_url)

Figure 4.7: Tee figure
\[(P_1 - P_2)_G + \frac{1}{2} \rho_G (V_{g1}^2 - V_{g2}^2) = K_{12} \frac{1}{2} \rho_G V_{g1}^2 \]

\[(P_1 - P_3)_G + \frac{1}{2} \rho_G (V_{g1}^2 - V_{g3}^2) = K_{13} \frac{1}{2} \rho_G V_{g1}^2 \]

\[(P_1 - P_2)_w + \frac{1}{2} \rho_w (V_{w1}^2 - V_{w2}^2) = K_{12} \frac{1}{2} \rho_G V_{w1}^2 \]

\[(P_1 - P_3)_w + \frac{1}{2} \rho_w (V_{w1}^2 - V_{w3}^2) = K_{13} \frac{1}{2} \rho_G V_{w1}^2 \]

(4.39)

where:

\( G, w = \) Gas and water phases

\( K_{12}, K_{13}, K'_{12}, K'_{13} = \) Frictional loss coefficients

Previous work conducted by Fortuin et al. (1990) have determined that the determination of these frictional loss coefficients can be accomplished with published Gardel (1957) correlations. As we can observe, a high amount of empiricism is needed, since many possible situations can be found that will change the values of those parameters. Fortuin (1990) shows how based on these equations, and assuming that \((P_2 - P_3)_c = (P_2 - P_3)_n\), the branch mass intake fraction \( \lambda_L \) for gas-liquid flow through a horizontal regular Tee junction can be predicted as:

\[
\frac{\rho_G W_{Gin}^2}{\rho_L W_{Lin}^2} \left[ W_{GR}^2 - W_{GB}^2 \right] - \left[ \frac{W_{LR}^2}{W_{Lin}^2} - \frac{W_{LB}^2}{W_{Lin}^2} \right] + \frac{2 g}{W_{Lin}^2} \left\{ \frac{\rho_G}{\rho_L} (Z_{GR} - Z_{GB}) - (Z_{LR} - Z_{LB}) \right\} \\
= \frac{\rho_G W_{Gin}^2}{\rho_L W_{Lin}^2} (K_{13} - K_{12}) - (K'_{13} - K'_{12}) 
\]

(4.40)

Equation (4.40) can be further simplified under the assumptions of equal liquid holdups for inlet, run and branch sides of the Tee and horizontal Tee junction with small liquid holdups to:
\[ \lambda_L = \lambda_0 + \alpha K_o (\lambda_G - \lambda_0) \]  

(4.41)

where:

\[ \lambda_0 = 0.5 (1 + K_{12} - K_{13}) \]

\[ K_0 = \frac{\rho_G V^2_{G1}}{\rho_L V^2_{L1}} \]

\[ \alpha = \text{constant dependent on velocity profile in the liquid film in the inlet} \]

Hart's trends (dashed lines) can be deduced from his paper "Route Selectivity for Gas-Liquid Flow in Horizontal T Junctions" (1990). This model shows good results for horizontal air-liquid flows with small liquid holdups values, as Figure 4.8 depicts.

Figure 4.8: Hart air water flow for small liquid holdup values
The same Equation (4.40) with different assumptions can lead to different behavior. For instance, if the pressure drop along each side of the Tee for each phase is the same it can be obtained that:

\[
\lambda_L = K_o \lambda_G + \frac{(1 - K_o)(K_{12} - K_{13} + 1)}{2}
\]  

(4.42)

Figure 4.9: New correlation Air water flow for small liquid holdup values

As Figure 4.9 depicts, this particular correlation does not agree as well as Hart's but this should be analyzed from the point of view that the friction loss coefficients are empirically calculated to agree with the specific Bernoulli equations, and another set of friction coefficients can be obtained to match the experimental data for specific conditions.
4.7 Numerical method challenges

A single-phase flow is, when treated as a transient problem, unconditionally stable for the fully-implicit numerical scheme. Although the single-pressure two-phase flow model is mathematically ill-posed due to the existence of complex characteristics, numerical discretizations take care of this challenge [Dinh, (2003)]. Many of the numerical methods employed are somehow empirical, since they are developed as a result of a trial-and-error process to make them work under certain specific conditions.

This work aims to show that the steady-state mass and momentum conservation equations can be used to solve complex two-phase flow network problems. The most difficult challenge is, since the Newton-Raphson method is used to solve the non-linear system of equations, the initial value that has to be given in order for the method to converge. Although it is not the answer to all the problems, implementation of the Global Convergent Method helps toward finding the roots of the system (Appendix D).

When a single phase appears in a control volume, the mass of the other phase should be substituted by a dummy equation that leads towards a zero or 1 solution, depending on the phase. At the same time, the momentum equation should be modified such that values close to 0 or 1 are used, avoiding the momentum equation from becoming singular.

4.8 Newton Raphson solution

In order to solve the non-linear system of equations derived from our discrete equations of mass, momentum and energy conservation at each CV, the Newton-Raphson method is
implemented. The basic idea consists of producing a Taylor series expansion and truncating it at the first partial derivative in order to obtain an improvement from the initial estimated solution.

Let us say that we have the following system of $n$ non-linear equations, expressed in their residual form:

\[
\begin{align*}
  f_1(x_1, x_2, x_3, \ldots, x_n) &= 0 \\
  f_2(x_1, x_2, x_3, \ldots, x_n) &= 0 \\
  f_3(x_1, x_2, x_3, \ldots, x_n) &= 0 \\
  \cdots \\
  f_n(x_1, x_2, x_3, \ldots, x_n) &= 0
\end{align*}
\]

(4.43)

If $x_1, x_2, x_3, \ldots, x_n$ are our initial values, we can produce a Taylor series expansion as truncated at the first derivative as follows:

\[
\begin{align*}
  0 &\equiv f_1(x_2, x_3, \ldots, x_n) + \Delta x_1 \frac{\partial f_1}{\partial x_1} + \Delta x_2 \frac{\partial f_2}{\partial x_2} + \Delta x_3 \frac{\partial f_3}{\partial x_3} + \ldots + \Delta x_n \frac{\partial f_n}{\partial x_n} \\
  0 &\equiv f_2(x_1, x_3, \ldots, x_n) + \Delta x_1 \frac{\partial f_1}{\partial x_1} + \Delta x_2 \frac{\partial f_2}{\partial x_2} + \Delta x_3 \frac{\partial f_3}{\partial x_3} + \ldots + \Delta x_n \frac{\partial f_n}{\partial x_n} \\
  0 &\equiv f_3(x_1, x_2, x_3, \ldots, x_n) + \Delta x_1 \frac{\partial f_1}{\partial x_1} + \Delta x_2 \frac{\partial f_2}{\partial x_2} + \Delta x_3 \frac{\partial f_3}{\partial x_3} + \ldots + \Delta x_n \frac{\partial f_n}{\partial x_n} \\
  \cdots \\
  0 &\equiv f_n(x_1, x_2, x_3, \ldots, x_n) + \Delta x_1 \frac{\partial f_1}{\partial x_1} + \Delta x_2 \frac{\partial f_2}{\partial x_2} + \Delta x_3 \frac{\partial f_3}{\partial x_3} + \ldots + \Delta x_n \frac{\partial f_n}{\partial x_n}
\end{align*}
\]

(4.44)

In matrix form we can put it as:
The system can be solved and the initial guess is updated as follows:

\[
\begin{bmatrix}
\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \cdots & \frac{\partial f_1}{\partial x_n} \\
\frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \cdots & \frac{\partial f_2}{\partial x_n} \\
\frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} & \cdots & \frac{\partial f_3}{\partial x_n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \frac{\partial f_n}{\partial x_3} & \cdots & \frac{\partial f_n}{\partial x_n}
\end{bmatrix}
\begin{bmatrix}
\Delta x_1 \\
\Delta x_2 \\
\Delta x_3 \\
\vdots \\
\Delta x_n
\end{bmatrix}
= -
\begin{bmatrix}
f_1 \\
f_2 \\
f_3 \\
\vdots \\
f_n
\end{bmatrix}
\]

(4.45)

The system can be solved and the initial guess is updated as follows:

\[
x_1 = x_1 + \Delta x_1 \\
x_2 = x_2 + \Delta x_2 \\
x_3 = x_3 + \Delta x_3 \\
\vdots \\
x_n = x_n + \Delta x_n
\]

(4.46)

Please refer to Appendix D for more detailed information regarding the employed Global Convergent Newton Raphson.

### 4.8.1 Straight pipe Newton Raphson example

For the previously described case of straight pipe (Figure 4.5) twelve residuals derived from the mass and momentum conservation equations can be obtained. \( R_{mki} \) represents the residual derived from the mass equations of phase k at block i, while \( R_{moki} \) represents the residual derived from the momentum equations of phase k at block i.
\[ R_{mg1} = \left( \rho_g v_g \alpha_g A \right)_1 - \dot{M}_g \]
\[ R_{mg2} = \left( \rho_g v_g \alpha_g A \right)_2 - \left( \rho_g v_g \alpha_g A \right)_1 \]
\[ R_{mg3} = \left( \rho_g v_g \alpha_g A \right)_3 - \alpha_{g2} \rho_{g2} \left( v_g A \right)_2 \]
\[ R_{mw1} = \left( \rho_w v_w \alpha_w A \right)_1 - \dot{M}_w \]
\[ R_{mw2} = \left( \rho_w v_w \alpha_w A \right)_2 - \left( \rho_w v_w \alpha_w A \right)_1 \]
\[ R_{mw3} = \left( \rho_w v_w \alpha_w A \right)_3 - \alpha_{w2} \rho_{w2} \left( v_w A \right)_2 \]
\[ R_{mg1} = \left( \alpha_g \rho_g v_g^2 \right)_1 - \left( \alpha_g \rho_g v_g^2 \right)_1 + \left( PA \right)_2 - \left( PA \right)_1 + \left( \alpha_g \vec{F}_{gw} + \vec{F}_{gw} - \vec{F}_i \right)_1 \]
\[ R_{mg2} = \left( \alpha_g \rho_g v_g^2 \right)_2 - \left( \alpha_g \rho_g v_g^2 \right)_2 + \left( PA \right)_3 - \left( PA \right)_2 + \left( \alpha_g \vec{F}_{gw} + \vec{F}_{gw} - \vec{F}_i \right)_2 \]
\[ R_{mg3} = \left( \alpha_g \rho_g v_g^2 \right)_3 - \left( \alpha_g \rho_g v_g^2 \right)_3 + \left( P_{sp1} \right)_3 - \left( PA \right)_3 + \left( \alpha_g \vec{F}_{gw} + \vec{F}_{gw} - \vec{F}_i \right)_3 \]
\[ R_{mw1} = \left( \alpha_w \rho_w v_w^2 \right)_2 - \left( \alpha_w \rho_w v_w^2 \right)_2 + \left( PA \right)_2 - \left( PA \right)_1 + \left( \alpha_w \vec{F}_{gw} + \vec{F}_{gw} + \vec{F}_i \right)_1 \]
\[ R_{mw2} = \left( \alpha_w \rho_w v_w^2 \right)_3 - \left( \alpha_w \rho_w v_w^2 \right)_3 + \left( PA \right)_3 - \left( PA \right)_2 = -\left( \alpha_w \vec{F}_{gw} + \vec{F}_{ww} + \vec{F}_i \right)_2 \]
\[ R_{mw3} = \left( \alpha_w \rho_w v_w^2 \right)_3 - \left( \alpha_w \rho_w v_w^2 \right)_3 + \left( P_{sp1} \right)_3 - \left( PA \right)_3 = -\left( \alpha_w \vec{F}_{gw} + \vec{F}_{ww} + \vec{F}_i \right)_3 \]
(4.47)
The structure of the Jacobian matrix can be observed in Equation (4.48).

$$
\begin{vmatrix}
\frac{\partial R_{mg1}}{\partial P_1} & \frac{\partial R_{mg1}}{\partial P_2} & \frac{\partial R_{mg1}}{\partial P_3} & \frac{\partial R_{mg1}}{\partial V_{g1}} & \frac{\partial R_{mg1}}{\partial V_{g2}} & \frac{\partial R_{mg1}}{\partial V_{g3}} & \frac{\partial R_{mg1}}{\partial V_{w1}} & \frac{\partial R_{mg1}}{\partial V_{w2}} & \frac{\partial R_{mg1}}{\partial V_{w3}} & \Delta P_1 \\
\frac{\partial R_{mg2}}{\partial P_1} & \frac{\partial R_{mg2}}{\partial P_2} & \frac{\partial R_{mg2}}{\partial P_3} & \frac{\partial R_{mg2}}{\partial V_{g1}} & \frac{\partial R_{mg2}}{\partial V_{g2}} & \frac{\partial R_{mg2}}{\partial V_{g3}} & \frac{\partial R_{mg2}}{\partial V_{w1}} & \frac{\partial R_{mg2}}{\partial V_{w2}} & \frac{\partial R_{mg2}}{\partial V_{w3}} & \Delta P_2 \\
\frac{\partial R_{mg3}}{\partial P_1} & \frac{\partial R_{mg3}}{\partial P_2} & \frac{\partial R_{mg3}}{\partial P_3} & \frac{\partial R_{mg3}}{\partial V_{g1}} & \frac{\partial R_{mg3}}{\partial V_{g2}} & \frac{\partial R_{mg3}}{\partial V_{g3}} & \frac{\partial R_{mg3}}{\partial V_{w1}} & \frac{\partial R_{mg3}}{\partial V_{w2}} & \frac{\partial R_{mg3}}{\partial V_{w3}} & \Delta P_3 \\
\frac{\partial \text{other terms}}{\partial P_1} & \frac{\partial \text{other terms}}{\partial P_2} & \frac{\partial \text{other terms}}{\partial P_3} & \frac{\partial \text{other terms}}{\partial V_{g1}} & \frac{\partial \text{other terms}}{\partial V_{g2}} & \frac{\partial \text{other terms}}{\partial V_{g3}} & \frac{\partial \text{other terms}}{\partial V_{w1}} & \frac{\partial \text{other terms}}{\partial V_{w2}} & \frac{\partial \text{other terms}}{\partial V_{w3}} & \Delta \text{other terms}
\end{vmatrix}
= -
\begin{vmatrix}
\Delta R_{mg1} \\
\Delta R_{mg2} \\
\Delta R_{mg3} \\
\text{other terms}
\end{vmatrix}

(4.48)

Equation (4.48) represents a system of simultaneous algebraic equations that needs to be solved. In our preliminary calculations LU Decomposed [Press et al. (1994)] has been implemented.

4.9 Closure relationships

In order to fully determine our model, some closure relationships, so pressure, phase velocities, temperature and hold-up can be defined as the principal unknowns to be solved. Appendix B and Appendix C shows the water and gas properties as handled by the model.
4.9.1 Mass transfer term

The amount of water vapor in gas will be governed by pressure, temperature, and gas composition. The water content of gas increases as a function of temperature. The higher the temperature, the more water is in the gas. In order to calculate the rate of gas transfer from liquid, our model uses the Bukacek (1990) correlation. This correlation allows us to determine the water content of natural gas for pressures ranging from 15 to 10,000 psia and for temperatures ranging from 60 to 460° F. Once this amount is determined, the rate of mass transfer to a phase k is calculated as the difference between the water content of two consecutive control volumes:

\[ W = 47.484 \frac{P_v}{P} + 10^{(-3083.87 \div 4596.7 + 6.69449)} \]  

(4.49)

where:

\[ P_v = \text{Pressure vapor of water} \]
\[ P = \text{Total Pressure} \]
\[ T = \text{Temperature (°F)} \]
\[ W = \text{Pounds of water in the gas per MMscf of gas} \]

For the Pressure vapor of water calculation, the following Hyland and Wexler (1983) correlation is valid over the range from 273.15 K to 473.15 K:

\[ P_v = \sum_{i=-1}^{3} c_i T^i + 6.5459673 \ln T \]  

(4.50)

where:

\[ T = \text{Temperature (K)} \]
\[ c_{-1} = -5.8002206 \times 10^3 \]
\[ c_0 = 1.3914993 \]
\[ c_1 = -4.8640239 \times 10^{-2} \]
\[ c_2 = 4.1764768 \times 10^{-5} \]
\[ c_3 = -1.4452093 \times 10^{-8} \]

Thermodynamic models provide reliable results for estimating the water content of natural gas, although since they depend on an Equation of State (EOS), the calculations tend to be long and difficult. The work currently in progress by Song et al. is interesting, named Project 032 "Water content in natural gas", in which a FORTRAN code is being developed by this researcher in collaboration with Rice University, in order to calculate the water content of any natural gas composition at different ranges of pressure and temperature. Figure 4.10 shows the results after applying the Bukacek (1990) correlation.
4.9.2 Wall shear stress forces

Ayala (2001) presented a comprehensive and detailed study for calculating wall shear and interfacial forces for four different flow patterns. The proposed model uses that same formulation. Figure 4.11 shows sketches for both mist and smooth stratified flow conditions.
Using geometrical considerations, the hydraulic diameter, wetted areas per unit volume and interphase areas per unit volume for each flow pattern can be deduced, as shown in Table 4.2.

Table 4.2: Hydraulic diameters and wetted areas per unit volume

<table>
<thead>
<tr>
<th>Flow pattern</th>
<th>$d_{gh}$</th>
<th>$d_{wh}$</th>
<th>$A_{gw}$</th>
<th>$A_{ww}$</th>
<th>$A_{gl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single Phase</td>
<td>$D$</td>
<td></td>
<td>$4/D$</td>
<td>N/A</td>
<td></td>
</tr>
<tr>
<td>Mist</td>
<td>$D$</td>
<td>$D$</td>
<td>$\frac{4}{D} \alpha_g$</td>
<td>$\frac{4}{D} \alpha_w$</td>
<td>$\frac{3\alpha_w}{r_p}$</td>
</tr>
<tr>
<td>Smooth Stratified</td>
<td>$D \left( \frac{\pi \alpha_g}{\pi - \varnothing + \sin (\varnothing)} \right)$</td>
<td>$D \left( \frac{\pi \alpha_w}{\varnothing} \right)$</td>
<td>$\frac{4}{D} \left( \frac{\pi - \varnothing}{\pi} \right)$</td>
<td>$\frac{4}{D} \left( \frac{\varnothing}{\pi} \right)$</td>
<td>$\frac{4}{D} \left( \frac{\sin (\varnothing)}{\pi} \right)$</td>
</tr>
</tbody>
</table>

For the Smooth Stratified pattern, since the water hold-up $\alpha_w$ is known, the angle $\varnothing$ is calculated solving the following correlation derived from geometrical considerations, implementing the Newton-Raphson iterative procedure:

$$\alpha_w = \frac{2\varnothing - \sin (2\varnothing)}{2\pi}$$

(4.51)
After obtaining the hydraulic diameter, the Reynolds number of the phase $k$ can be calculated as:

$$\text{Re}_k = \frac{\rho_k \bar{v}_k d_{kh}}{\mu_k}$$

(4.52)

where:

- $\text{Re}_k$ = Reynolds number of phase $k$
- $\rho_k$ = Density of phase $k$
- $\bar{v}_k$ = Velocity of the phase $k$

Then the Fanning friction factor of the phase $k$ ($f_{kw}$) is calculated depending on whether it is laminar flow ($\text{Re}_k < 2100$) or turbulent flow ($\text{Re}_k > 2100$).

In the case of laminar flow:

$$f_{kw} = \frac{16}{\text{Re}_k}$$

(4.53)

In the case of turbulent flow Colebrooke correlation (Colebrook, 1939) is used:

$$\frac{1}{\sqrt{f_{kw}}} = -4 \log \left[ \frac{\varepsilon}{3.7065d_{kh}} \right] - \frac{5.0452}{\text{Re}_k} \log \left( \frac{(\varepsilon/d_{kh})}{2.8257} + \frac{5.8506}{\text{Re}_k^{0.8981}} \right)$$

(4.54)

where:

- $\varepsilon$ = Pipe roughness

The phase $k$ wall friction force per unit volume ($\overline{f}_{kw}$) is finally defined as:

$$\overline{f}_{kw} = A_{kw} f_{kw} \frac{\rho_k |\bar{v}_k| \bar{v}_k}{2}$$

(4.55)

where:

- $A_{kw}$ = Phase $k$ wetted wall area per unit volume
\[ f_{kw} = \text{Phase k Fanning friction factor} \]

### 4.9.3 Interfacial forces

In the case of mist flow, the maximum droplet size is calculated using the Weber number (We) as:

\[
\text{We} = \frac{2\rho_g (v_g - v_w)^2 r_{\text{max}}}{\sigma}
\]  \hspace{1cm} (4.56)

where:

- \( \rho_g \) = Gas density
- \( \sigma \) = Interfacial surface tension
- \( r_{\text{max}} \) = Maximum droplet radius

Assuming a Weber number of 12, \( r_{\text{max}} \) is calculated using Equation (4.57). Then, a modified Weber number can be calculated for viscous fluids as:

\[
\text{We} = 12 \left[ 1 + \left( \frac{\mu_w}{2\rho_f r_{\text{max}} \sigma} \right)^{0.36} \right]
\]  \hspace{1cm} (4.57)

Using this new Weber number we can calculate again \( r_{\text{max}} \) with Equation (4.58). Then the mean droplet radius (\( r_p \)) is calculated as:

\[ r_p = 0.06147 r_{\text{max}} \]  \hspace{1cm} (4.58)

The interfacial force is then calculated as:
\[ \bar{\tau}_i = A_{gl}f_i \rho_g \left| \bar{v}_g - \bar{v}_w \right| \frac{(\bar{v}_g - \bar{v}_w)}{2} \]

(4.59)

where:

- \( A_{gl} \) = Interphase area per unit volume
- \( f_i \) = Interfacial friction factor
- \( \mu_k \) = Viscosity of the phase \( k \)

In the case of mist flow pattern, a new Reynolds number is defined as:

\[ Re = \frac{\rho_g 2r_p (\bar{v}_g - \bar{v}_w)}{\mu_g} \]

(4.60)

The following table shows the different correlations for the various Reynolds numbers of the drag coefficient \( C_d \) for rigid spheres presented by Cliff et al. (1978):

<table>
<thead>
<tr>
<th>Range</th>
<th>Correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re &lt; 0.01</td>
<td>( C_d = \frac{24}{Re} \left( 1 + \frac{3}{16} Re \right) )</td>
</tr>
<tr>
<td>0.01 &lt; Re &lt; 20</td>
<td>( C_d = \frac{24}{Re} \left( 1 + 0.1315 Re^{0.082-0.05w} \right) )</td>
</tr>
<tr>
<td>20 &lt; Re &lt; 260</td>
<td>( C_d = \frac{24}{Re} \left( 1 + 0.1935 Re^{0.6305} \right) )</td>
</tr>
<tr>
<td>260 &lt; Re &lt; 1500</td>
<td>( C_d = 10^{1.6435-1.1242w+0.1558w^2} )</td>
</tr>
<tr>
<td>1500 &lt; Re &lt; 12000</td>
<td>( C_d = 10^{-2.4571+2.558w-0.9295w^2+0.1049w^3} )</td>
</tr>
<tr>
<td>12000 &lt; Re &lt; 44000</td>
<td>( C_d = 10^{-1.9181+0.6370w-0.0636w^2} )</td>
</tr>
<tr>
<td>44000 &lt; Re &lt; 338000</td>
<td>( C_d = 10^{-4.3390+1.5809w-0.1546w^2} )</td>
</tr>
<tr>
<td>338000 &lt; Re &lt; 400000</td>
<td>( C_d = 29.78 - 5.3w )</td>
</tr>
<tr>
<td>400000 &lt; Re &lt; 10^6</td>
<td>( C_d = 0.1w - 0.49 )</td>
</tr>
</tbody>
</table>
Re > 10^6

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd = 0.19 - \frac{8 \cdot 10^4}{Re}</td>
<td></td>
</tr>
</tbody>
</table>

The interfacial friction factor for the mist flow is then calculated as $C_d/4$.

For the smooth stratified flow pattern, Baker et al. (1988) proposed an expression for the equivalent roughness ($\varepsilon_i$) assuming that the interfacial velocity is approximated to the liquid velocity. Applying this new equivalent to the Colebrook correlation (Colebrook, 1939) and applying it to the gas phase, the Fanning friction factor for the interface can be easily calculated.

$$\varepsilon_i = \begin{cases} 
\frac{34\sigma}{\rho_g v_w^2} & \text{if } \frac{\rho_g v_w^2 \mu_w^2}{\rho_w \sigma^2} \leq 0.005 \\
170\sigma \left( \frac{\rho_g v_w^2 \mu_w^2}{\rho_w \sigma^2} \right)^{0.30} & \text{if } \frac{\rho_g v_w^2 \mu_w^2}{\rho_w \sigma^2} > 0.005
\end{cases}$$

(4.61)
CHAPTER 5
RESULTS

5.1 Single pipe study

Studies of air-water co-current flow have been considered, as well as single air flow in horizontal pipes. The water density and compressibility factor of air are considered as constant. Figure 5.1 depicts the single pipe case considered. Pipe gas and water properties are summarized in Table 5.1.

Table 5.1: Single pipe system properties

<table>
<thead>
<tr>
<th>System Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (F)</td>
<td>85.7</td>
</tr>
<tr>
<td>Air molecular weight (lmb/lbmol)</td>
<td>29</td>
</tr>
<tr>
<td>Roughness (ft)</td>
<td>0.008</td>
</tr>
<tr>
<td>Water density (lbm/ft³)</td>
<td>32.303</td>
</tr>
<tr>
<td>Air viscosity (cp)</td>
<td>0.01827</td>
</tr>
<tr>
<td>Water viscosity (cp)</td>
<td>1.78</td>
</tr>
<tr>
<td>Surface tension (lbf/ft)</td>
<td>0.048</td>
</tr>
<tr>
<td>Pipe diameter (in)</td>
<td>2</td>
</tr>
<tr>
<td>Pipe length (ft)</td>
<td>3000</td>
</tr>
</tbody>
</table>

Figure 5.1: Horizontal pipe
Simulations were run for the case of single-phase gas running through the pipe as well as two-phase flow mist and smooth stratified flow patterns. Figure 5.2 depicts the pressure loss along the pipe for the different flow conditions. It is observed that as distance from the inlet increases, pressure decreases due to frictional forces created as a result of the contact of the fluid with the pipe wall. In the case of two-phase flow, there are additional friction forces due to the interfacial forces. Additional pressure loss can also be observed due to the two-phase flow in comparison with the single phase flow.

Figure 5.2: Single horizontal pipe pressure profiles
Similarly, Figure 5.3 and Figure 5.4 depict gas and liquid velocities along the pipe. The mist flow pattern presents a relatively homogeneous distribution of liquid phase in the gas phase with respect to the smooth stratified flow pattern. As a result, gas and liquid velocities tend to be closer for the mist flow pattern since the liquid droplets have a tendency of being carried by the gas phase.

Figure 5.3: Single horizontal pipe gas velocity profiles
Figure 5.4 shows the liquid hold-up variation along the pipe for both flow patterns. It is fair to be noted that the liquid hold-up variation along the pipe for the smooth stratified flow pattern is greater than the one experimented by the mist flow pattern. Again, the homogeneous distribution of the liquid phase in the gas phase in the case of mist flow holds the answer to justify that behavior.
5.2 Importance of the discretization methodology

Although the conservation equations and their deduction are straightforward, the discretization of them leads to intrinsic difficulties. To illustrate the importance of this point, two different discretizations have been employed. The difference between them is that the gas holdup used in the momentum conservation equations has not been averaged between the two adjacent CVs in the first formulation as it is supposed to be according to the proposed formulation. The fluid properties are the same as the ones used in

Table 5.1. For each case, the gas holdup at the outlet of the pipe has been specified using three different formulations: 1) calculating the gas holdup in such a way that mass is conserved
also in the last momentum CV, 2) applying zero curvature and 3) specifying a fixed zero curvature at the user's will. Figure 5.6 depicts the horizontal pipe under smooth stratified flow conditions.

![Horizontal Pipe](image)

**Figure 5.6: Horizontal pipe smooth stratified flow**

Figure 5.7 and Figure 5.8 depict the pressure profile under each formulation and each different gas holdup specification. By not averaging the gas holdups between two adjacent CVs, different pressure profiles are created under different holdup specifications at the outlet of the pipe; in contrast, by averaging the gas holdups, the same pressure profiles are created for all of the gas holdup outlet specifications. The same situation occurs with gas and liquid velocity profiles and with the holdups. Figure 5.9 depicts the water holdup profile, which is greater than the one depicted in Figure 5.5. This was expected due to the fact that the water flow rate has been increased. It can be also observed how in the case of an arbitrarily fixed holdup specified at the outlet, averaging adjacent holdups is capable of generating a consistent profile with the exception of the last CV, where the numbers are forced by way of the user's will to show the effect of the different discretization schemes.
Figure 5.7: Single horizontal pipe pressure profile with no hold-up averaging

Figure 5.8: Single horizontal pipe pressure profile with hold-up averaging
Figure 5.9: Single horizontal pipe water holdup profile with hold-up averaging

5.3 One-phase flow at a Tee-junction

The following Tee-junction has been analyzed for the case of natural gas single phase flow. Gas properties are obtained as detailed in Appendix C. The implemented Tee-junction for this case model does not account for the additional irreversible losses that occur at the Tee, assuming that such losses are negligible compared to the actual pipe pressure drops. Figure 5.10 depicts the number of CVs used to discretize the system. All three pipes are 4.0" in diameter and have a roughness of 0.0006'. Gas gravity is 0.5524 and the temperature is considered constant and equal to 75 degrees Fahrenheit. In order to simulate the Tee, the CV representing the regular
junction (CV number 6) is only 1’ long, compared to the length of the rest of the CVs (2000’). Pressures at the outlets are also depicted in Figure 5.10.

![Diagram of Tee-junction discretization](image)

Figure 5.10: Single-phase gas flow at Tee-junction discretization

The analytical solution of this junction using PSUGasNet software for the pressure at the junction and assuming that twice the gas flow rate goes into the run compared to the branch is 650.5 psia. Our model gives us a junction pressure of 649.6 being the difference between them 0.1%. Figure 5.11: Single-phase gas flow at Tee-junction depicts the pressure distribution along the inlet, run and branch pipes. It can be observed how the pressure drop in the run is higher than in the branch, something expected since more gas is diverted into it. In order to run the model, it was specified that out of the 12 MMSCF/D of gas rate in the inlet, two-thirds (2/3) of that gas would go into the run. Our model predicts that 66.45% of the initial gas will go into the run, being the difference between both models 0.3%.
Figure 5.11: Single-phase gas flow at Tee-junction

If irreversible losses want to be accounted for in our modeled junction, Bernoulli's equation has to be implemented. Equations (5.1) state the Bernoulli equation as applied to the Double Stream Models and where water and gas inlet velocities serve as a reference from which the differences in pressure between the run and branch can be calculated based on friction loss coefficients. The implementation of the two first equations for the case of single phase flow will allow our model to conserve the Bernoulli equations at the junction.
For illustration, a simulation has been performed on the Tee-junction with 4" diameter pipes, which is depicted in Figure 5.12. Since the outlet pressures are specified to be the same value if there was not a different pressure sensed at the junction by run and branch, the pressure and velocity profiles would be the same in both of them. For this particular case the friction loss coefficients \( K_{12} \) and \( K_{13} \) have been set at 0.4 and 1.0 values, respectively.

\[
(P_1 - P_2)_g + \frac{1}{2} \rho_g (V_{g1}^2 - V_{g2}^2) = K_{12} \frac{1}{2} \rho_g V_{g1}^2
\]

\[
(P_1 - P_3)_g + \frac{1}{2} \rho_g (V_{g1}^2 - V_{g3}^2) = K_{13} \frac{1}{2} \rho_g V_{g1}^2
\]

\[
(P_1 - P_2)_w + \frac{1}{2} \rho_w (V_{w1}^2 - V_{w2}^2) = K'_{12} \frac{1}{2} \rho_w V_{w1}^2
\]

\[
(P_1 - P_3)_w + \frac{1}{2} \rho_w (V_{w1}^2 - V_{w3}^2) = K'_{13} \frac{1}{2} \rho_w V_{w1}^2
\]

(5.1)

Figure 5.13 depicts the phenomenon that occurs at the junction, conserving Bernoulli’s equation and creating a different pressure profile at the junction outlets that will be, in the end, responsible for the amount of mass flux that goes into the run and the branch. Knowing in depth
the pressure loss coefficients for the specific junction is key to determining those different pressures experienced at the junction.

![Single-phase gas flow pressure profile at Tee-junction with Bernoulli](image)

It is very important to note that these new pressures observed at the outlet of the junction cause a change to our equations in the sense that phases densities and all the properties of the phase that depend on the pressure have to be modified and calculated using these new pressures.

**5.4 Two-phase flow at a Tee-junction**

From analyzing Equation (5.1), it can be observed that in formulation, both phases face a different set of pressures. In our proposed model we are stating that those pressures, the ones that both phases undergo, have to be the same. At any rate, it is possible to formulate Bernoulli's
conservation equation as long as the loss coefficients are calculated in accordance with that formulation, but also and most importantly, in such a way that agrees with the discretized model employed. Since our discretized model aims towards a common shared pressure for both phases, the mass split of the liquid phase can be obtained as a function of the gas split, which must be known in order to obtain the gas and water splits.

Shoham et al (1987) produced some experimental results for two-inch diameter horizontal Tee-junctions. The experiment consisted of injecting air and water at atmospheric conditions, varying the pressure at the end of the branch while keeping the rest of the variables constant, and then analyzing the route selectivity of the air and the water. Fortuin et al (1990) formulated a model to predict the route selectivity based on the double stream model and the Bernoulli equation at the Tee-junction. His model requires several empirical parameters including frictional loss coefficients taken from Gardel (1957), liquid hold-up (obtained from a semi-empirical correlation that they formulated in 1989 for small liquid hold-ups) and some coefficients that depend on whether the fluid is turbulent or laminar. In doing so, a series of straight lines on a plot of liquid branch fraction versus gas branch fractions were obtained. Hart's trends (dashed lines) can be deduced from his paper, "Route Selectivity for Gas-Liquid Flow in Horizontal T Junctions" (1990). For the particular case studied, the equations of those lines are as follows:

\[
\lambda_L = 0.07 + 1 \cdot 0.554997(\lambda_G - 0.07) \text{ for } UL = 0.0313 \frac{m}{s}
\]

\[
\lambda_L = 0.07 + 0.65 \cdot 1.495897(\lambda_G - 0.07) \text{ for } UL = 0.00724 \frac{m}{s}
\]

\[
\lambda_L = 0.07 + 0.65 \cdot 4.658191(\lambda_G - 0.07) \text{ for } UL = 0.00156 \frac{m}{s}
\]

(5.2)
Figure 5.14 depicts the liquid branch fraction ($\lambda_L$) versus the gas branch fraction ($\lambda_B$) when injecting gas at a superficial velocity at the inlet of 12.4 m/s for different water injection superficial velocities (UL) at the inlet and varying the pressure at the branch outlet. The dashed line represents the straight lines calculated using Fortuin's et al model (1990) while the black points represent some experimental results obtained by the University of Amsterdam.

Figure 5.14: Shoham experimental and Hart trends branch fractions

Our challenge is to validate our code with this experimental data under smooth stratified flow conditions and to somehow compare our results to those obtained by Fortuin et al (1990) and the experimental ones. To do this, a simulation was carried out using a regular five-foot length Tee-junction with a very small roughness parameter (0.0003 in), in order to obtain minimum pressure losses along the Tee-junction. The flow rate ratios (air superficial velocity over water superficial velocity) are the same as the ones used by the data collected at the University of
Amsterdam using 0.26% of the air flow rate used in their experiment. Figure 5.15 depicts the liquid branch fraction ($\lambda_L$) versus the gas branch fraction ($\lambda_B$) when injecting gas at a superficial velocity at the inlet of 12.4 m/s for different water injection superficial velocities (UL) at the inlet and varying the pressure at the branch outlet. The solid lines are the results of our simulations.

![Figure 5.15: Validation Shoham and Hart branch fractions experiment](image)

An important observation to be made is that, since the liquid fraction is a function of the gas fraction, it is possible to match the experimental results, as long as the right correlation is used. For the simulation result that appears circled as depicted in the previous figure pressure, liquid holdup and gas and water velocities profiles can be obtained. Although we simulated a small Tee-junction and no major changes in the profile are expected, it has to be noted the
importance of the route selectivity of the water since it occurs although the existence of minor profile changes. The following four figures show the different profiles along the Tee-junction.

Figure 5.16: Shoham and Hart simulation pressure profile

Figure 5.17: Shoham and Hart simulation water holdup profile
Figure 5.18: Shoham and Hart simulation gas velocity profile

Figure 5.19: Shoham and Hart simulation water velocity profile
5.5 Solving a Two-phase flow Network

The following example will solve the network depicted in Figure 5.20 under different conditions to demonstrate how our software can handle the resolution of them according with the equations of the proposed model. The model consists of 9 different pipes with internal diameters of 3" and roughness parameters of 0.003'. All of the CVs are 1000' in length, except those that are in a junction, where the length is only 1'. Gas and water fluid properties are handled as described in Appendices B and C.

The results of the simulation under isothermal (85.7°F) smooth stratified flow conditions and assuming that gas and water fractions are equal at the junction represented by CV 6 are presented in Table 5.2.
Table 5.2: Gas-water network solution

<table>
<thead>
<tr>
<th>CV</th>
<th>Pressure (psia)</th>
<th>Water Holdup</th>
<th>Gas Velocity (ft/s)</th>
<th>Water Velocity (ft/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>715.94</td>
<td>0.04478</td>
<td>4.8860</td>
<td>2.4565</td>
</tr>
<tr>
<td>2</td>
<td>712.88</td>
<td>0.04466</td>
<td>4.9082</td>
<td>2.4630</td>
</tr>
<tr>
<td>3</td>
<td>709.80</td>
<td>0.04454</td>
<td>4.9306</td>
<td>2.4697</td>
</tr>
<tr>
<td>4</td>
<td>706.71</td>
<td>0.04442</td>
<td>4.9534</td>
<td>2.4764</td>
</tr>
<tr>
<td>5</td>
<td>703.60</td>
<td>0.04434</td>
<td>4.9767</td>
<td>2.4810</td>
</tr>
<tr>
<td>6</td>
<td>702.04</td>
<td>0.02935</td>
<td>2.4589</td>
<td>1.8749</td>
</tr>
<tr>
<td>7</td>
<td>701.27</td>
<td>0.02933</td>
<td>2.4618</td>
<td>1.8763</td>
</tr>
<tr>
<td>8</td>
<td>699.74</td>
<td>0.02928</td>
<td>2.4675</td>
<td>1.8790</td>
</tr>
<tr>
<td>9</td>
<td>698.19</td>
<td>0.02924</td>
<td>2.4733</td>
<td>1.8817</td>
</tr>
<tr>
<td>10</td>
<td>696.65</td>
<td>0.02920</td>
<td>2.4791</td>
<td>1.8844</td>
</tr>
<tr>
<td>11</td>
<td>695.10</td>
<td>0.02915</td>
<td>2.4850</td>
<td>1.8877</td>
</tr>
<tr>
<td>12</td>
<td>701.28</td>
<td>0.02933</td>
<td>2.4555</td>
<td>1.8747</td>
</tr>
<tr>
<td>13</td>
<td>699.74</td>
<td>0.02928</td>
<td>2.4612</td>
<td>1.8774</td>
</tr>
<tr>
<td>14</td>
<td>698.20</td>
<td>0.02924</td>
<td>2.4670</td>
<td>1.8801</td>
</tr>
<tr>
<td>15</td>
<td>696.66</td>
<td>0.02920</td>
<td>2.4728</td>
<td>1.8828</td>
</tr>
<tr>
<td>16</td>
<td>695.11</td>
<td>0.02915</td>
<td>2.4786</td>
<td>1.8861</td>
</tr>
<tr>
<td>17</td>
<td>699.76</td>
<td>0.02928</td>
<td>2.4643</td>
<td>1.8782</td>
</tr>
<tr>
<td>18</td>
<td>698.99</td>
<td>0.02926</td>
<td>2.4672</td>
<td>1.8795</td>
</tr>
<tr>
<td>19</td>
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<tr>
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<td>5.1370</td>
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<td>0.04332</td>
<td>5.1625</td>
<td>2.5398</td>
</tr>
</tbody>
</table>

Velocities at entrance of CV 12: 2.4527, 1.8734
Figure 5.21 represents the pressure and liquid holdup profiles in a schematic way to visualize the change of pressure within the network.

Figure 5.21: Pressure profile at gas-water network
A more practical way of representing the network is by giving the inlet and outlet pressures of each pipe and averaging the velocities and holdups along those pipes. Calculating the actual mass flow rates along each pipe helps us to double check the material balance. Table 5.3 depicts the different parameters characteristic of each pipe.
Table 5.3: Gas-water network pipes smooth stratified flow conditions

<table>
<thead>
<tr>
<th>Pipe</th>
<th>Pin (psia)</th>
<th>Pout (psia)</th>
<th>Delta P (psia)</th>
<th>Water Holdup</th>
<th>Gas Velocity (ft/s)</th>
<th>Water Velocity (ft/s)</th>
<th>Qgas (MMscf/D)</th>
<th>Qwater (lbm/D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>717.47</td>
<td>702.04</td>
<td>1.53</td>
<td>0.0445</td>
<td>4.920</td>
<td>2.466</td>
<td>1.00</td>
<td>29000</td>
</tr>
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<td>694.32</td>
<td>7.73</td>
<td>0.0292</td>
<td>2.471</td>
<td>1.881</td>
<td>0.50</td>
<td>14500</td>
</tr>
<tr>
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<td>7.71</td>
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</tr>
<tr>
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<td>698.99</td>
<td>1.16</td>
<td>0.0293</td>
<td>2.464</td>
<td>1.878</td>
<td>0.50</td>
<td>14500</td>
</tr>
<tr>
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<td>698.99</td>
<td>694.33</td>
<td>4.65</td>
<td>0.0292</td>
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<td>1.883</td>
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<td>14500</td>
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<td>694.33</td>
<td>678.25</td>
<td>16.09</td>
<td>0.0436</td>
<td>5.094</td>
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<td>1.00</td>
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</tr>
<tr>
<td>7</td>
<td>678.25</td>
<td>644.02</td>
<td>34.23</td>
<td>0.0591</td>
<td>10.749</td>
<td>3.712</td>
<td>2.00</td>
<td>58000</td>
</tr>
<tr>
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<td>4.66</td>
<td>0.0292</td>
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<td>678.25</td>
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<td>5.101</td>
<td>2.519</td>
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</tr>
</tbody>
</table>

Table 5.4 depicts the same run but under mist flow conditions. It can be observed that, as expected, the pressure losses along the pipes are lower than in the smooth stratified flow conditions.

Table 5.4: Gas-water network pipes mist flow conditions

<table>
<thead>
<tr>
<th>Pipe</th>
<th>Pin (psia)</th>
<th>Pout (psia)</th>
<th>Delta P (psia)</th>
<th>Water Holdup</th>
<th>Gas Velocity (ft/s)</th>
<th>Water Velocity (ft/s)</th>
<th>Qgas (MMscf/D)</th>
<th>Qwater (lbm/D)</th>
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<tbody>
<tr>
<td>1</td>
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<td>6.59</td>
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<td>29000</td>
</tr>
<tr>
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<td>673.17</td>
<td>1.62</td>
<td>0.0351</td>
<td>2.587</td>
<td>1.572</td>
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</tr>
<tr>
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<td>674.79</td>
<td>673.18</td>
<td>1.61</td>
<td>0.0351</td>
<td>2.580</td>
<td>1.567</td>
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<td>14500</td>
</tr>
<tr>
<td>4</td>
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<td>674.16</td>
<td>0.24</td>
<td>0.0351</td>
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<td>0.50</td>
<td>14500</td>
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<tr>
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<td>673.18</td>
<td>0.98</td>
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<td>2.583</td>
<td>1.565</td>
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<td>6.72</td>
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</tr>
<tr>
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<td>666.46</td>
<td>644.02</td>
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<td>0.0269</td>
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<tr>
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<td>674.15</td>
<td>673.17</td>
<td>0.98</td>
<td>0.0352</td>
<td>2.583</td>
<td>1.566</td>
<td>0.50</td>
<td>14500</td>
</tr>
<tr>
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<td>673.17</td>
<td>666.46</td>
<td>6.70</td>
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<td>5.175</td>
<td>3.613</td>
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</tr>
</tbody>
</table>

Table 5.5 depicts the same run but under a single gas phase. It can be observed that, as expected, the pressure losses along the pipes are lower than in the smooth stratified and mist flow conditions, which emphasizes the importance of accurate pressure drop calculations in multiphase flow.
In all of the previous runs, we have been assuming that gas and water split fractions that occur at the control volume 6 are equal. But as we have seen, this is not always the case and it is the key to solving the route preferential phenomena. The next run will show how the model can handle this fact and how water route preferential can be determined if the Tee-junction is fully discretized with the corresponding friction loss factors or the water fraction split can be calculated as a function of the gas fraction split. We are again assuming smooth stratified flow conditions.

The pressure at the outlet is now specified at 630 psia and it is assumed that the mass for the run (Pipe 2), the water mass fraction, is 1.28 times the gas mass fraction in the same pipe. Under these conditions, the results of the simulation are presented in Table 5.6. In this case, and following the DSM model for natural gas and water, the simplified equation used to determine the different split fractions at the Tee is:

\[
\lambda_L = 0.07 + 1 \cdot 1.28(\lambda_G - 0.07)
\]

Table 5.5: Single-phase gas network pipes

<table>
<thead>
<tr>
<th>Pipe</th>
<th>Pin (psia)</th>
<th>Pout (psia)</th>
<th>Delta P (psia)</th>
<th>Gas Velocity (ft/s)</th>
<th>Qgas (MMscf/D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pipe 1</td>
<td>668.35</td>
<td>663.95</td>
<td>4.39</td>
<td>5.042</td>
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</tr>
<tr>
<td>Pipe 2</td>
<td>663.95</td>
<td>662.83</td>
<td>1.12</td>
<td>2.540</td>
<td>0.5</td>
</tr>
<tr>
<td>Pipe 3</td>
<td>663.95</td>
<td>662.84</td>
<td>1.11</td>
<td>2.527</td>
<td>0.5</td>
</tr>
<tr>
<td>Pipe 4</td>
<td>663.69</td>
<td>663.52</td>
<td>0.17</td>
<td>2.533</td>
<td>0.5</td>
</tr>
<tr>
<td>Pipe 5</td>
<td>663.52</td>
<td>662.84</td>
<td>0.68</td>
<td>2.535</td>
<td>0.5</td>
</tr>
<tr>
<td>Pipe 6</td>
<td>662.84</td>
<td>658.38</td>
<td>4.46</td>
<td>5.082</td>
<td>1.0</td>
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<tr>
<td>Pipe 7</td>
<td>658.38</td>
<td>644.02</td>
<td>14.36</td>
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</tr>
<tr>
<td>Pipe 8</td>
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<td>662.83</td>
<td>0.68</td>
<td>2.535</td>
<td>0.5</td>
</tr>
<tr>
<td>Pipe 9</td>
<td>662.83</td>
<td>658.38</td>
<td>4.45</td>
<td>5.094</td>
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</table>
Figure 5.23: Complex gas-water network with differential phase split at CV 6

Table 5.6: Gas-water network pipes smooth stratified flow conditions and differential split at CV 6

<table>
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<tr>
<th>Pipe</th>
<th>Pin (psia)</th>
<th>Pout (psia)</th>
<th>Delta P (psia)</th>
<th>Water Holdup</th>
<th>Gas Velocity (ft/s)</th>
<th>Water Velocity (ft/s)</th>
<th>Q_gas (MMscf/D)</th>
<th>Q_water (lbm/D)</th>
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<tr>
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<td>689.52</td>
<td>15.75</td>
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<td>681.11</td>
<td>8.42</td>
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<td>689.52</td>
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<td>7.74</td>
<td>0.0228</td>
<td>2.655</td>
<td>1.833</td>
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<td>687.73</td>
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<td>1.18</td>
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<td>2.512</td>
<td>1.900</td>
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</table>

We observe that our predictions are consistent with what was expected. The gas and water fractions obtained are a consequence of the type of junction that has been analyzed. Table
5.7 shows the comparison between both simulations. All the results are consistent with what should physically be expected.

Table 5.7: Gas-water network pipes smooth stratified flow conditions comparison

<table>
<thead>
<tr>
<th></th>
<th>$Q_{\text{gas}}$ (MMscf/D)</th>
<th>$Q_{\text{water}}$ (lbm/D)</th>
<th>Water Holdup</th>
<th>Gas Velocity (ft/s)</th>
<th>Water Velocity (ft/s)</th>
</tr>
</thead>
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<td>0.1%</td>
<td>1.9%</td>
<td>1.1%</td>
</tr>
<tr>
<td>Pipe 2</td>
<td>-6.1%</td>
<td>20.0%</td>
<td>-0.6%</td>
<td>-3.5%</td>
<td>-2.1%</td>
</tr>
<tr>
<td>Pipe 3</td>
<td>6.2%</td>
<td>-20.0%</td>
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<td>0.0%</td>
<td>1.9%</td>
<td>1.2%</td>
</tr>
<tr>
<td>Pipe 5</td>
<td>0.0%</td>
<td>0.0%</td>
<td>0.0%</td>
<td>1.9%</td>
<td>1.2%</td>
</tr>
<tr>
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</tr>
<tr>
<td>Pipe 7</td>
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<td>0.0%</td>
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<td>1.2%</td>
</tr>
<tr>
<td>Pipe 8</td>
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<td>0.0%</td>
<td>0.0%</td>
<td>2.0%</td>
<td>1.3%</td>
</tr>
<tr>
<td>Pipe 9</td>
<td>-3.1%</td>
<td>10.0%</td>
<td>-0.4%</td>
<td>-0.6%</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

The following figures depict the comparison between both scenarios. It can be observed that water and gas are not equally split at the Tee-junction.
Figure 5.25: Network water amount comparison

Figure 5.26: Network water holdup comparison
Figure 5.27: Network gas velocity comparison

Figure 5.28: Network water velocity comparison

- Red = +20%
- Green = -20%
5.6 Verification and validation of the code for Tee-junctions

In numerical simulations, verification and validation are important steps for understanding the behavior of a physical system. A simple definition of both is provided by Roache (1998): "Verification demonstrates that you are solving the equations right. Validation demonstrates that you are solving the right equations". Verification always comes before validation.

Because of the complexity of the physical phenomena that we are trying to model, a major challenge presents itself when fine-tuning our runs since the initial guesses have to be "good enough" in order for our Jacobian to converge properly. It is also important to analyze the consequences of the mesh size and its implications, as we have done in the previous point. In order to ensure that our code is doing what was intended, we referred to the Method of Manufactured Solutions (MMS). The idea is quite simple: to create a solution for our PDE system of equations and to run the code to make sure that that the solution is being obtained. We did that with the help of several spreadsheets in Excel to solve different cases of two-phase flow Tee-junctions. The code was able to arrive at the same solution and if that solution was fed into the code as our initial guess, only one iteration was necessary, proving that the Jacobian structure and the code were solving the equations correctly. As depicted in Figure 5.29, an Excel spreadsheet was built to verify the code for a two-phase isothermal flow pipe divided into three CVs. The light yellow cells around the graphic represent the input or entry data needed to define the system. Since this system contains 18 unknowns (3 pressures, 3 gas velocities, 3 water velocities, 3 gas fractions, 3 gas forces and 3 water forces) and we count with 12 conservation equations (3 gas mass conservation, 3 water mass conservation, 3 gas momentum conservation and 3 water momentum conservation), 6 unknowns have to be fixed. In this particular case, the 3 pressures
and the 3 gas velocities were our selected fixed unknowns, permitting us to create a manufactured solution.

Figure 5.29: Excel sheet for code verification

The numbers in orange in the spreadsheet represent the calculations performed to solve the non-linear system of equations. The grey cell is a check showing that the sum of the residuals of the conservation equations is equal to zero, showing again the full mass and momentum conservation of the equations. Another way to check the conservation of the equations and to verify the code is by plotting the mass and momentum fluxes divided by the initial mass and momentum that enters the pipe at the inlet. In doing this, the material and momentum balances can be obtained for the two phases and, if conservation is achieved, these values must be equal to

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<th>Entry data</th>
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<tr>
<td>Qw= 100 bbl/D</td>
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</tbody>
</table>

<table>
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<th>dx</th>
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<th>Eq mass</th>
<th>Moment out</th>
<th>Moment in</th>
<th>Pressures</th>
<th>Fg</th>
<th>Eq momentum</th>
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<th>Pressures</th>
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one for this to be true. Figure 5.30 depicts the material balances for the case previously studied of a straight pipe summarized in Table 5.1 and under smooth stratified two phase flow conditions.

![Figure 5.30: Verification of material and momentum balances]
CHAPTER 6

CONCLUDING REMARKS

An FVM one-dimensional, steady-state, isothermal, two-phase model has been developed to solve complex networks and to address the uneven split phenomenon that currently available software is not handling under two common flow patterns such as mist and smooth stratified. Liquids, especially water, are the major culprits of excessive losses not only in the wellbore but throughout the surface production system. Work has to be done on developing, testing, deploying and demonstrating an analytical tool that would serve the primary purpose of increasing throughput capacity and improving operational reliability of natural gas gathering network infrastructure by tracking the development of two-phase flow in the network system. Although industry has not been indifferent to the problem, the lack of predictive technology to tell them precisely where and how the liquid is distributed within the system and to determine the best strategy to get rid of it is still an unsolved problem.

6.1 Conclusions

During this comprehensive study the following conclusions capture the observations and recommendations that were made:

- The pressure drop calculated assuming single-phase flow is significantly lower than the one experienced when liquid and gas flow co-currently. FVM enables us to solve complex networks in single- and two-phase flow under mist and smooth stratified flow pattern conditions. Other flow pattern conditions are implemented
by using semi-empirical correlations that define the friction losses specific for those conditions.

- The two-phase flow physical reality is approximated by the two-fluid model. The accurate mapping of the pressure, velocities of both phases and fluid redistribution inside the network is proven critical since it can reduce additional compression costs caused by the liquid phase and help to make decisions regarding water removal and enhance system performance, so capacity can be maintained as close as possible to the designed maximum and supply-demand flow rates can be established to maximize operations.

- Wall roughness changes over time are due to erosion, corrosion, and deposits on specific areas with vortex and pipeline geometry changes. Time-dependent wall roughness should be studied to see the effects of this change in pipe deliverability.

- The water-tracking model can be complemented with corrosion models for a better understanding and design of natural gas networks, especially regarding its maintenance.

- Implementation of the energy conservation equation will solve for non-isothermal conditions. Incorporation of the temperature effect to study its influence in the uneven split phenomenon is important as well as the study of any implemented corrosion model under different temperature conditions.
• The need for a close initial guess is not as large an issue when solving for a single-phase flow. The major challenge arises when trying to solve for a two-phase flow, doubling the number of unknowns (isothermal case). The fact is that small changes in pressure result in a different route selectivity and that the inherent nature of the Newton-Raphson procedure, as an iterative method, makes it extremely difficult for the system to converge. The amount of time employed in coming up with an initial guess that was sufficient for convergence of the steady-state system of non-linear equations made us suspicious of the proposed practical steady-state solution. The set of equations is defined, but the numerical treatment to effectively solve them is the biggest challenge. A Global Convergent method helps to solve the initial guess challenge and its implementation is critical to solving complicated networks.

• The use of the imaginary staggered grid approach causes some inconvenience in terms of boundary conditions, both in diverging and converging structures. In the case of diverging, the challenge derives from the fact that the center of the staggered CV does not coincide with the spatial position of the velocity. To solve this challenge, our study proposes small CVs to discretize the junction CV. In a convergent junction, as depicted in Figure 6.1, it can be observed that the evaluation of the momentum flux for the momentum CV at the edge closest to the Tee needs a velocity that is not there physically. An easy solution employed by the industry is to consider that velocity is zero, since beyond it there is no velocity in that direction because of the wall, but that is not completely correct and creates some numerical error. A backward staggered approach solves this
issue within the converging junction, but creates the same dilemma when treating the diverging Tee-junction.

Figure 6.1: Converging Tee-junction velocity approximation

- Solve the conservation equations using transient analysis instead of steady-state conditions, although some stabilization techniques are required because of the ill-posed nature of multi-phase flow. Transient studies were conducted on single phase and preliminary results were satisfactory. Since single-phase flow is unconditionally stable no additional stabilization techniques were required.

- A more general deduction of the Bernoulli equation is proposed in this work. This new Bernoulli equation, expressed in terms of momentum, agrees better with the general procedure that has been employed to derive momentum conservation equations. Again, our starting point is the Euler Equation of Inviscid Motion:
\[ \rho u \nabla \cdot u = -\Delta P - \delta_{irr} \]

where:

\[ \Delta P = \text{Pressure drop} \]

\[ \delta_{irr} = \text{Irreversible losses} \]  \hspace{1cm} (6.1)

Integrating over the volume it can be obtained that:

\[ \int \nabla \cdot \rho u \, dV + \int (-\Delta P - \delta_{irr}) \, dV = 0 \]  \hspace{1cm} (6.2)

And applying now the divergence and gradient theorems to Equation (6.2),

\[ \int \rho uu \, dA + \int (-\Delta P) \, dA \int (-\delta_{irr}) \, dV = 0 \]  \hspace{1cm} (6.3)

Under the assumption of a regular CV (same areas) and discretizing and dividing for the volume, the final expression is obtained:

\[ \rho_2 v_2^2 - \rho_1 v_1^2 + P_2 - P_1 = \delta_{irr} \]  \hspace{1cm} (6.4)

The way the irreversible losses are calculated in terms of the different friction loss coefficients will determine the values of those losses, but now all the terms are expressed in momentums, obtaining a more homogeneous formulation to the problem. Once the irreversible losses are known, a general form of the liquid branch intake fraction as a function of downstream velocities and friction loss coefficients can be used to obtain the amount of each phase that goes into the different sides of the Tee-junction.

\[ \lambda_L = f(\lambda_g, K_o, K_{12}, K_{13}) \]  \hspace{1cm} (6.5)
• Comprehensive study of the type or types of Tee-junctions of the networks is fundamental to accurately define friction loss coefficients that will define the uneven split accordingly with the Bernoulli equation used.

• In the transition from two-phase to single phase, difficulties are encountered since the set of equations become singular. Following Frepoli's (2003) recommendations, creating a dummy equation is a possible way to solve this problem.
REFERENCES


Euler, L.: *Solutio Problematis ad geometriam situs*, 1736.


APPENDIX A

INTEGRAL THEOREMS

A.1 Divergence or Gauss-Ostrogradsky theorem

This theorem relates the flux of a vector field through a surface to the behavior of the vector field inside the volume defined by the closed surface. Figure A.1 represents a volume defined by a surrounded boundary area where $\mathbf{\hat{n}}$ is the outward pointing unit normal field of the boundary and the vector field is the mass flux term $\rho \mathbf{v}$. The divergence theorem states that the volume integral of the divergence is equal to the net flow across the closed boundary.

\[
\int_{V} \rho \mathbf{v} \cdot dV = \oint_{S} \rho \mathbf{v} \cdot d\mathbf{A}
\]

(A.1)

Figure A.1: Volume figure and vector field

A.2 Gradient theorem

Similar to the divergence theorem is the gradient theorem. The main difference is that now it is applied to any scalar field instead of to a vector field. Figure A.2 depicts the volume,
boundary area and scalar field pressure. The divergence theorem states that the volume integral of the gradient of a scalar field is equal to the net flow across the closed boundary.

![Figure A.2: Volume figure and scalar field](image)

\[ \int_V \nabla P \, dV = \oint_S P \, dA \]  
(A.2)

**A.3 Application to momentum conservation in a pipe CV**

Figure A.3 depicts a CV of a cylindrical pipe where both theorems will be applied to a single phase momentum equation conservation.

![Figure A.3: Control volume of pipe for momentum](image)

The momentum conservation equation states:

\[ \frac{d(\rho \vec{v})}{dt} + \rho \vec{v} \cdot \nabla \vec{v} = -\nabla P - \vec{F}_{kg} - \vec{F}_{kw} \]  
(A.3)
When Equation (A.3) is integrated over the control volume the following expression is obtained:

$$
\int_V \frac{d(\rho \bar{v})}{dt} dV + \int_V \rho \bar{v} \nabla \cdot \bar{v} dV = -\int_V \nabla P dV - \int_V \bar{F}_{kg} + \bar{F}_{kw} dV
$$

(A.4)

Divergence theorem can be applied to the second integral as follows:

$$
\int_V \rho \bar{v} \cdot \nabla \bar{v} dV = \rho \bar{v} \oint_S \bar{v} d\bar{A} = \rho \bar{v} \left( \oint_S \bar{v} d\bar{A}_1 + \oint_S \bar{v} d\bar{A}_2 + \oint_S \bar{v} d\bar{A}_3 \right)
$$

(A.5)

Recalling the definition of vector product:

$$
\bar{v} d\bar{A} = |\bar{v}||d\bar{A}| \cos(\bar{v} \wedge d\bar{A})
$$

(A.6)

It is observed that $d\bar{A}_3$ is perpendicular to $\bar{v}$, so the integral $\oint_S \bar{v} d\bar{A}_3$ is zero. Finally is the following expression is obtained for the integral:

$$
\int_V \rho \bar{v} \cdot \nabla \bar{v} dV = \rho \bar{v} \bar{v} A_1 - \rho \bar{v} \bar{v} A_2
$$

(A.7)

Gradient theorem can be applied for the third integral of Equation (A.4).

$$
\int_V \nabla P dV = \oint_S P d\bar{A}_1 + \oint_S P d\bar{A}_2 + \oint_S P d\bar{A}_3
$$

(A.8)

Recalling that the flow is unidirectional, the gradient of the pressure in any other direction is zero. For this reason it can be established that:

$$
\int_V \nabla P dV = P \bar{A}_1 - P \bar{A}_2
$$

(A.9)
APPENDIX B

WATER PROPERTIES

B.1 Water density


\[
\rho_w = 1000 \left( 1 - \frac{(T + 288.9414)}{508929.2(T + 68.12963)} \right) (T - 3.9863)^2
\]  

(B.1)

where:

\[
\rho_w = \text{Water density (Kg/m}^3) \]

\[
T = \text{Temperature (°C)}
\]

The values calculated via this correlation are compared with the ones provided by the National Institute of Standards and Technology (NIST) at atmospheric pressure. As seen in Figure B.1, the results are satisfactory. The model considers that liquid water density depends solely on temperature.
B.2 Water viscosity

The following exponential correlation suggested by Toh (2002) has been used to calculate the water viscosity at atmospheric conditions. Values using this correlation are in agreement with the ones provided by NIST as shown in Figure B.2.

\[
\mu_w = 0.02414 \cdot 10^{\left(\frac{247.8}{T-273}\right)}
\]

(B.2)

where:

\[
\mu_w = \text{Water viscosity (cp)}
\]

\[
T = \text{Temperature (K)}
\]
B.3 Water surface tension

The following correlation has been used to calculate the water viscosity at atmospheric conditions depending on the temperature. Values using this correlation are in agreement with the ones provided by NIST as shown in Figure B.3.

\[
\sigma_w = 0.07275 \left(1 - 0.002 \cdot (T - 291)\right) \cdot \frac{0.22480894387}{3.280839895}
\]

(B.3)

where:

\[
\sigma_w = \text{Water surface tension (lbf/ft)}
\]

\[
T = \text{Temperature (K)}
\]
Figure B.3: Water surface tension comparison
APPENDIX C

GAS PROPERTIES

C.1 Gas compressibility factor. Dranchuk and Abou-Kaseem

Dranchuk and Abou-Kassem (1990) fits an EOS with 11 constants to generate Standing and Katz z-factor chart. These charts are used once the pseudoreduced pressure, $P_r$, and pseudoreduced temperature, $T_r$, are calculated as:

$$P_r = \frac{P}{P_{pc}}$$

$$T_r = \frac{T}{T_{pc}}$$

(C.1)

where:

$P$= Pressure

$P_{pc}$= Pseudocritical pressure

$T$= Temperature

$T_{pc}$= Pseudocritical temperature

The z factor predicted through this EOS is accurate over the following ranges: The Dranchuk and Abou-Kassem EOS can be written as:

$$z = 1 + c_1(T_r)\rho_r + c_2(T_r)\rho_r^2 - c_3(T_r)\rho_r^5 + c_4(T_r,\rho_r)$$

(C.2)

where:

$$\rho_r = \frac{0.27 P_r}{z T_r}$$
\begin{align*}
  c_1(T_r) &= 0.3265 - \frac{1.0700}{T_r} - \frac{0.5339}{T_r^3} + \frac{0.01569}{T_r^4} - \frac{0.05165}{T_r^5} \\
  c_2(T_r) &= 0.5475 - \frac{0.7361}{T_r} + \frac{0.1844}{T_r^2} \\
  c_3(T_r) &= 0.1056 + \frac{0.6134}{T_r} + \frac{0.7210}{T_r^2} \\
  c_4(T_r, \rho_r) &= 0.6134(1 + 0.7210\rho_r^2) \left(\frac{\rho_r^2}{T_r^3}\right) \exp(-0.7210\rho_r^2)
\end{align*}

Since \( z \) is in both sides of Equation (C.1) this one needs to be arranged in the form:

\[
  z - [1 + c_1(T_r)\rho_r + c_2(T_r)\rho_r^2 - c_3(T_r)\rho_r^5 + c_4(T_r, \rho_r)] = 0
\]  

(C.8)

The root of this equation can be solved using Newton-Raphson iterative procedure. This correlation is considered accurate for engineering purposes within the following ranges:

\[
  0.2 \leq P_r < 30 \text{ and } 1.0 \leq T_r < 3.0
\]

\[
  P_r < 1.0 \text{ and } 0.7 < T_r < 1.0
\]

C.2 Gas viscosity

For the gas viscosity calculation, the Lee, Gonzalez and Eakin (1966) correlation is employed.

\[
  \mu_G = 1 \cdot 10^{-4} k_v e^{x_v \left(\frac{P_g}{62.4}\right)^{y_v}}
\]

(C.9)
The units of the viscosity are centipoises (cp) if temperature in Rankine degrees and density of the gas in lbm/ft$^3$ are given.
APPENDIX D

A GLOBALLY CONVERGENT METHOD FOR NONLINEAR SYSTEMS OF EQUATIONS

D.1 Newton Raphson (NR) general strategy

NR is applied to the multidimensional root finding of a non-linear set of $N$ equations to be zeroed, by finding $n$-independent variables $x_i, \ i=1,2,..., N$ that satisfy them. Let $F$ be the vector of functions that represent each equation of the non-linear system.

$$F_i(x_1,x_2,...,x_N) = 0 \quad i = 1,2,...,N$$

(D.1)

Let $x$ denote the vector of values of $x_i$. Each of the functions $F_i$ can be expanded using Taylor series and neglecting the second order terms of the expansions of the proximity of any vector $x$ as:

$$F(x + \delta x) = F(x) + J \cdot \delta x$$

(D.2)

where $J$ is the Jacobian matrix whose entries can be calculated as:

$$J = \frac{\partial F_i}{\partial x_j}$$

(D.3)

When $F(x + \delta x)$ is set to zero a set of linear equations is obtain for the corrections $\delta x$ that makes that each function moves closer to zero:

$$J \cdot \delta x = -F$$

(D.4)

This process is iterated until a convergence criteria is achieved updating the solution vector as follows:

$$x_{new} = x_{old} + \delta x$$

(D.5)
The main drawback of using NR is related to the closeness of the initial guess to the root. When the initial guess is not sufficiently close it method has the tendency to diverge. The number of iterations needed to achieve the convergence criteria also highly depends on the closeness of the initial guess. This the reason why pure NR is also called local convergent method.

**D.2 A Globally Convergent Method**

A global convergent method is one that converges to a solution from almost any initial guess. The following strategy is taken from Press et al. (1992) [pp. 376-378]. The main idea of the strategy is to minimize a function $f$ by taking Newton steps designed to bring $F$ to zero. The function $f$ is defined as:

$$f = \frac{1}{2} F \cdot F$$

(D.6)

The whole idea is to find values of $\lambda$ that guarantee that the function $f$ is decreasing to a rate at the least some fraction of the initial rate of decrease. These two conditions can be written as:

$$x_{new} = x_{old} + \lambda \cdot \delta x$$

(D.7)

$$f(x_{new}) \leq f(x_{old}) + 10^{-4} \nabla f \cdot (x_{new} - x_{old})$$

(D.8)

The strategy implementation can be summarized in the following steps:

1) Define the following function and its derivative:

$$g(\lambda) = f(x_{old} + \lambda \cdot \delta x)$$
\[ g'(\lambda) = \nabla f \cdot \delta x \]

(D.9)

At this moment \( g(0) \) and \( g'(0) \) were available once the NR step \( \delta x \) is known.

2) Start with a full Newton step \((\lambda = 1)\). If this step is not acceptable then calculate \( g(1) \) and \( g'(1) \). Let's model \( g(\lambda) \) as a quadratic:

\[
g(\lambda) \approx [g(1) - g(0) - g'(0)]\lambda^2 + g'(0)\lambda + g(0)
\]

(D.10)

Taking the derivative of the quadratic and making it equal to zero it can be obtained a minimum value of \( \lambda \). This minimum value has to be set greater than 0.1.

\[
\lambda = -\frac{g'(0)}{2[g(1) - g(0) - g'(0)]}
\]

(D.11)

3) If more backtracks are needed \( g(\lambda) \) will be modeled as a cubic in \( \lambda \):

\[
g(\lambda) = a\lambda^3 + b\lambda^2 + g'(0)\lambda + g(0)
\]

(D.12)

where \( g(\lambda_1) \) is the previous value and \( g(\lambda_2) \) is the second most recent value. It must also be enforced that \( \lambda \) is greater than \( 0.1\lambda_1 \) and less than \( 0.5\lambda_1 \).
VITA

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Juan Emilio Fernández Luengo was born in Madrid, Spain, on January 6th 1973. He holds Bachelor and MS degrees in Mining Engineering in the specialty of Energy and Combustibles from the Polytechnic University of Madrid, Spain. His master thesis was based on comprehensive study of the natural gas deregulation process in Spain. He started pursuing his PhD studies in Petroleum and Natural Gas Engineering at The Pennsylvania State University on January 2006. His research interest includes numerical simulation of two-phase flow, phase behavior, natural gas and LNG solid precipitation and reservoir simulation. He holds a P.E. license in Spain in mining engineering and is a continuing member of the Society of Petroleum Engineers since 2006.