LARGE-EDDY SIMULATION OF IN-CYLINDER FLOWS IN
MOTORED RECIPROCATING-PISTON INTERNAL
COMBUSTION ENGINES

A Dissertation in
Mechanical Engineering
by
Kai Liu

© 2012 Kai Liu

Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

December 2012
The dissertation of Kai Liu was reviewed and approved* by the following:

Daniel C. Haworth
Professor of Mechanical Engineering
Dissertation Advisor, Chair of Committee

André L. Boehman
Professor of Fuel Science and Materials Science and Engineering

James G. Brasseur
Professor of Mechanical Engineering, Bioengineering, and Mathematics

Stephen R. Turns
Professor of Mechanical Engineering

Karen A. Thole
Professor of Mechanical Engineering
Head of the Department of Mechanical and Nuclear Engineering

*Signatures are on file in the Graduate School.
Abstract

Two key bottlenecks prevent engines from reaching their performance, efficiency, and emissions potential. The first bottleneck is limited understanding of turbulence hydrodynamics for in-cylinder flows including cycle-to-cycle variations (CCV), and the second one is the absence of an objective approach for making quantitative comparisons between simulation and experiment, beyond ensemble averaging. In this thesis, the CCV phenomenon in IC engines and its effects on IC-engine performance are introduced. Previous studies of CCV, its root causes, and its influences on engine performance are reviewed. The limitations of current practices for IC engine simulation and analysis are discussed. Large-eddy simulation (LES) has shown promise in internal combustion (IC) engine applications, and proper orthogonal decomposition (POD) has been proposed as an objective way to analyze complex turbulent flows and to make comprehensive comparisons between simulation and measurements.

In the research performed here, LES and POD have been performed for two simplified motored IC engines: the Imperial College piston-cylinder assembly with and without swirl and the Transparent Combustion Chamber (TCC) engine. For the first configuration, the sensitivity of LES to key numerical and physical model parameters has been investigated. Results are especially sensitive to mesh and to
the subfilter-scale (SFS) turbulence models. Satisfactory results can be obtained using simple viscosity-based SFS turbulence models, although there is room for improvement. No single model gives uniformly best agreement between model and measurements at all spatial locations and at all times. Compared to Reynolds-averaged Navier-Stokes (RANS) modeling, LES shows advantages in accuracy and in capturing more details of the complex in-cylinder flow dynamics. In particular, LES is able to capture CCV using computational meshes that are comparable to those that are used for RANS, in that case, the high computational cost of LES is mainly due to the need to compute multiple engine cycles. POD is then used to study the dynamics of the in-cylinder turbulent flow. Systematic parametric studies are performed, including two-dimensional (2-D) POD versus three-dimensional (3-D) POD, phase-dependent POD versus phase-invariant POD, and sensitivities of POD mode structure and mode convergence rate to spatial and temporal resolution. The use of POD to identify and quantify CCV is explored, and the ability of POD to distinguish between organized and disorganized flows is demonstrated.

The LES and POD experience from the piston-cylinder assembly is then extended to a more realistic engine configuration (TCC engine) with full four-stroke motored cycles, where detailed particle image velocimetry (PIV) measurements are being made. The complex in-cylinder flows, including characterization of CCV, are analyzed by using LES and POD. Initial quantitative comparisons with PIV measurements are also performed. It is found that many of the key conclusions that were drawn from the POD analysis of the piston-cylinder assembly carry over to the more realistic engine. This suggests that the POD tools that have been developed will be useful in analyzing real engine flows.
Table of Contents

List of Figures viii
List of Tables xvi
List of Symbols xviii
List of Abbreviations xxi
Acknowledgments xxiii

Chapter 1
Introduction 1
1.1 Background and motivation ............................... 1
    1.1.1 Large-eddy simulation (LES) ....................... 11
    1.1.2 Proper orthogonal decomposition (POD) ........ 17
1.2 Objectives and hypotheses ............................... 21
1.3 Organization of dissertation ........................... 22

Chapter 2
Turbulent combustion in a homogeneous-charge spark-ignition Engine 24
2.1 The HCSI combustion system .............................. 25
2.2 Other combustion systems ............................... 28
2.3 Premixed turbulent flame propagation .................. 30
2.4 CFD-based turbulence hydrodynamics:
    Current practice for in-cylinder flows ................ 32
2.5 Key issues to be addressed in the proposed research 35

v
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.2.2 Swirling Imperial College piston-cylinder assembly</td>
<td>75</td>
</tr>
<tr>
<td>5.3 POD analysis</td>
<td>80</td>
</tr>
<tr>
<td>5.3.1 Phase-dependent POD</td>
<td>81</td>
</tr>
<tr>
<td>5.3.2 Phase-invariant POD</td>
<td>86</td>
</tr>
<tr>
<td>5.3.3 Flow reconstruction from POD modes</td>
<td>93</td>
</tr>
<tr>
<td>5.3.4 Cycle-to-cycle variations</td>
<td>96</td>
</tr>
<tr>
<td>5.3.5 Swirling flow</td>
<td>96</td>
</tr>
<tr>
<td>5.4 Chapter summary</td>
<td>102</td>
</tr>
<tr>
<td><strong>Chapter 6</strong></td>
<td></td>
</tr>
<tr>
<td><strong>A motored two-valve, four-stroke-cycle engine</strong></td>
<td>106</td>
</tr>
<tr>
<td>6.1 Geometric configuration and operating conditions</td>
<td>106</td>
</tr>
<tr>
<td>6.1.1 Experimental measurements</td>
<td>107</td>
</tr>
<tr>
<td>6.1.2 Numerical method</td>
<td>109</td>
</tr>
<tr>
<td>6.1.2.1 Computational mesh</td>
<td>109</td>
</tr>
<tr>
<td>6.1.2.2 Initial and boundary conditions and the estimation of mean quantities</td>
<td>111</td>
</tr>
<tr>
<td>6.1.2.3 Postprocessing</td>
<td>112</td>
</tr>
<tr>
<td>6.2 Results</td>
<td>113</td>
</tr>
<tr>
<td>6.2.1 Global in-cylinder quantities and monitoring points</td>
<td>113</td>
</tr>
<tr>
<td>6.2.2 Ensemble-averaged velocity fields</td>
<td>119</td>
</tr>
<tr>
<td>6.2.3 POD analysis</td>
<td>122</td>
</tr>
<tr>
<td>6.2.3.1 Phase-dependent POD</td>
<td>123</td>
</tr>
<tr>
<td>6.2.3.2 Phase-invariant POD</td>
<td>129</td>
</tr>
<tr>
<td>6.2.3.3 Flow reconstruction from POD modes</td>
<td>136</td>
</tr>
<tr>
<td>6.2.4 Velocity at spark-plug gap</td>
<td>138</td>
</tr>
<tr>
<td>6.3 Chapter summary</td>
<td>138</td>
</tr>
<tr>
<td><strong>Chapter 7</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Conclusions and Future Work</strong></td>
<td>141</td>
</tr>
<tr>
<td>7.1 Summary and principal conclusions</td>
<td>141</td>
</tr>
<tr>
<td>7.2 Future Work</td>
<td>145</td>
</tr>
<tr>
<td><strong>Bibliography</strong></td>
<td>146</td>
</tr>
</tbody>
</table>
### List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Schematic illustrations of four IC-engine combustion systems.</td>
<td>25</td>
</tr>
<tr>
<td>2.2</td>
<td>CCV in pressure of a IC engine.</td>
<td>28</td>
</tr>
<tr>
<td>2.3</td>
<td>Turbulent premixed flame propagation in a flamelet regime.</td>
<td>31</td>
</tr>
<tr>
<td>4.1</td>
<td>2-D cross section through the channel for the turbulent planar channel flow.</td>
<td>51</td>
</tr>
<tr>
<td>4.2</td>
<td>Baseline computational mesh for the turbulent planar channel flow.</td>
<td>51</td>
</tr>
<tr>
<td>4.3</td>
<td>$y$- and $z$- velocity components (m/s) versus time (s) at $x, y, z = 0.1047$ m, 0.00253 m, $-1.225$ m.</td>
<td>54</td>
</tr>
<tr>
<td>4.4</td>
<td>Contour plot of the streamwise velocity component (m/s) (a) Instantaneous velocity. (b) Mean velocity.</td>
<td>55</td>
</tr>
<tr>
<td>4.5</td>
<td>Mean streamwise velocity profile for the baseline case.</td>
<td>55</td>
</tr>
<tr>
<td>4.6</td>
<td>Reynolds-stress-component profiles for the baseline case. (a) Component $&lt;u'u'&gt;$, (b) Component $&lt;v'v'&gt;$, (c) Component $&lt;w'w'&gt;$. (d) Component $&lt;u'v'&gt;$.</td>
<td>56</td>
</tr>
<tr>
<td>4.7</td>
<td>Mean streamwise velocity profile for the baseline case.</td>
<td>57</td>
</tr>
<tr>
<td>4.8</td>
<td>Reynolds-stress-component profiles with variations in wall-normal mesh spacing. (a) Component $&lt;u'u'&gt;$, (b) Component $&lt;v'v'&gt;$, (c) Component $&lt;u'v'&gt;$, (d) Component $&lt;u'w'&gt;$.</td>
<td>58</td>
</tr>
<tr>
<td>5.1</td>
<td>Axisymmetric piston-cylinder assembly.</td>
<td>61</td>
</tr>
<tr>
<td>5.2</td>
<td>2-D sections through the computational mesh for the axisymmetric piston-cylinder assembly. (a) Cross section containing the axis of symmetry. (b) Cross section normal to the axis of symmetry.</td>
<td>63</td>
</tr>
<tr>
<td>5.3</td>
<td>Contour plot showing the integral length scale $l_0$ for the baseline mesh. (a) $36^\circ$ aTDC. (b) $144^\circ$ aTDC.</td>
<td>65</td>
</tr>
<tr>
<td>5.4</td>
<td>Contour plot showing the ratio $l_0/\Delta$ for the baseline mesh. (a) $36^\circ$ aTDC. (b) $144^\circ$ aTDC.</td>
<td>65</td>
</tr>
<tr>
<td>5.5</td>
<td>Computed (lines) and measured (symbols) radial profiles at $36^\circ$ aTDC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.</td>
<td>66</td>
</tr>
</tbody>
</table>
5.6 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.7 Computed (lines) and measured (symbols) radial profiles at 90° aT-DC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.8 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.9 Computed (lines) and measured (symbols) radial profiles at 270° aT-DC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.10 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for two approaches to accommodate piston motion. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.11 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for two approaches to accommodate piston motion. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.12 Computed axial velocity at a fixed spatial location for LES (resolved velocity) and RANS (mean velocity).

5.13 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for $k - \varepsilon$ RANS and for the baseline LES case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.14 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for $k - \varepsilon$ RANS and for the baseline LES case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.15 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for three meshes. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.16 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for three meshes. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.17 Computed (lines) and measured (symbols) radial profiles of axial RMS velocity at 36° aTDC. (a) Coarse mesh. (b) Baseline mesh. (c) Fine mesh.

5.18 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for three computational timesteps. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.
5.19 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for three computational timesteps. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.20 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC with variations in SFS model. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.21 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC with variations in SFS model. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.22 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for the swirling case. (a) Mean azimuthal velocity profiles. (b) Azimuthal RMS velocity profiles.

5.23 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for the swirling case. (a) Mean radial velocity profiles. (b) Radial RMS velocity profiles.

5.24 Computed (lines) and measured (symbols) radial profiles at 36° aT-DC for the swirling case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.25 Computed (lines) and measured (symbols) radial profiles at 90° aT-DC for the swirling case. (a) Mean azimuthal velocity profiles. (b) Azimuthal RMS velocity profiles.

5.26 Computed (lines) and measured (symbols) radial profiles at 90° aT-DC for the swirling case. (a) Mean radial velocity profiles. (b) Radial RMS velocity profiles.

5.27 Computed (lines) and measured (symbols) radial profiles at 90° aT-DC for the swirling case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.28 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for the swirling case. (a) Mean azimuthal velocity profiles. (b) Azimuthal RMS velocity profiles.

5.29 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for the swirling case. (a) Mean radial velocity profiles. (b) Radial RMS velocity profiles.

5.30 Computed (lines) and measured (symbols) radial profiles at 144° aT-DC for the swirling case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.31 Fractions of kinetic energy in the first few modes from 2-D phase-dependent POD analysis for the nonswirling case for a cutting plane that contains the cylinder axis.
5.32 Fraction of kinetic energy versus mode number and number of
snapshots from 2-D phase-dependent POD analysis for the non-
swirling case for a cutting plane that contains the cylinder axis. (a)
30° aTDC. (b) TDC. .................................................. 82
5.33 Phase-dependent 2-D POD modes and normalized ensemble average
velocity vectors for a cutting plane that contains the cylinder axis
at 30° aTDC for the nonswirling case. (a) Mode 1. (b) Mode 2. (c)
Mode 3. (d) Normalized ensemble average. .......................... 83
5.34 Phase-dependent 2-D POD modes and normalized ensemble average
velocity vectors for a cutting plane that contains the cylinder axis
at TDC for the nonswirling case. (a) Mode 1. (b) Mode 2. (c)
Mode 3. (d) Normalized ensemble average. .......................... 84
5.35 Phase-dependent 2-D POD modes for the fluctuating velocity field
for a cutting plane that contains the cylinder axis for the non-
swirling case. (a) Mode 1, 30° aTDC. (b) Mode 2, 30° aTDC. (c)
Mode 1, TDC. (d) Mode 2, TDC. ...................................... 85
5.36 Differences between the velocity-fluctuation-based POD modes and
the original-flow POD modes, from phase-dependent 2-D POD for
a cutting plane that contains the cylinder axis for the nonswirling
case. (a) Figure 5.35(a)–Figure 5.33(b). (b) Normalized Fig-
ure 5.36(a). (c) Figure 5.35(b)+Figure 5.33(c). (d) Normalized
Figure 5.36(c). .......................................................... 86
5.37 Comparison of eigenvalues obtained using raw versus interpolated
velocity data from phase-dependent 3-D POD at 90° aTDC for the
nonswirling case. ....................................................... 87
5.38 Fraction of kinetic energy versus mode number and number of snap-
shots from 3-D phase-dependent POD analysis for the nonswirling
case. (a) 30° aTDC. (b) TDC. ........................................ 87
5.39 Phase-dependent 3-D POD modes for a cutting plane that contains
the cylinder axis at 30° aTDC for the nonswirling case. (a) Mode
1. (b) Mode 2. ....................................................... 88
5.40 Phase-dependent 3-D POD modes for a cutting plane normal to the
cylinder axis (z = 10 mm) at 30° aTDC for the nonswirling case.
(a) Mode 1. (b) Mode 2. ................................................ 88
5.41 Phase-dependent 3-D POD modes for a cutting plane that contains
the cylinder axis at TDC for the nonswirling case. (a) Mode 1. (b)
Mode 2. ............................................................. 89
5.42 Phase-dependent 3-D POD modes for a cutting plane normal to the
cylinder axis (z = 10 mm) at TDC for the nonswirling case. (a)
Mode 1. (b) Mode 2. .................................................. 89
5.43 Fractions of kinetic energy in the first 15 modes from 2-D phase-invariant POD analysis for the nonswirling case for a cutting plane that contains the cylinder axis. (a) Data from all 360 phases used, with variations in the number of cycles. (b) Data from all 30 cycles used, with variations in the number of phases. 90

5.44 Phase-invariant 2-D POD modes for a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1. (b) Mode 2. 90

5.45 Phase-dependent 2-D POD modes for a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1, 90° aTDC. (b) Mode 1, 270° aTDC. 91

5.46 Fraction of kinetic energy versus mode number and number of cycles from 3-D phase-invariant POD for the nonswirling case. All phases have been included. 91

5.47 Phase-invariant 3-D POD modes on a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1. (b) Mode 2. 92

5.48 Phase-invariant 3-D POD modes on a cutting plane normal to the cylinder axis (z = 10 mm) for the nonswirling case. (a) Mode 1. (b) Mode 2. 92

5.49 Phase-invariant 2-D POD modes on a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1, without dilatation correction. (b) Mode 2, without dilatation correction. (c) Mode 1, without kinetic energy normalization. (d) Mode 2, without kinetic energy normalization. 93

5.50 Reconstruction of the instantaneous velocity field (velocity component $w$) at TDC of the third cycle using different numbers of 2-D phase-dependent POD modes for the nonswirling case on a cutting plane that contains the cylinder axis. (a) First three modes. (b) First five modes. (c) First ten modes. (d) Original flow. 94

5.51 Time-varying coefficients from 2-D phase-invariant POD for the nonswirling case for a cutting plane that contains the cylinder axis. (a) Coefficients of the first three POD modes versus phase for 30 engine cycles. (b) Standard deviation of the coefficients over 30 engine cycles versus phase. 97

5.52 Fractions of kinetic energy in the first few modes from 2-D phase-dependent POD analysis for the swirling case for a cutting plane that contains the cylinder axis. 98

5.53 Fraction of kinetic energy versus mode number and number of snapshots from 2-D phase-dependent POD analysis for the swirling case for a cutting plane that contains the cylinder axis. (a) 30° aTDC. (b) TDC. 98
5.54 Phase-dependent 2-D POD modes for a cutting plane that contains the cylinder axis at 30° aTDC for the swirling case. (a) Mode 1. (b) Mode 2. .................................................... 99

5.55 Fraction of kinetic energy versus mode number and number of snapshots from 3-D phase-dependent POD analysis for the swirling case. (a) 30° aTDC. (b) BDC. .................................................... 99

5.56 Phase-dependent 3-D POD modes for a cutting plane that contains the cylinder axis at 30° aTDC for the swirling case. (a) Mode 1. (b) Mode 2. .................................................... 100

5.57 Phase-dependent 3-D POD modes on cutting plane normal to the cylinder axis (z = 10 mm) at 30° aTDC for the swirling case. (a) Mode 1. (b) Mode 2. .................................................... 100

5.58 Fractions of kinetic energy in the first 15 modes from phase-invariant POD analysis for the swirling case, with variations in the number of engine cycles considered. (a) 2-D POD for a cutting plane that contains the cylinder axis. (b) 3-D POD. .................................................... 101

5.59 Phase-invariant 2-D POD modes for a cutting plane that contains the cylinder axis for the swirling case. (a) Mode 1. (b) Mode 2. .................................................... 101

5.60 Phase-invariant 3-D POD modes on a cutting plane that contains the cylinder axis for the swirling case. (a) Mode 1. (b) Mode 2. .................................................... 102

5.61 Phase-invariant 3-D POD modes on a cutting plane normal to the cylinder axis (z = 10 mm) for the swirling case. (a) Mode 1. (b) Mode 2. .................................................... 102

5.62 Time-varying coefficients from 2-D phase-invariant POD for the swirling case. (a) Coefficients of the first three POD modes versus phase for 30 engine cycles. (b) Standard deviation of the coefficients over 30 engine cycles versus phase. .................................................... 103

6.1 Computational domain for LES of the TCC engine. The locations of five monitoring points are shown. .................................................... 107

6.2 Schematic of the experimental configuration for the TCC engine. .................................................... 108

6.3 Valve lift profiles for TCC engine. .................................................... 109

6.4 Port-and-cylinder computational mesh for the TCC engine. .................................................... 110

6.5 The cutting plane that contains the cylinder axis and the two valve stems. .................................................... 111

6.6 In-cylinder pressure versus crank angle. .................................................... 113

6.7 In-cylinder mass versus crank angle. .................................................... 113

6.8 Zoomed view of in-cylinder pressure versus crank angle near TDC. .................................................... 114

6.9 Zoomed view of in-cylinder mass versus crank angle near TDC. .................................................... 114

6.10 LES 60-cycle RMS of in-cylinder pressure versus crank angle. .................................................... 114
6.11 LES 60-cycle RMS of in-cylinder mass versus crank angle. 114
6.12 LES 60-cycle normalized RMS of in-cylinder pressure versus crank angle. 115
6.13 LES 60-cycle normalized RMS of in-cylinder mass versus crank angle. 115
6.14 Pressure histories for five cycles at five monitoring points (Figure 6.1). (a) Intake plenum inlet. (b) Exhaust plenum outlet. (c) Intake port. (d) Exhaust port. (e) In-cylinder. 116
6.15 (a) Trapped mass versus cycle number. (b) Peak in-cylinder pressure versus cycle number. (c) Peak in-cylinder temperature versus cycle number. 117
6.16 Instantaneous in-cylinder mass versus instantaneous intake-port pressure. (a) 118° aTDC. (b) 180° aTDC. 118
6.17 Trapped mass versus mean intake-port pressure while the intake valve is open. 119
6.18 Ensemble-averaged 2-D velocity vectors and contours of RMS velocity magnitude on a cutting plane that contains the cylinder axis from LES and PIV. (a) Mean 2-D velocity vectors at 100° aTDC from LES. (b) Mean 2-D velocity vectors at 100° aTDC from PIV. (c) RMS velocity magnitude at 100° aTDC from LES. (d) RMS velocity magnitude at 100° aTDC from PIV. (e) Mean 2-D velocity vectors at 300° aTDC from LES. (f) Mean 2-D velocity vectors at 300° aTDC from PIV. (g) RMS velocity magnitude at 300° aTDC from LES. (h) RMS velocity magnitude at 300° aTDC from PIV. (PIV data courtesy of V. Sick, D. L. Reuss and P. Abraham, personal communication, December, 2011) 120
6.19 Fraction of kinetic energy in the first few modes from 2-D phase-dependent POD analysis for a cutting plane that contains the cylinder axis. 123
6.20 Fraction of kinetic energy in the first 10 modes versus number of snapshots from 2-D phase-dependent POD analysis for a cutting plane that contains the cylinder axis. (a) 100° aTDC. (b) 300° aTDC. 124
6.21 Phase-dependent 2-D POD modes and normalized ensemble-average velocity vectors for a cutting plane that contains the cylinder axis at 100° aTDC. (a) Mode 1. (b) Mode 2. (c) Mode 3. (d) Normalized ensemble average. 125
6.22 Phase-dependent 2-D POD modes and normalized ensemble-average velocity vectors for a cutting plane that contains the cylinder axis at 300° aTDC. (a) Mode 1. (b) Mode 2. (c) Mode 3. (d) Normalized ensemble average. 126
6.23 Phase-dependent 2-D POD modes for the fluctuating velocity field on a cutting plane that contains the cylinder axis. (a) Mode 1, 100° aTDC. (b) Mode 2, 100° aTDC. (c) Mode 1, 300° aTDC. (d) Mode 2, 300° aTDC.

6.24 Fraction of kinetic energy in the first 10 modes from 3-D phase-dependent POD analysis at 100° aTDC and 300° aTDC.

6.25 Velocity vectors and contours (axial velocity component \( w \)) of phase-dependent 3-D POD modes. (a) Mode 1, 100° aTDC. (b) Mode 2, 100° aTDC. (c) Mode 1, 300° aTDC. (d) Mode 2, 300° aTDC.

6.26 Fractions of kinetic energy in the first 10 modes from 2-D phase-invariant POD analysis for a cutting plane that contains the cylinder axis. (a) Data from all 720 phases used, with variations in the number of cycles. (b) Data from all 60 cycles used, with variations in the number of phases.

6.27 Phase-invariant 2-D POD modes for a cutting plane that contains the cylinder axis. (a) Mode 1. (b) Mode 2. (c) Mode 3.

6.28 Time-varying coefficients from 2-D phase-invariant POD for a cutting plane that contains the cylinder axis. (a) Coefficients of the first three POD modes versus phase for 60 engine cycles. (b) RMS of the coefficients over 60 engine cycles versus phase.

6.29 Phase-invariant 2-D POD modes for a cutting plane that contains the cylinder axis, for intake and compression strokes only. (a) Mode 1. (b) Mode 2. (c) Mode 3.

6.30 Time-varying coefficients from 2-D phase-invariant POD for a cutting plane that contains the cylinder axis for intake and compression strokes only. (a) Coefficients of the first three POD modes versus phase for 60 engine cycles. (b) RMS of the coefficients over 60 engine cycles versus phase.

6.31 Reconstruction of the instantaneous velocity field (velocity component \( w \)) at 100° aTDC of the eleventh cycle using different numbers of 2-D phase-dependent POD modes on a cutting plane that contains the cylinder axis. (a) First 10 modes. (b) First 30 modes. (c) All modes. (d) Original flow field.

6.32 Ensemble-averaged velocity magnitude and RMS velocity at the spark-plug gap.
# List of Tables

1.1 Summary of CCV causing factors. ........................................ 6  
1.2 Summary of factors influencing the extent of CCV. .................. 8  
1.3 Summary on LES applications in IC engines. .......................... 16  
1.4 Comparison between POD and Fourier analysis. ........................ 18  
1.5 A summary of POD studies in IC engine. ................................. 20  
3.1 The constants used in the $k - \varepsilon$ turbulence model. .............. 42  
4.1 LES run matrix for the swirling case. Values in bold font correspond to the baseline case. ........................................ 53  
5.1 LES run matrix for the nonswirling case. Values in bold font correspond to the baseline case. ........................................ 67  
5.2 LES run matrix for the swirling case. ..................................... 75  
5.3 Relevance index between reconstructed velocity fields (using 2-D phase-dependent POD modes) and the original velocity field of the third cycle for the nonswirling case on a cutting plane that contains the cylinder axis. ........................................ 94  
5.4 Relevance index between reconstructed velocity fields (using 3-D phase-invariant POD modes) and the original velocity field of the third cycle for the nonswirling case. ........................................ 95  
6.1 Parameters for the TCC engine. ............................................. 107  
6.2 Relevance indices between mean and RMS velocities with different averaging windows.  
A: Average over the last 60 cycles ($11^{th} - 70^{th}$ cycle),  
B: Average over the last 50 cycles ($21^{st} - 70^{th}$ cycle),  
C: Average over the last 40 cycles ($31^{st} - 70^{th}$ cycle),  
D: Average over the last 30 cycles ($41^{st} - 70^{th}$ cycle),  
E: Average over the first 50 cycles ($11^{th} - 60^{th}$ cycle),  
F: Average over the first 40 cycles ($11^{th} - 50^{th}$ cycle),  
G: Average over the first 30 cycles ($11^{th} - 40^{th}$ cycle). .................. 122
6.3 Relevance indices between POD modes obtained using different numbers of input snapshots. A: Input the last 60 cycles (11th – 70th cycle), B: Input the last 50 cycles (21st – 70th cycle), C: Input the last 40 cycles (31st – 70th cycle), D: Input the first 50 cycles (11th – 60th cycle), E: Input the first 40 cycles (11th – 50th cycle). 124

6.4 Relevance index between the n-th mode for velocity fluctuations and the (n + 1)-th mode for the original flow. 128

6.5 Relevance indices between modes for velocity fluctuations and the original flow. 128

6.6 Relevance index between reconstructed velocity fields (using 3-D phase-invariant POD modes) and the original velocity field of the eleventh cycle. 137
List of Symbols

\[ \| ( . ) \| \quad \text{Frobenius norm} \]
\[ \| ( . ) \|_2 \quad \text{$l^2$ norm} \]
\[ \langle ( . ) \rangle \quad \text{Ensemble averaged quantity} \]
\[ \hat{( . )} \quad \text{Density-weighted (Favre) averaged quantity} \]
\[ \overline{ ( . )} \quad \text{Spatially filtered quantity} \]
\[ \tilde{( . )} \quad \text{Density-weighted (Favre) filtered quantity} \]
\[ ( . )'' \quad \text{Fluctuation associated with spatial filter} \]
\[ ( . )' \quad \text{Fluctuation associated with ensemble average} \]
\[ a^{(k)} \quad \text{The coefficient of the $k$-th POD mode} \]
\[ b \quad \text{Bore} \]
\[ f \quad \text{Relevance index} \]
\[ k \quad \text{Turbulence kinetic energy} \]
\[ k_{SFS} \quad \text{SFS turbulent kinetic energy} \]
\[ l_0 \quad \text{Turbulence integral length scale} \]
\[ s \quad \text{Stroke} \]
\[ t \quad \text{Time} \]
\[ u \quad \text{Velocity} \]
$u^+$ Normalized velocity
$u_\tau$ Wall friction velocity
$w_{\text{piston}_{\text{ms}}}$ Piston $z$-velocity component at mid-stroke
$w_{\text{piston}}$ Piston $z$-velocity component
$x_i$ $i$ spatial coordinate
$y^+$ Wall-normal distance
$z_{\text{piston}_{\text{ms}}}$ Piston location at mid-stroke
$z_{\text{piston}}$ Piston location
$A(k)$ The $k$-th eigenvector in method of snapshots
$C$ Matrix in method of snapshots
$C_s, C_I, C_K$ LES empirical constants
$C_\mu, C_\varepsilon$ $k - \varepsilon$ RANS model empirical constants
$E$ Wall model empirical constant
$S_{ij}$ Rate of strain
$T$ Temperature
$\bar{V}_p$ Mean piston speed
$\delta_{ij}$ Kronecker delta function
$\varepsilon$ Turbulence dissipation
$\kappa$ von Karman constant
$\lambda^{(k)}$ The eigenvalue of the $k$-th POD mode
$\mu$ Dynamic viscosity
$\mu_{\text{SFS}}$ Apparent SFS turbulent viscosity
$\mu_t$ Turbulence viscosity
$\nu$ Kinematic viscosity

xix
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>Density</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Viscous stress tensor</td>
</tr>
<tr>
<td>$\sigma_k, \sigma_\varepsilon$</td>
<td>$k - \varepsilon$ RANS model empirical constants</td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>Turbulence integral time scale</td>
</tr>
<tr>
<td>$\tau_{SFS}$</td>
<td>Apparent SFS stress</td>
</tr>
<tr>
<td>$\tau_w$</td>
<td>Wall shear stress</td>
</tr>
<tr>
<td>$\psi^{(k)}$</td>
<td>The $k$-th POD mode</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>LES filter width</td>
</tr>
<tr>
<td>$\Omega_{CS}$</td>
<td>Crankshaft rotational speed</td>
</tr>
</tbody>
</table>
List of Abbreviations

1-D, 2-D, 3-D  One-dimensinal, two-dimensinal, three-dimensinal
aTDC     After top-dead-center
BDC      Bottom-dead-center
CAD      Crank angle degree
CCV      Cycle-to-cycle variations
CFD      Computational fluid dynamics
CFM      Coherent flame model
DI       Direct-injection
DNS      Direct numerical simulation
EGR      Exhaust gas recirculation
FSD      Flame surface density
HCCI     Homogeneous-charge compression-ignition
HCSI     Homogeneous-charge spark-ignition
IC       Internal combustion
LDA      Laser Doppler anemometry
LES      Large-eddy simulation
PFI      Port-fuel-injection
PISO  Pressure implicit with splitting of operators
PIV  Particle image velocimetry
PLIF  Planar laser induced fluorescence
POD  Proper orthogonal decomposition
RANS  Reynolds-averaged Navier-Stokes
RMS  Root-mean-square
RPM  Run per minute
SCCI  Stratified-charge compression-ignition
SCSI  Stratified-charge spark-ignition
SFS  Subfilter-scale
SG-SIDI  Spray-guided spark-ignited direct-injection
SIMPLE  Semi-implicit method for pressure-linked equations
SI  Spark ignition
TCC  Transparent combustion chamber
TDC  Top-dead-center
TKE  Turbulence kinetic energy
UHC  Unburned hydrocarbons
WG-SIDI  Wall-guided spark-ignited direct-injection
Foremost, I would like to express my deepest gratitude to my advisor Prof. Daniel C. Haworth for his continuous support, patience and guidance throughout my PhD study. His knowledge and personality make me regard him as my career model. It is my honor to be his student.

Besides my advisor, I would like to thank the rest of my dissertation committee: Prof. Stephen R. Turns, Prof. André L. Boehman, and Dr. James G. Brasseur, for their encouragement and insightful comments.

My sincere thanks also goes to Dr. Tang-Wei Kuo, Dr. Venkatesh Gopalakrishnan, Dr. Shengming Chang, and Dr. Xiaofeng Yang for offering me the GM summer internship opportunities. Thanks for their guidance and help during my summer internships and my PhD study.

I am grateful to Prof. Volker Sick and Dr. David Reuss of the University of Michigan for their helpful discussion regarding to the TCC engine and POD work. I appreciate Mr. Stefano Duranti, Mr. Navtej Singh and Mr. Erwan Gautier of CD-adapco for many helpful discussions related to STAR-CD and es-ice. Mr. Jason Holmes of Penn State Research Computing and Cyberinfrastructure deserves special mention for prompt support whenever I turned to him for help on HPC.

I would like to thank my colleagues and friends at Penn State, particularly Dr. Yuhui Wu, Dr. Yongzhe Zhang, Dr. Anquan Wang, Dr. Ranjan Mehta, Dr.
Eugene Kung, Dr. Ankur Gupta, Dr. Jaishree Sharma, Ms. Hedan Zhang, Mr. Subhasish Bhattacharjee, Mr. Somesh Roy, Ms. Xinyu Zhao, Mr. Vivek Raja, Mr. Adhiraj Dasgupta, Mr. Yajuvendra Shekhwat, Dr. Yanxing Wang, Dr. Fuhua Ma, Dr. Hongfa Huo and Dr. Dongjun Ma. Thanks for their help, encouragement and for all the good times we have had in the last six years.

I thank my former professor Lipeng Lu at Beijing University of Aeronautics and Astronautics for inspiring my interest in turbulence, for his help and encouragement all these years. I also thank my colleagues and friends in China, particularly Dr. Jian Ye, Dr. Xianjun Yu, Dr. Wei Sun, Mr. Qiao Tian. Thanks for their helpful comments and discussions on my dissertation work.

Thanks also to the mechanical engineering department of Penn State, who brought me to the United States, to this old university and accepted me as a “Penn Stater”. As an international student and the first time to study aboard, I will never forget the help and support Penn State gives me. The six year’s life at Penn State has brought me lot of beautiful memories. In my mind, Penn State and Pennsylvania is my second hometown.

Lastly, and most importantly, I wish to thank my parents, Qian Liu and Wenfen Wei for their endless love, support and encouragement throughout my life. Especially, I would like to give my special thanks to my wife Fang Mei whose patient love enabled me to complete this work and the happiness that she brought to my life.

Financial support from CD-adapco and from the GM R&D Center for my dissertation project is gratefully acknowledged.
Chapter 1

Introduction

1.1 Background and motivation

The 20\textsuperscript{th} century has been a time of great development for the automobile industry. According to a report from Ward’s Auto, the global number of cars exceeded 1.015 billion in 2010, jumping from 980 million in 2009 [1]. Approximately 60 million new cars and light trucks are built annually worldwide [2], and reciprocating-piston internal combustion (IC) engines power nearly all of them [3].

Automobile engines burn over a billion cubic meters (260 billion US gallons) of petrol/gasoline and diesel fuel yearly [2]. Approximately 28\% of the energy consumption and CO\textsubscript{2} emissions in the United States is contributed by automobiles [4]. Automobiles are also responsible for nearly 80\% of CO emissions, over 50\% of NO\textsubscript{X} emissions, and over 40\% of volatile organic compound emissions in the United States [4]. The development of advanced IC engines thus is particularly important technically, economically, and socially.

A major challenge for IC engine combustion scientists and engineers is to optimize engine combustion to improve fuel economy, lower pollutant emissions, and provide alternative-fuels capabilities while maintaining outstanding performance, durability, and reliability at an affordable price. Although significant progress has been made in the past century, energy sustainability and vehicle emissions will remain significant issues for the foreseeable future [5].

The analysis of in-cylinder flows in IC engines is a primary concern for IC engine developers. In-cylinder aero-thermal-chemical processes in piston engines
are rich and complex, and they have strong influences on engine efficiency and pollutant emissions [6, 7]. The stochastic nature of in-cylinder processes has been identified as one of two key areas that must be targeted to realize further significant reductions in fuel consumption for IC engines in transportation applications [8].

In IC engines, the flow and combustion events are not repeated from one engine cycle to another, and this phenomena is called cycle-to-cycle variations (CCV) or cyclic variability. CCV are very common in IC engines; for example, CCV can be found in the in-cylinder pressure, temperature, trapped mass, flow structure, mixture equivalence ratio and combustion events.

CCV are especially noticeable at low loads and engine speeds (such as idle conditions) and for lean or highly diluted operating conditions, such as with exhaust gas recirculation (EGR) operation, which is widely used to reduce NO\textsubscript{X} emissions by reducing the combustion temperature.

The main challenges for engine designers are to improve engine fuel consumption and reduce pollution emissions. However, these goals are restricted to a large extent by CCV, which have long been recognized as one of the main limiting factors for IC-engine development. IC-engine designers must calibrate the engine so that it operates even under the most extreme deviations from the nominal operating condition. If there were no CCV, the turbulence mixing and combustion events would take place at the designed operating conditions and the engine could be calibrated closer to the limits of stable operation for improved efficiency. However, in reality, each combustion event takes place at different conditions, and this may lead to incomplete combustion or even misfire, in which case the design targets can not be achieved.

To ensure that all the engine cycles operate within specified ranges (e.g., within the limits for peak in-cylinder pressure or temperature), the engine must be calibrated to operate away from optimal conditions. For example, CCV result in some engine cycles that burn faster than the ensemble average. In these fast combustion cycles, the in-cylinder peak pressure is higher, and the knock tendency is increased, which has the potential to damage an engine [6, 8]. These outlier cycles impose the lower limit for fuel octane number and the upper limit for engine compression ratio. On the other hand, on the slow-burning combustion cycles, the combustion may not be complete by the time of exhaust-valve opening, the in-cylinder peak
pressure and temperature are lower, and higher hydrocarbon and soot emissions are expected. In extreme cases, partial burns or misfires may occur.

CCV in the engine output power and torque result in poor driveability of the vehicle, and affect the the overall engine performance characteristics for some kinds of transmissions [9]. It is shown by Young [10] that CCV of the in-cylinder pressure also contribute to engine noise, and reducing the CCV can suppress engine noise.

The root causes of CCV in IC engines and their influencing factors have been studied for more than 50 years. It has been found that several factors affect the CCV during the combustion process [9]. Therefore, before we discuss CCV during the combustion events and its influencing factors, it is worthwhile to first introduce the main combustion stages and their governing mechanisms. Generally, the combustion process in a successful working cycle of a spark-ignition (SI) IC engine can be divided into four main stages [6, 9]:

- Sparking and flame initiation;
- Initial flame kernel development;
- Turbulent flame propagation (main stage of combustion);
- Flame termination.

CCV in the combustion can occur or be influenced at one or more of the first three of these stages, and the variations in each stage will affect the subsequent stages. The flame termination stage does not affect the CCV and will not be discussed here.

The first stage is the sparking and flame initiation stage. It is initiated by a voltage rise between electrodes followed by an electrical breakdown in the spark gap in a very short time [6, 11]. It includes three subphases: the discharge breakdown phase, the electrical arc phase and the glow discharge phase. The CCV of the plasma kernel properties in the first subphase are caused by fluctuations in the mixture strength, density, and the local flow velocity. At the second subphase, the mean velocity fluctuations and their directions may lead to variations in the spark duration and energy input. The flame kernel at the third subphase is more sensitive than the other two subphases. Several factors can affect the CCV during this subphase, including combustion-related, flowfield-related, mixture-composition-related, spark-energy-related, and spark-plug-geometry-related factors [9].
The initial flame development stage is the second stage, and this is the most crucial stage for CCV development. It starts when the burnt mass fraction reaches 1% to 2% and lasts for approximately 30% of the total combustion duration in the cycle [9, 12]. The flame starts as a roughly smooth spherical kernel in the spark gap at about 1 crank-angle degrees (CAD) after spark breakdown, and it lasts until the kernel size is comparable to the turbulent scales, which is usually about 3 CAD after breakdown. During this period, the flame kernel expansion velocity is close to the laminar flame speed. Therefore, the combustion CCV development during this phase is mainly attributed to the local equivalence-ratio fluctuations, the extent of dilution and the local thermodynamic conditions which determine the laminar flame speed [9].

When the flame kernel reaches a size at which it is simultaneously influenced by a few large turbulent eddies, it continues its growth in a flamelet regime [13], and this stage is usually referred to as turbulent flame propagation stage. In this stage, the burning rate depends on the laminar flame speed and the active flame front area. Similar to the previous stage, the overall equivalence ratio and the turbulence intensity affect the burning rate through the laminar flame speed, thus leading to cyclic variations. However, the flame front area wrinkling and distortion are more important during this stage. The flame front is usually assumed to propagate spherically from the center of the flame kernel, which is randomly located around the spark plug for each cycle. The random flame kernel location together with the spark-plug orientation and the chamber configuration determine the flame front area by flame distortion and quenching to the wall for each cycle, which introduce further CCV in the combustion burning rate. In this stage, the CCV of the turbulent flow motion in the vicinity of flame kernel will also affect the flame front area, thus contributing to CCV of the combustion burning rate. A higher burning rate generally corresponds to less deviation and distortion of the flame shape from a sphere, thus leading to less CCV during the flame propagation [9].

Young [10] reviewed combustion CCV in homogeneous-charge spark-ignition engines in 1981. The scope of the review ranged from the mid 1960s, when the systematic investigations of CCV phenomenon began, to the 1980s. The main CCV influencing factors were summarized into two categories: chemical and physical factors. Chemical factors include mixture equivalence ratio, dilution and fuel
type. Physical factors include ignition characteristics (spark-plug location, spark timing and number of ignition sources), combustion-chamber geometry, engine speed, compression ratio and the mixture flow motion, especially in the vicinity of the spark plug before ignition. All these factors were reviewed in detail, and the relative importance of several influencing factors was discussed. It is generally agreed that CCV in combustion are the fundamental cause of CCV in pressure and engine output; the combustion CCV originate as early as the time of spark ignition, when the flame kernel development is determined; and the combustion burning rate is one of the most important causes for CCV, because several factors affect the CCV by influencing the combustion rate. Usually, a faster-burning combustion cycle produces smaller CCV than a slower-burning one.

However, the effects of some factors on CCV were still unclear at the time of Young’s review, and some hard evidence and data were still lacking. Ozdor [9] made a more complete review of CCV in 1994, which covered more recent studies of CCV since Young’s review. In [9], two groups of CCV influencing factors were discussed: the “CCV causing factors” (as shown in Table 1.1), from which CCV can originate, and the “CCV influencing factors” (as shown in Table 1.2), that determine the relative magnitude and sensitivity of the CCV. For example, the overall air/fuel (A/F) ratio, spark-plug location and fuel type do not cause CCV in IC engines by themselves, but they influence the magnitude of the CCV development. A more complete review of CCV-related factors including those already discussed in Young’s review [10] is covered in [9]. These CCV influencing factors are categorized into four groups according to their sources:

- Mixture-composition-related factors;
- Cyclic cylinder charging-related factors;
- Spark- and spark-plug-related factors;
- In-cylinder mixture-motion-related factors.

The main mechanisms of each factor, as well as its relative contribution, are summarized in Table 1.1 and 1.2.
<table>
<thead>
<tr>
<th>CCV causing factors</th>
<th>Influenced combustion stages</th>
<th>Kind of caused primary variations</th>
<th>Relative contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulence intensity and scales</td>
<td>2</td>
<td>Flame stretching, local quenching, flame kernel convection</td>
<td>Significant</td>
</tr>
<tr>
<td>CCV in the overall A/F ratio</td>
<td>2</td>
<td>Laminar flame speed affecting flame kernel growth rate</td>
<td>(a)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Laminar flame speed affecting flame propagation velocity</td>
<td>Unstudied</td>
</tr>
<tr>
<td>CCV in the fraction of diluents</td>
<td>2</td>
<td>Laminar flame speed affecting flame kernel growth rate</td>
<td>(a)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Laminar flame speed affecting flame propagation velocity</td>
<td>(b)</td>
</tr>
<tr>
<td>Mixture spatial inhomogeneity</td>
<td>2</td>
<td>Mixture composition in the &quot;first eddy burnt&quot;</td>
<td>Depends on the scale of non-uniformities</td>
</tr>
<tr>
<td>CCV in cylinder charging</td>
<td>3</td>
<td>Amount of fuel burned per cycle</td>
<td>Significant</td>
</tr>
<tr>
<td>CCV in mean flow vector</td>
<td>1</td>
<td>Length of spark channel affecting spark discharge characteristics</td>
<td>Small</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Kernel convection velocity vector</td>
<td>Small (c)</td>
</tr>
<tr>
<td>CCV in spark discharge characteristics</td>
<td>1</td>
<td>Initial size of the hot plasma kernel</td>
<td>Unstudied (d)</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Energy amount and rate of its deposition into the flame kernel</td>
<td>Unstudied (d)</td>
</tr>
<tr>
<td>“Spark jitter”</td>
<td>1</td>
<td>Thermodynamic conditions affecting spark breakdown energy</td>
<td>Negligible in modern electronic systems</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Combustion phasing in the cycle</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.1. Summary of CCV causing factors [9].
Comments [9]:

(a) Only a combined effect of spatial inhomogeneity and CCV in both overall A/F ratio and fraction of diluents can be drawn from the studies with local mixture sampling; this combined effect is estimated to be significant.

(b) The effect is coupled with the effect of CCV in cylinder charging (reduced amount of residuals in the cycle is usually accompanied by increased amount of fuel to be burned, thereby the total effect is amplified). As a matter of fact, we are not aware of any experimental data on CCV in both fraction of diluents and cylinder charging.

(c) CCV in flame kernel convection can be caused by both random turbulent fluctuations and CCV in mean flow velocity. The latter source seems to be less important, therefore its contribution is estimated as small.

(d) CCV in spark discharge characteristics are mostly a secondary effect of the CCV in mean flow velocity. There is a lack of data on the magnitude of these variations; only the effect of mean values of spark characteristics was reported.

Influenced combustion stages:

1. Sparking and flame initiation;
2. Initial flame kernel development;
3. Turbulent flame propagation.
<table>
<thead>
<tr>
<th>Factor influencing the extent of CCV</th>
<th>Influenced combustion stage</th>
<th>Mechanism of influence</th>
<th>Best for minimum CCV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of fuel</td>
<td>2 and 3</td>
<td>Laminar flame speed</td>
<td>Providing maximum laminar flame speed</td>
</tr>
<tr>
<td>Overall A/F ratio</td>
<td>2 and 3</td>
<td>Laminar flame speed</td>
<td>Close to stoichiometric</td>
</tr>
<tr>
<td>Overall fraction of diluents</td>
<td>2 and 3</td>
<td>Laminar flame speed</td>
<td>Minimum possible</td>
</tr>
<tr>
<td>Spark timing</td>
<td></td>
<td>Combustion phasing in the cycle</td>
<td>Maximum brake torque</td>
</tr>
<tr>
<td>Spark discharge characteristics</td>
<td>1</td>
<td>Hot plasma kernel expansion rate</td>
<td>High breakdown energy, long spark duration, aggravated spark current</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Spark contribution to the flame kernel energy balance</td>
<td></td>
</tr>
<tr>
<td>Spark gap</td>
<td>1</td>
<td>Size of initial hot plasma kernel breakdown energy</td>
<td>As wide as possible</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Relative heat loss affected by flame kernel volume to &quot;wetted&quot; surface area ratio</td>
<td></td>
</tr>
<tr>
<td>Electrode shape</td>
<td>2</td>
<td>Relative heat loss affected by contact area fraction</td>
<td>Thin and/or sharp-pointed</td>
</tr>
<tr>
<td>Spark plugs number and location</td>
<td>3</td>
<td>Flame travel distance</td>
<td>Multi-point ignition; single spark location depends on the flow pattern</td>
</tr>
<tr>
<td>Spark plug orientation with respect to mean flow velocity vector</td>
<td>Heat losses affected by flame kernel convection with respect to the side electrode</td>
<td>Perpendicular to mean flow velocity vector</td>
<td></td>
</tr>
<tr>
<td>Mean flow vector at the spark gap vicinity</td>
<td>2</td>
<td>Flame kernel convection</td>
<td>3 - 5 m/s, crossflow</td>
</tr>
<tr>
<td>Overall in-cylinder flow pattern</td>
<td>2</td>
<td>Flame kernel convection</td>
<td>Intensive swirl coupled with tumble or squish component</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Convection of the fully developed flame</td>
<td></td>
</tr>
<tr>
<td>Spark discharge characteristics</td>
<td>1</td>
<td>Hot plasma kernel expansion rate</td>
<td>High breakdown energy, long spark duration, aggravated spark current</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Spark contribution to the flame kernel energy balance</td>
<td></td>
</tr>
<tr>
<td>Turbulence scales in the spark gap vicinity</td>
<td>2</td>
<td>Dispersion in “first eddy burn times”</td>
<td>Small Taylor microscale at the time of ignition</td>
</tr>
<tr>
<td>Turbulence intensity</td>
<td>2</td>
<td>Flame kernel growth rate</td>
<td>Increased to a value giving incipient local flame quenching</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Turbulent flame propagation velocity</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.2. Summary of factors influencing the extent of CCV [9].
Although [9] was a relatively complete review, the effects of some factors were still unclear due to insufficient data, such as the effects of mixture inhomogeneity and the CCV in spark-discharge characteristics. All of the work that was reviewed was experimental work. On the modeling side, several semi-empirical CCV models [14, 15, 16] have been developed to relate the pressure or combustion variations to velocity variations. The basic assumption behind these models is that the combustion CCV are mainly attributed to the CCV of turbulence characteristics in the vicinity of the spark plug during the early stage of combustion; chemical factors are included in the models via the laminar flame speed. Daw and Kahl [17], applied a mathematical technique - chaotic time series analysis - to cylinder pressure data from a SI four-stroke engine fueled with both methanol and iso-octane. The objective was to look for the presence of “deterministic chaos” dynamics in peak pressure variations and to investigate the potential of that approach as a diagnostic tool for CCV. Daw et al. [18] then proposed a simple, physical model to explain the combustion cyclic variations in spark-ignited engines. The interaction between stochastic, small-scale fluctuations in engine parameters and nonlinear deterministic coupling between successive engine cycles were considered in the model. The predictions from the model were found to agree well with experimental data. Although some of the combustion theories were considered, these semi-empirical models are based on significant assumptions and simplifications. The advantage of such models is that they can rapidly simulate thousands of engine cycles and predict statistical characteristics of CCV; however, they are not good tools to investigate the root causes and influencing factors of CCV.

More recent CCV works focus on using the advanced optical diagnostics (e.g., particle-image velocimetry - PIV) and advanced three-dimensional computational fluid dynamics (e.g., large-eddy simulation - LES), which enable a closer scrutiny of the CCV development process. Early attempts of PIV or LES focused on capturing the CCV of large-scale flow or flame structures. Reuss [19] applied two-dimensional PIV to measure the CCV of large-scale flow-structures in a motored, two-valve, four-stroke engine. LES was performed on the same configuration by Haworth [20]. However, due to computational limitations, a relatively coarse mesh was used, and only a small number of engine cycles was simulated. Cairns and Sheppard [21] developed a dual-seeding method to capture the cyclically resolved
simultaneous flame images and associated velocity fields in an optically accessible single-cylinder SI engine. The interaction between the flame propagation and in-cylinder flow motion was studied, and it was shown that local unburned-gas motion had significant effects on the flame propagation, thus leading to CCV in the combustion process.

One example of recent CCV work using optical diagnostics and CFD was a study of misfire phenomenon in spray-guided spark-ignited direct-injection (SG-SIDI) engines. SG-SIDI engines have a significant fuel economy advantage over the traditional wall-guided spark-ignited direct-injection (WG-SIDI) engines, with a wider stratified-charge operating range [5]. It was reported that the misfires were correlated to the cyclic variations in conditions near the spark plug. High gradients near the spark plug made ignition very sensitive to spark-plug location (i.e., a 1 mm shift lowered ignitability in both measurements and simulations) and to cyclic variations in spray angle [5, 22]. Peterson et al. [23] investigated the rare misfire and partial burn cycles in a SG-SIDI optical engine using high-speed 2-D PIV and planar laser induced fluorescence (PLIF). It was found that the partial burns and misfires are not the result of failed ignition, but rather of failure during the flame propagation process due to the CCV of flow structures and equivalence ratio in the spark-plug vicinity. With the same PIV data, Chen et al. [24] further investigated how the flow motion, and fuel/air distribution near the spark plug lead to misfire by comparing the well burned cycles with the misfire cycles using conditional sampling and proper orthogonal decomposition (POD).

One the modeling side, Enaux et al. [25] applied LES to a single-cylinder SI engine. It was shown that CCV were essentially due to velocity fluctuations at the spark plug, which induce variations of the early flame kernel growth and of the overall combustion duration. These large-scale aerodynamic variations manifested themselves through changes in the location of the tumble residual motion at spark timing from cycle to cycle. Granet et al. [26] also performed LES on the same engine configuration where experiment data was available for two operating points: a stable point characterized by low CCV and an unstable one with high CCV. Acoustic effects were also considered by including the exhaust and intake plenums. A detailed comparison between experiments and LES was carried out, it was found that LES was able to predict qualitatively and quantitatively the CCV of real fired
operating points, and it was able to distinguish a stable point from an unstable one. Special attention was paid to comparing the flow motion, flame structure, and temperature distribution in the vicinity of the spark plug at ignition timing. It was found that LES mimicked well the evolution of the flame in terms of shape, position and timing, which were essential for the CCV development. A more complete review of LES studies on CCV is included in Section 1.1.1.

In summary, CCV in IC engines have greatly limited IC-engine development. They have a negative impact on the drivability of the vehicle, large levels of CCV and pre-ignition have the potential to damage an engine, and they also lead to increased levels of pollutant emissions and higher fuel consumption. The review of Ozdor [9] suggests that a 10% increase in the power output could be obtained for the same fuel consumption by the elimination of CCV. Reducing the level of CCV in IC engines will enable the engine to operate under conditions that are closer to the optimal conditions, thus improving the vehicle’s drivability, and reducing both fuel consumption and pollution emissions.

1.1.1 Large-eddy simulation (LES)

Modern engines are already at a high level of refinement. Further increases in performance, and reductions in fuel consumption and emissions will require effective use of high-spatial-and-temporal-resolution optical diagnostics and numerical simulations [5]. High-resolution optical diagnostics (e.g., PIV) and numerical models (LES) are increasingly being used to develop advanced combustion systems for next-generation piston engines. PIV in IC engines was pioneered by Reuss et al. [27], and it has become an effective investigation tool in both gasoline engines [28, 19, 29, 30, 31, 24] and diesel engines [32, 33, 34].

On the modeling side, LES is increasingly used as a tool for advanced IC engine design. In LES one explicitly captures the dynamics of the large eddies (larger than the filter width $\Delta$), while modeling the effects of the smaller eddies (smaller than the filter width $\Delta$) on the larger ones. The filter width should be an order of magnitude smaller than the integral scale. Because the statistics of small-scale turbulence are expected to be more universal than those of the large scales, LES offers the promise of wider generality and more accurate results compared
to Reynolds-averaged Navier-Stokes (RANS), where the effects of all turbulence scales are modeled, while requiring smaller computational resources compared with direct numerical simulation (DNS) where all turbulence scales are resolved.

There are important differences between RANS and LES [20]. A RANS methodology converges to an exact solution of the Reynolds-averaged Navier-Stokes equations with increasing spatial and temporal resolution. Thus the numerical accuracy can be improved, but the dynamic range of scales that is resolved cannot be increased with grid refinement. In LES, similar convergence to an exact solution of the spatially-filtered governing equations could be realized. In principle, the LES filter width $\Delta$ is proportional to the grid cell dimension and the grid cells have aspect ratios of order one. In that case, the dynamic range of scales that is resolved increases with increasing spatial and temporal resolution, and a consistent LES may converge to an exact solution of the unfiltered Navier-Stokes equations: to DNS. Usually grid independence in LES can be established only in a statistical sense: the sum of resolved and subfilter-scale (SFS) contributions to mean quantities should be independent of numerical parameters such as mesh size and computational time step, for example.

LES is expected to capture more flow structures, eddies and vortices than RANS on the same computational grid. Such flow structures and turbulence in general arise from the non-linear terms in the momentum equation. To resolve finer flow structures, the non-linear terms must be treated accurately, which requires a denser mesh with higher-order numerics and less dissipative numerical methods.

LES is also expected to provide better predictive capability compared to RANS, with less empirical input required. The effects of unresolved scales on resolved scales must be modeled. The small eddies tend to be more universal, and thus easier to model. An example is the “dynamic approach” for SFS modeling in LES, where the value of the model coefficients is determined automatically according to the local resolved flow structures [35].

There are additional considerations in simulations of flows in IC engines. In RANS simulations of reciprocating-piston IC engines, the local instantaneous value of a computed variable represents an ensemble- or phase-average over many engine cycles at a specified spatial location and crank phasing, while in LES these variables are spatially filtered. It has long been argued that turbulence
modeling based on spatial filtering offers advantages compared to time- or phase-averaging [36], and these advantages are particularly compelling for the IC-engine application [3, 20, 37, 38]. A key bottleneck preventing engines from reaching their performance, efficiency and emissions potential is our limited understanding of the turbulence hydrodynamics for in-cylinder flows. This includes cycle-to-cycle flow and combustion variabilities, which are not accessible from RANS, but can be captured by LES, at least in principle.

In addition, LES is expected to be better than RANS at capturing the impact of relatively small changes in geometry (such as combustion chamber geometry, spark plug shape and location, piston bowls, valves and port design), fuel injection (such as fuel injection angle, injection timing and total injected fuel mass), and operating conditions (such as spark timing, valve timing, etc.). These types of "sensitivity studies," as well as CCV, are very important for IC engine design, and LES has a significant potential advantage over RANS in these respects.

Since LES can better capture the details of the turbulence dynamics including CCV, the transition from RANS to LES is a natural direction. El Tahry and Haworth [37] argued that the computational meshes typically used for RANS modeling of practical in-cylinder configurations should be sufficient to capture 80-90% of the flow’s kinetic energy. For IC engines at moderate Reynolds numbers, it has been estimated that grid independent (to within 10-20%) profiles of dependent mean variables in RANS computations of in-cylinder flow and combustion would require at least $10^6$ mesh points using second-order or higher numerical methods [38]. This corresponds to sub-millimeter mesh spacing in a typical automotive IC engine, and it is not far beyond current RANS practice. Other arguments for pursuing LES for in-cylinder CFD have been made in [3] and [5]. Even if comparable meshes are used, LES will require more computational effort compared with RANS, because smaller computational time steps may be required and simulations may need to be carried through multiple engine cycles.

For fundamental LES studies in simple geometries, the filter size is usually taken to be in the inertial subrange of an isotropic turbulence spectrum. For these studies, dense grids with simple SFS models are usually used. Also, high accuracy numerical methods are necessary to make the schemes less dissipative [39]. This approach is common when LES is applied to study basic or fundamental
aspects of turbulence, such as the dynamics of homogeneous turbulence in a simple geometry. However, the inertial subrange filtering requirement was not part of the original LES definition [39]. The use of very fine meshes with high-order numerical methods is not practical for IC engines, where the flows are almost never homogeneous. Traditional concepts, such as the inertial subrange, rely on a sufficient statistical population that often does not exist at the smaller scale subgrid level in a complex evolving flow [39]. In most LES applications in IC engines, relatively coarse meshes (approximately millimeter-size meshes) with second-order numerics have been used.

There are many complex physical process that occur in IC engines, and all of them require modeling; these include turbulence modeling, combustion modeling, scalar transport/mixing modeling, and fuel-spray modeling. In many of the current LES applications in IC engines, researchers use LES-type modeling for turbulence and, in some cases, for scalar fluxes. However, they often still rely on RANS-type submodels for other physical process. This type of hybrid approach is very common and is a reasonable way to proceed [39], given the practical limitations. The turbulence model provides the key scales that are required for the models of other physical processes in IC engines. Therefore, improving the turbulence model (using LES versus RANS) is expected to improve RANS-type submodels for other processes. The LES turbulence models can provide better accuracy, capture more large-scale structures and provide greater sensitivity, so that many advantages of LES can be realized, even when combined with RANS-type submodels for other processes [39]. Because the scope of this thesis is limited to cold flow in motored engines, only LES turbulence modeling is discussed here.

Similar to RANS-based turbulence models, the most widely used LES models are based on an apparent turbulence viscosity, where the modeled stress is proportional to the local rate of strain through a turbulence viscosity. The simplest SFS model is to simply set the turbulence viscosity to be zero. It has been argued that the effect of numerical dissipation is similar to that of the turbulence viscosity, and this approach can give satisfactory results in some cases [39]. However, this approach mixes the physics and the numerics in a way that is different to control and to understand.

The Smagorinsky model [40] was the first, and remains most widely used, LES
turbulence model. It is a zero-equation model with one model coefficient. It is simple to implement and has shown great success in both fundamental LES studies and IC-engine applications. However, the model coefficient needs to be specified, and different values have been found to be required for different flows. Germano et al. [35] improved the Smagorinsky model by introducing the dynamic approach to estimate the adjustable model coefficient. A test filter is applied to the filtered equation, and the value of the model coefficient is found from the difference between the test- and base- filtered equations on the CFD grid. This dynamic approach is widely used in both fundamental and IC-engine LES applications, and it has proven to be very successful. However, the additional filtering operation results in a modest (approximately 20%) increase in computational cost [39].

The kinetic-energy-equation approach is a viscosity-based one-equation LES model. A SFS kinetic energy transport equation is solved and the turbulence viscosity is formed from the SFS turbulence kinetic energy (TKE) and the filter size. The use of a kinetic energy equation has several advantages over the Smagorinsky model, and these advantages are particularly attractive for IC-engine applications. First, more physical processes are captured in the turbulence model, including the production, convection and dissipation of SFS turbulence kinetic energy. Second, the SFS turbulence kinetic energy provides a velocity scale that can be used in other models, such as combustion, scalar transport and spray modeling. Third, a model that uses a SFS turbulence kinetic energy equation is expected to provide a better model for the SFS stress, and it works better on the relatively coarse meshes that are commonly used in IC engines [39].

Over the last twenty years, significant progress has been made in LES for IC engines. Early reviews of LES applications to IC engines include Celik et al. [41] and Haworth [20]. Haworth and Jansen [38] applied LES to predict the ensemble-averaged mean and root-mean-square (RMS) velocity profiles for a simplified motored engine configuration. Celik et al. [42, 43] studied turbulence statistics using KIVA [44] for a motored engine configuration. Although these are simple engine configurations without combustion, they demonstrated the capability of LES to capture CCV and the potential for improved accuracy compared to RANS.

Early attempts to apply LES with combustion in IC engines include Naitoh
et al. [45] (LES for turbulent premixed-flame propagation in IC engines on relatively coarse grids) and Smirnov et al. [46, 47] (LES of diesel fuel injection and combustion for IC engines using KIVA).

For more realistic configurations, Vermorel et al. [48] and Richard et al. [49] applied LES with a flame-surface-density-based combustion model (coherent flame model) to a real single-cylinder, spark-ignited four-valve engine. Vermorel et al. [50] studied the same engine using LES with a more advanced combustion model (extended coherent flame model). Laget et al. [51] performed LES for a four-cylinder engine based on the work of Vermorel et al. [48, 49, 50]. The main focus of these works was to estimate the CCV and to study the root causes for the CCV in IC engines using a high fidelity LES code. Although only a small number (approximately ten) of engine cycles were simulated in these works, the results showed encouraging qualitative and quantitative agreement with experiments.

Other examples of in-cylinder LES include Hu et al. [52, 53, 54] (LES of diesel engine combustion with CHEMKIN and a flamelet time scale combustion model), Enaux et al. [55] (validation of CCV for a motored single-cylinder piston engine using LES), Banerjee et al. [56] (LES of diesel engine combustion with a multi-mode combustion model) and Zhang et al. [57, 58] (LES of scalar dissipation rate in an IC engine). A recent review of LES applications in IC engines has been made by Rutland [39]. Dedicated conferences were organized in 2008 [59] and in 2010 [60], and those are good sources of up-to-date information and entry points to the literature. LES applications in IC engine are summarized in Table 1.3.

While LES is being applied to real engine configurations, there is still something to be learned from simpler configurations, such as the behavior of the SFS models and numerical algorithms that are used for LES. In this dissertation, LES is first applied to a simplified motored engine configuration with and without swirl to explore the effects of physical model parameters and numerical parameters. A systematic study is carried out to quantify the relative magnitudes of resolved-

<table>
<thead>
<tr>
<th>CFD mesh size</th>
<th>1 mm</th>
<th>~ 1 mm</th>
<th>~ 2-4 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical process</td>
<td>Cold flow</td>
<td>Scalar mixing</td>
<td>Combustion</td>
</tr>
<tr>
<td>Numerics</td>
<td>Second order</td>
<td>Third order</td>
<td>Higher order</td>
</tr>
<tr>
<td>Configuration</td>
<td>Simplified geometry</td>
<td>Real engine geometry</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.3. Summary on LES applications in IC engines.
scale and SFS fluctuations. A real geometry engine configuration is studied next where PIV measurements are available, and initial comparisons between LES and PIV are made.

1.1.2 Proper orthogonal decomposition (POD)

As discussed above, PIV and LES have been increasingly used to study the dynamics of turbulent flows in IC engines. However, to date, quantitative comparisons between PIV and LES have been limited mainly to ensemble- (phase-) averaged mean quantities. The absence of alternative approaches for making quantitative comparisons between high-fidelity simulations and experiments beyond ensemble averaging has been another bottleneck for IC-engine design.

POD (also known as the Karhunen-Loéve transform, the Hotelling transform, or principal component analysis) [61] has been proposed as an approach for analyzing the dynamics of complex in-cylinder processes, and as the basis for making quantitative comparisons between PIV and LES that goes beyond ensemble averaging. For example, POD may provide insight into the nature of the CCV that limit the increases in performance and reductions in fuel consumption and emissions that can be realized in advanced spark-ignition and compression-ignition piston engines.

POD provides an objective way to extract and identify the most energetic structures in a turbulent flow [62]. POD was first introduced into the turbulence field by Lumley in 1967 [63], and has several attractive properties: the original flow field can be expressed as a linear combination of POD modes and corresponding coefficients; the POD modes are mutually orthogonal and they are functions of space only, independent of time, while the coefficients are functions of time only and independent of space; and the POD modes are optimal in the sense that a higher fraction of the original flow’s kinetic energy can be captured using fewer POD modes compared to any other orthogonal basis [64]. These properties suggest that POD may be an attractive tool for the analysis of turbulent flows in multiple applications.

POD can be compared with Fourier-based analysis, as they are both orthogonal decomposition methods that share some common properties. A comparison between them is shown in Table 1.4. In both POD and Fourier analysis, the basis
Fourier transform

Common points
- Flow field can be represented as a linear combination of basis functions (modes)
- Modes are mutually orthogonal
- Modes are normalized with unity magnitude

Differences
- Modes not predefined
- Modes are ordered by energy
- Variance-based orthogonal decomposition

<table>
<thead>
<tr>
<th>POD</th>
<th>Fourier transform</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow field can be represented as a linear combination of basis functions (modes)</td>
<td></td>
</tr>
<tr>
<td>Modes are mutually orthogonal</td>
<td>Modes predefined</td>
</tr>
<tr>
<td>Modes are normalized with unity magnitude</td>
<td>Modes are ordered by wavelength</td>
</tr>
<tr>
<td></td>
<td>Scale-based orthogonal decomposition</td>
</tr>
</tbody>
</table>

Table 1.4. Comparison between POD and Fourier analysis.

functions or modes are orthogonal to (or independent of) each other; the modes are normalized with the same magnitudes; only the flow structure information is included in the context of turbulence; and the original flow fields can be represented as a linear combination of the modes and corresponding coefficients. However, POD and Fourier analysis differ in the way that their modes are obtained. For Fourier transformation, the modes are predefined and they represent the flow structure for a certain wavelength, while the POD modes are not predefined; POD modes are obtained by maximizing the energy content when projecting the original flow fields onto the POD modes. That is to say, if the flow fields are projected onto a POD mode, the average energy content is larger than if they are projected onto any other structure, such as a Fourier mode. One property of POD and Fourier analysis is that in a statistically homogeneous system, the POD modes are the same as the Fourier modes [64]. In general, Fourier transformation is a scale-based orthogonal decomposition, while POD is an energy-based (or variance-based) orthogonal decomposition.

However, POD analysis is computationally intensive, and for that reason, there are few examples of its application before the 1980’s. Early applications of the POD include those by Bakewell and Lumley [65] (turbulent pipe flow), Payne and Lumley [66] (turbulent wake behind a cylinder) and Hilberg et al. [67] (turbulent shear layer); further examples can be found in [64]. The application of POD in the turbulence field was explored in these studies, where POD was mainly used as a “coherent structure” identification or visualization tool. In some cases, it has been found that the energy-based orthogonal decomposition of POD has an advantage over the length-scale-based orthogonal decomposition of Fourier transformation.
in capturing the most important turbulence structures while filtering out the
dynamically less important structures.

POD is an attractive candidate for the analysis of in-cylinder flows in IC
engines, where large-scale flow structures, turbulence generation and CCV are
primary concerns. The first application of POD to flows in piston engines appeared
in the early 2000’s, using datasets obtained from experiments and simulations.
Erdil et al. [68] applied POD to flow in a motored test engine; the velocity fields
were obtained by using a hot wire to measure two velocity components at a single
fixed location in the flow for different engine configurations. Different analysis
methods, such as turbulence filtering or phase averaging also were applied to
the same datasets and results from these different decomposition techniques were
compared with each other. It was found that POD can effectively be used in the
analysis of turbulence in IC engines towards better understanding of combustion
processes, in addition to the conventional phase averaging methods and turbulence
filtering. By examining the POD energy spectrum for a shrouded and a standard
valve configuration, it was found that more than 50% of the kinetic energy was
contained in the first mode for the shrouded valve configuration, and that POD
could be used as a way to quantify the flow’s level of complexity or organization.

Raposo et al. [69] and Boreé [70, 71] applied POD to experimental datasets
of motored flows obtained using PIV. In addition to looking at the POD mode
structures and energy spectrums as in previous POD studies, they focused on
analyzing the dynamic behavior of the large-scale flow structures by studying the
time-varying coefficients of low-order POD modes. The modes represent the main
flow structures or fluctuations, while the time-varying coefficients give an idea of
how energy is transferred from one structure to another. For example, it was shown
in [70, 71] that this method could be used to analyze the production, compression
and break-up process of a large-scale tumble vortex in a simplified engine. The
energy transformation between modes during the intake and compression strokes
could be inferred from the time-varying mode coefficients. POD also has been
suggested as a good method to describe the CCV of in-cylinder flows.

Fogleman et al. [72, 73] used a similar method to analyze the tumble breakup
in a simplified IC engine in more detail; they focused more on analyzing the CCV
using POD. They reviewed previous POD works and applications in IC engines
Extract the most energetic flow structure/scalar distribution and main fluctuations [30, 32, 74, 75]
Describe dynamic behavior and energy transformation [69, 70, 71, 72, 73, 76]
Quantify the level of flow's organization using phase-dependent POD [68, 72, 73, 75]
Study CCV using phase-invariant POD [33, 72, 73, 77, 75]
POD modes used as basis for low-dimensional model [72, 73]
Make comprehensive comparisons between LES and experiments
Reconstruct information between consecutive measurements [29, 32, 33, 74]

<table>
<thead>
<tr>
<th>POD variants</th>
<th>Phase-dependent POD [30, 32, 33, 68, 69, 70, 71, 72, 73, 74, 77, 75]</th>
<th>Phase-invariant POD [72, 73, 75]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Datasets</td>
<td>Hot-wire anemometry [68]</td>
<td>LES [72, 73, 75]</td>
</tr>
<tr>
<td>Engine geometry</td>
<td>Simplified engine [70, 71, 72, 73, 75]</td>
<td>Gasoline engine [30, 68, 69, 74, 77]</td>
</tr>
<tr>
<td>Combustion</td>
<td>Motored engine [30, 32, 33, 68, 69, 70, 71, 72, 73, 75]</td>
<td>Combustion engine [74, 77]</td>
</tr>
<tr>
<td>Dimension</td>
<td>1-D [74, 77]</td>
<td>2-D [30, 32, 33, 68, 69, 70, 71, 72, 73, 75]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3-D [75]</td>
</tr>
</tbody>
</table>

Table 1.5. A summary of POD studies in IC engine.

and proposed the “phase-invariant POD,” in contrast with the previous “phase-dependent POD.” In “phase-dependent POD,” the flow fields at a particular phase from different engine cycles are analyzed. However, in “phase-invariant POD,” the flow fields from all phases are analyzed to obtain the POD modes. These modes then contain information for all phases. As will be discussed in more detail in Chapter 3, three modifications are required compared to the phase-dependent POD. These modifications resolve the geometry change issue, and the inherent differences of kinetic energy over an engine cycle in piston engines. The CCV then can be quantified by studying the time-varying coefficients. These modifications are expected to be reasonable proposals, although they have not been rigorously justified; the effect of each modification is explored in this thesis. Fogleman et al. [72, 73] also proposed to use the POD modes as the basis for a low-dimensional turbulence model, in which a set of simplified equations is solved for mode coefficients coupled with the POD modes, as an alternative to solving the Navier-Stokes equations.

Other examples of POD analysis in IC engines include Cosadia et al. [32, 33] (CCV of the swirling flow in an optically accessible diesel engine), Druault et al. [29] (use of POD for time interpolation from PIV data to study CCV) and Kapitza
et al. [30] (examination of turbulent structures generated by the intake port of a direct-injection spark-ignition engine). More recent examples of POD application in IC engines can be found in [24] and [75]. In addition to the analysis of cold flow in the motored engine, POD also has been used to analyze the combustion or scalar distribution in optical engines [34, 77]. A summary of POD studies in IC engines is provided in Table 1.5; only the key references are listed in the table.

1.2 Objectives and hypotheses

As discussed above, two key bottlenecks that prevent further improvements in IC engines are our limited understanding of turbulence hydrodynamics for in-cylinder flows, especially CCV, and the absence of an objective approach for quantitative comparisons between simulation and experiment, beyond ensemble averaging. With this in mind, the objectives of the thesis are:

1. Study complex in-cylinder turbulent flows, especially the CCV in IC engines by using LES.

2. Assess and develop the POD approach as a tool to analyze complex turbulent flows in piston engines, and as a basis for making quantitative, objective comparisons between in-cylinder velocity fields obtained using high-speed optical diagnostics and numerical simulations.

This thesis addresses the following hypotheses:

1. Multiple-cycle LES is expected to provide more accurate predictions of in-cylinder turbulence compared to RANS, and to provide new insight into the dynamics of in-cylinder flows, especially CCV.

2. POD provides an objective basis for quantifying CCV and for quantitative comparisons between simulations and experiments that goes beyond ensemble averaging.

In this dissertation, multiple-cycle LES will be performed for two motored engine configurations where detailed experimental measurements are available, and these hypotheses will be tested.
As discussed earlier, LES is a good candidate for reciprocating engines at moderate Reynolds numbers due to the arguments that LES can provide more insight into the complex in-cylinder flows such as CCV on typical RANS meshes (approximately sub-millimeter mesh spacing) without significant mesh refinement. The CCV of flow structures before ignition, especially the flow motions in the vicinity of spark plug, greatly influence the CCV during combustion. We will focus on motored engines without combustion in this dissertation. A planar channel flow configuration is studied first to test the suitability of the finite-volume code for LES: STAR-CD. Then two simplified engine configurations are studied: the Imperial College piston-cylinder assembly with and without swirl [78, 79, 80, 81] and the Transparent Combustion Chamber (TCC) engine [19, 82]. The Imperial College configuration is used to address important outstanding issues for in-cylinder LES in the context of a simplified engine-like configuration. These include: a systematic comparison between a conventional two-equation RANS model and LES; a systematic parametric study of the effects of physical model parameters and numerical parameters; quantification of the grid quality of the LES solutions through an examination of the relative magnitudes of resolved-scale and SFS fluctuations; and the first LES results reported to date for the configuration with swirl. The LES is next extended to a more realistic engine configuration with full four-stroke motored cycles (TCC engine) where detailed PIV measurements are being made. Initial quantitative comparisons with PIV measurements are performed.

POD is applied to the LES data for both engine configurations to analyze the complex in-cylinder flows, including characterization of CCV. The application of POD to quantify the CCV is explored. A systematic study is performed to explore several POD variants and the influence of key parameters for both the simplified engine and the real-geometry four-stroke engine. These findings are expected to provide guidance to researchers who apply POD to analyze PIV and LES data in real engines.

1.3 Organization of dissertation

The remainder of this dissertation is organized as follows:
• Chapter 2: A brief review of the combustion systems used in IC engines is given. Particular attention is paid to the homogeneous-charge spark-ignition (HCSI) combustion system. The characteristics of premixed turbulent flame propagation in IC engines are discussed.

• Chapter 3: The mathematical formulation, physical models, and numerical methods for LES and POD are shown. The numerical method (method of snapshots) used to obtain POD results is introduced, and issues specific to POD in IC engines are discussed.

• Chapter 4: The LES capability of STAR-CD is assessed by studying a turbulent planar channel flow case. The mean streamwise velocity and Reynolds-stress profiles are compared with DNS results.

• Chapter 5: LES results for a simplified-piston-cylinder assembly (Imperial College engine) with and without swirl are presented. This includes a systematic parametric study of the physical models and numerical parameters. A comprehensive POD analysis is performed on the LES data. The application of POD to IC engines is explored.

• Chapter 6: LES and POD are performed for a more realistic engine configuration with full four-stroke motored cycles (TCC engine) where detailed PIV measurements are being made. Initial quantitative comparisons with PIV measurements are performed.

• Chapter 7: Key findings and contributions of the dissertation are summarized. The conclusions of the dissertation are drawn, and future work is proposed.
Chapter 2

Turbulent combustion in a homogeneous-charge spark-ignition Engine

For many years, the combustion process in an IC engine had been idealized as either a premixed turbulent flame propagation (in the case of spark-ignition gasoline engines) or as a turbulent diffusion flame (in the case of compression-ignition diesel engines). However, due to new insights into in-cylinder combustion processes and the development of advanced IC engines, the boundary between pure premixed and pure diffusion combustion in IC engine has been blurred, and alternative combustion systems have been introduced and studied [3].

Engine combustion systems can be categorized by the mode of ignition (spark-ignition or compression-ignition) and by the degree of homogeneity of the fuel-air mixture at the time of ignition (homogeneous-charge or stratified-charge). This yields four basic combustion systems [3]:

- Homogeneous-charge spark-ignition (HCSI).
- Stratified-charge spark-ignition (SCSI).
- Homogeneous-charge compression-ignition (HCCI).
- Stratified-charge compression-ignition (SCCI).

Schematics of these combustion systems are provided in Figure 2.1. There spark-ignition systems are in the top row, which are usually used in gasoline-fueled
engines, and compression-ignition systems are in the bottom row, which include diesel-fueled engines. Essentially homogeneous systems are in the left column, and essentially stratified systems are in the right column. Here we focus on the HCSI gasoline engine which is currently the most widely used in automobiles, although a brief introduction to the other three combustion systems will be included.

2.1 The HCSI combustion system

The HCSI gasoline engine has been in production for decades, and advanced HCSI gasoline engines are expected to remain competitive in vehicle applications for many years [5]. As illustrated in Figure 2.1, liquid gasoline is injected upstream of the combustion chamber, typically onto the back of the intake valve by a relatively low-pressure fuel injector mounted in the intake port. Fuel and air are drawn into the combustion chamber as the valve opens and the piston descends. The fuel, air, and residual gas (ideally) are well mixed at the molecular level and fuel-air mixing time is usually sufficient to ensure an approximately homogeneous mixture prior
to ignition, usually 20 - 30 CAD before top-dead-center (TDC).

The combustion process for a warmed-up HCSI gasoline engine is generally idealized as premixed turbulent flame propagation through homogeneous reactants, although further study has shown that the fuel/air/residual mixture in HCSI engines is considerably less homogeneous than previously thought [83, 84]. The maximum power for HCSI engines is limited by air flow capacity. A supercharger or turbocharger can be used to increase the power by allowing more fuel to be burned and more work to be done per cycle. The compression ratio for HCSI engines is limited to approximately 10:1 due to knock, and this limits the fuel economy. Fuel economy at part load is reduced greatly by pumping (throttling) losses [5]. Over-fueling is necessary for ignition during cold start, which also reduces the fuel efficiency.

For a warmed-up HCSI gasoline engine in steady-state operation, the engine-out unburned hydrocarbons (UHC) are dominated by oil-film absorption/desorption and by combustion-chamber crevices rather than directly by the combustion process itself [5, 85]. Engine-out NO\textsubscript{X} is dominated by thermal NO (Zeldovich or extended Zeldovich mechanisms [86]) due to the high temperature. Tailpipe emissions (UHC, CO, and NO\textsubscript{X}) are controlled effectively using a conventional three-way catalytic aftertreatment system. Fuel and air are in stoichiometric proportion (air-to-fuel mass ratio of approximately 14.6:1) to ensure effective operation of the three-way catalytic aftertreatment system in simultaneously oxidizing UHC and CO and in reducing NO\textsubscript{X}. Exhaust gas recirculation (EGR) may be used to improve efficiency and to lower engine-out NO\textsubscript{X} [3]. Three-way catalytic aftertreatment systems and closed-loop stoichiometric control (with an exhaust O\textsubscript{2} sensor) remove more than 99.5% of engine-out UHC, CO, and NO\textsubscript{X} emissions, so that most tailpipe emissions occur during cold starts before the catalyst has reached its operating temperature.

Further improvements in fuel efficiency demand closer scrutiny of the HCSI combustion process. Attention is focused increasingly on cold-start and transients rather than on warmed-up steady-state operation. This is because cold start remains the dominant source of tailpipe UHC emissions. Fuel additives and alternative fuels are being explored. Highly fuel-lean and/or highly dilute combustion (the latter corresponding to high levels of EGR) are of interest for their reduced
fuel consumption potential. Combustion stability issues become acute near the
lean and/or dilute limits of operation; cycle-to-cycle combustion variations then
limit the fuel consumption and emissions benefits that can be realized.

An essential aspect of HCSI combustion-system design is the balance between
low-speed part-load combustion efficiency and wide-open-throttle torque and pow-
er. This tradeoff can be addressed using CFD-based turbulent combustion mod-
elling [3]. At low-speed light-load operating conditions, fast burn generally is
desirable for its positive impact on idle stability, fuel consumption, NO\textsubscript{X} emis-
sions, EGR tolerance, and knock propensity. Fast burn requires high in-cylinder
turbulence levels which can be achieved by manipulation of the large-scale in-
cylinder flow structure [87]. Retarded ignition timing reduces engine-out NO\textsubscript{X},
knock propensity, and CCV. Cycle-to-cycle variations in pressure are illustrated
in Figure 2.2 [48]. It can be seen that the in-cylinder pressure history varies from
cycle to cycle, so that the combustion events occur at different conditions (such
as pressure, temperature and A/F ratio), thus leading to CCV in the combustion
duration, timing and products. As discussed in Chapter 1, these cycle-to-cycle
(and also cylinder-to-cylinder) differences limit the optimization of the combustion
system.

Engines with the fuel injector mounted in the intake port are called port-fuel-
injection (PFI) engines, while for direct-injection (DI) engines, the fuel injectors
are mounted in the combustion chamber. For a DI engine, a side- or center-
mounted high-pressure (usually 5 - 20 MPa) injector sprays fuel directly into
the combustion chamber. The spray process must be early enough in the cycle
to promote homogeneous fuel/air mixing before ignition. Fuel wetting of the
piston or cylinder walls is reduced due to the high-pressure fuel injector, which
produces a more finely atomized spray (Sauter mean drop diameter of \(~15\mu m, 
versus \(~120\mu m for PFI) and faster vaporization [5]. Direct-injection engines
have the potential to reduce emissions, increase power, and improve fuel economy
compared to PFI engines. The increased power (up to \(~15\%) and fuel economy
(3 - 5\%) is because of the charge cooling from the evaporating fuel spay and
reduced knock propensity allowing a higher (\(~12:1\)) compression ratio [5]. The
fuel economy can be further improved with cylinder deactivation or stratified-
charge-start options [88]. The hydrocarbon emissions are reduced by eliminating
port-fuel “capacitance” effects during transients and over-fueling during cold start. It is forecast that the DI engine will replace the PFI engines because of its better efficiency and emissions. More detailed discussions about HCSI-DI gasoline engines are beyond the scope of this dissertation, and can be found in [3, 5, 88].

2.2 Other combustion systems

Stratified globally fuel-lean combustion systems offer the potential for increased fuel efficiency compared with homogeneous stoichiometric systems. As shown in Figure 2.1, the high-pressure fuel injector is moved from the intake port into the combustion chamber. Stratified-charge engines operate in at least two modes depending on the load and speed: at high load and high speed, the fuel is injected early in the intake stroke, the air and fuel are well mixed to reach a stichometric homogeneous state at ignition, which is essentially the same as the HCSI-DI engine discussed above; at low load and low speed, less fuel is injected, and the average equivalence ratio is too lean to burn if the fuel mixture were well mixed. In that case, the fuel is injected just before ignition, which results in a local fuel-
rich mixture close to the spark-plug area at the time of ignition [89]. Because the power of the engine is not controlled by throttling the intake air, there is no throttling loss. Complex optimization is required for the critical design parameters such as in-cylinder flow with variable swirl or tumble, fuel-spray shape, drop size, penetration and targeting, piston surface geometry, and injector and spark timing.

In stratified-charge engines, combustion proceeds from premixed turbulent flame propagation near the spark plug, to diffusion-controlled combustion as partially reacted rich zones mix with fuel-lean zones. For reliable ignition, the fuel-air stratification must be optimized at each engine speed/load condition to maintain a somewhat fuel-rich mixture at the spark plug at the time of spark. A compact near-stoichiometric mixture is required in the vicinity of the spark plug for robust flame propagation, and steep gradients in equivalence ratio at the edge of the fuel cloud are required to minimize the overly lean fringes that are the source of unburned hydrocarbon emissions [5]. The complexity of stratified-charge engines requires much tighter control of cycle-to-cycle and cylinder-to-cylinder variability to minimize bad engine cycles (i.e., misfires) [5].

The SCCI engine (diesel engine) has the highest thermal efficiency of any regular internal or external combustion engine due to its very high compression ratio and absence of throttling. It is widely used in the heavy-duty market [3, 5]. However, a key diesel emissions issue is the soot/NO\textsubscript{X} tradeoff: in general, strategies that reduce emission levels for one of these pollutants tend to increase the other.

In HCCI engines, the fuel is injected into the combustion chamber early in the intake stroke to form a nearly homogeneous fuel-air mixture at ignition time. The mixture is highly diluted by EGR, or is very lean. This system has the potential for diesel-like thermal efficiency with near-zero NO\textsubscript{X} and particulate-matter emissions. There has been ongoing interest in HCCI engines for more than 25 years [5]. Compared to the combustion systems discussed so far, HCCI engines are extremely sensitive to small variations in in-cylinder pressure, temperature, and composition. Understanding and controlling the spatial nonhomogeneities, temporal unsteadiness, and CCV in aero-thermo-chemical quantities for the nominally homogeneous HCCI combustion process is expected to be a key to successful engine design [3]. More detailed discussion of these combustion systems can be
found in [3, 5].

\section{2.3 Premixed turbulent flame propagation}

As discussed in the last section, the combustion process for a warmed-up HCSI gasoline engine can be idealized as premixed turbulent flame propagation. Premixed combustion processes are usually characterized by the Damköhler ($Da$) and the Karlovitz ($Ka$) numbers. These are defined as \[90\]

\begin{equation}
Da = \frac{\tau_t}{\tau_c}, \tag{2.1}
\end{equation}

\begin{equation}
Ka = \frac{\tau_c}{\tau_k}, \tag{2.2}
\end{equation}

where $\tau_t$ is the turbulence integral time scale, $\tau_k$ is the Kolmogorov time scale and $\tau_c$ is a chemical time scale estimated from the laminar premixed flame speed and thickness. If $Da >> 1$ and $Ka << 1$, the chemical reactions occur much faster than all turbulent scales. In that case, turbulence does not alter the internal flame structure and the local flame structure is essentially laminar. For piston engines these nondimensional numbers can be estimated as: $10 < Da < 500$ and $0.01 < Ka < 5$. Combustion in spark-ignition engines thus mainly occurs in the flamelet regime \[50, 90\].

In this regime, chemical reactions take place in very thin regions whose local structure is essentially that of a one-dimensional (1-D) premixed laminar flame. The principal effect of turbulence is to wrinkle the flame, thereby increasing the active flame surface area. The turbulent flame front may then be considered as a collection of wrinkled interfaces separating cold unburned reactants from hot burned products (Figure 2.3).

Among the combustion models that have been developed for the flamelet regime, the flame-surface-density-based models such as the Coherent Flame Model (CFM) are particularly well-suited to piston IC engines. The flame surface density (FSD) $\Sigma$ is defined as

\begin{equation}
\Sigma = \lim_{\delta V \to 0} \frac{\delta A}{\delta V}, \tag{2.3}
\end{equation}

where $\delta V$ is the flame area in a volume $\delta A$. The principal idea of the CFM model
Figure 2.3. Turbulent premixed flame propagation in a flamelet regime [91, 92].

is to model the rate of fuel consumption per unit volume $\tilde{\omega}_F$ as the product of flame surface density $\Sigma$ and the local consumption rate of the fresh mixture per unit flame area, which is proportional to the laminar flame speed $S_l$:

$$\tilde{\rho}\tilde{\omega}_F = \tilde{\rho}_u \tilde{Y}_{TF} S_l \tilde{\Sigma}, \quad (2.4)$$

where ‘$-$’ denotes a spatially filtered quantity, ‘$\sim$’ denotes a density-weighted (Favre) filtered quantity $\tilde{Q}_i \equiv \rho \tilde{Q}_i / \tilde{\rho}$, $\tilde{\rho}_u$ is the fresh gases density and $\tilde{Y}_{TF}$ is the “fuel tracer,” which is the fuel mass fraction conditioned on being in the fresh gases [48, 50]:

$$\tilde{Y}_{TF} = \tilde{\rho}_F / \tilde{\rho}_u, \quad (2.5)$$

where $\tilde{\rho}_F$ is the mass of fuel in the fresh gases per unit volume (there can also be fuel in the burned gases in the case of rich mixtures), and $\tilde{\rho}_u$ is the fresh-gases mass per unit volume.

The FSD $\Sigma$ can be determined via modeled transport equations proposed in [49], for example, in the context of LES. The mixture composition is computed by solving transport equations for the filtered mass of chemical species. The laminar flame speed $S_l$ can be computed using a correlation based on the Metghalchi and Keck experiments [93]. More details of the CFM model can be found in [50].

The advantage of flamelet modeling is that it permits a decoupling between detailed chemical kinetics and turbulent hydrodynamics, while maintaining tight local coupling between chemical kinetics and molecular transport [87]. However,
the coupling is correct only under specific (boundary-layer-like) conditions that are not always valid in practical combustion devices. In cases where flamelet combustion does occur (e.g., homogeneous flame propagation in a stoichiometric premixed spark-ignition engine), flamelet models have been highly successful [87].

A review of early work on in-cylinder fluid mechanics has been made by Lumley [94]. The in-cylinder turbulence can increase the overall burn rate by increasing the active flame surface density. This is because flame front wrinkling increases the turbulent flame area. The FSD is approximately proportional to the RMS turbulence level \( u' \) in the engine; \( u' \) is proportional to the mean piston speed \( \bar{V}_p \); and \( \bar{V}_p \) is proportional to the crankshaft rotational speed \( \Omega_{CS} \) [3]. Therefore, the overall burn rate scales in direct proportion to engine speed. This explains why SI piston engines can operate over a wide range of speeds (600 RPM < \( \Omega_{CS} \) < 6,000 RPM) with only minor variations in ignition timing [3]. Damköhler’s studies of turbulent combustion in [95] were partly motivated by this remarkable and fortuitous scaling.

## 2.4 CFD-based turbulence hydrodynamics:

### Current practice for in-cylinder flows

The current mainstream turbulence modeling approach for in-cylinder CFD is a \( k - \varepsilon \) RANS model with standard wall functions. As discussed in Chapter 1, CCV are not accessible with this level of modeling. This is because in RANS, the local instantaneous value of a computed variable represents an ensemble- or phase-average over many engine cycles at a specified spatial location and crank phasing. A simulation through a single engine cycle represents the ensemble average, and simulations through multiple engine cycles should give same result on every cycle, after reaching a statistically periodic state. In practice, it usually is necessary to carry a RANS-based calculation through more than a single engine cycle to ensure that the result corresponds to a cyclic steady state; a small number of cycles (two to five) usually is sufficient [3, 87].

All fluctuations about the ensemble average are represented by the turbulence model. However, classical equilibrium turbulence notions and analysis tools for
homogeneous isotropic turbulence may not be relevant for complex in-cylinder turbulent flows. Anisotropy effects, intermittency due to large-scale motions such as tumble precession, CCV and rare deviations from the average, such as those caused by misfires, are not the same as the effects of turbulent fluctuations in a given engine cycle. These cannot be accurately predicted using RANS [48]. It is generally agreed that the next generation of turbulence modeling for IC engines will be LES. As discussed earlier, LES modeling based on spatial filtering offers the following advantages compared to RANS, and these advantages are particularly compelling for the IC-engine application.

1. LES is capable to capture CCV in IC engines; this is because the variables in LES are spatially filtered, rather than ensemble-averaged as in RANS.

2. LES can capture more flow structures, eddies and vortices on the computational grid than RANS. This is due to smaller modeled turbulence viscosity and higher-order numerical algorithms, which lead to smaller dissipation.

3. LES should be better than RANS at capturing the impact of relatively small changes in geometry (such as combustion-chamber shape, piston-bowl profile, spark-plug geometry and location, port design, valve design, etc.), fuel injection, and operation parameters (such as spark timing, injection timing, valve timing, etc.). The improved “design sensitivity” will help LES contribute to engine optimization.

4. LES models are expected to require less configuration-specific tuning than RANS models, thus providing better predictive capability for engine design. This is because in LES, models are only required for the effects of small unresolved eddies, and the behavior of smaller eddies tend to be more universal and thus easier to model. The main-stream LES models involve fewer adjustable coefficients, especially for the “dynamic approach” discussed above, where there are no adjustable coefficients.

5. Although LES is computationally more expensive than RANS, it remains affordable in IC engines, where the Reynolds number is relatively low. The sub-millimeter grids that are used in RANS can be used to perform LES
without significant refinement, although a large number of engine cycles may need to be simulated for LES.

In LES, the variables are spatially filtered rather than ensemble averaged. This is an advantage when LES is used to study new phenomena. This is because the local instantaneous quantities such as temperature, mass fraction and A/F ratio are more complete than ensemble-averaged quantities in modeling the combustion process. However, it can be a disadvantage when comparing the LES results with experimental data that are often averaged over many cycles. LES has to be run through multiple cycles in order to obtain statistically converged ensemble-averaged results. Therefore, LES will still require more CPU time than RANS. The increased computational cost is not necessarily due to a finer computational mesh, but because of the multiple engine cycles that are needed.

After LES is performed, it is necessary to decide how to interpret LES results and how to make quantitative comparisons with experiment. As Pope mentioned in [96], one can not compare the instantaneous resolved flow field from LES directly with experiments; they can only be compared in a statistical way. The most straight-forward way in the case of an IC engine is to make comparisons based on phase-averaged quantities between LES and experiments. The RMS of the flow quantities such as velocity, temperature and pressure also can be obtained and compared. These give an indication of the magnitude of the cycle-to-cycle fluctuations and CCV.

Phase-averaging is simple and intuitive; however, it provides limited information into the turbulence and combustion process of interest. For example, phase-averaged quantities do not necessarily represent the most energetic or the most dynamically important flow structures. Alternative techniques can provide more insight into turbulence in IC engines. Fourier transforms and POD are two candidates.

In Fourier transformation, a time series of flow fields can be represented as a series of Fourier modes (or basis functions) and their corresponding time-varying coefficients. The mutually orthogonal Fourier modes represent the flow structures at each wavenumber or length scale; the energy spectrum of Fourier modes represents the energy contained at different length scales. Classic Fourier transforms requires spatial homogeneity or periodicity, which we do not have in an engine.
POD is similar to Fourier transformation in the sense that it is also an orthogonal decomposition method: a time series of flow fields can be represented as a linear combination of basis function (POD modes) and corresponding time-varying coefficients. However, in contrast to Fourier transformation in which the modes correspond to different length scales; POD modes are related to energy content. POD modes are obtained by maximizing the kinetic energy when projecting the original flow fields onto the modes. For example, if the flow fields are projected onto the first mode, the average energy content is larger than if the flow field is projected onto any other basis, such as a Fourier mode. In the space orthogonal to this mode, the maximization process is repeated, and in this way, a set of orthogonal POD modes can be obtained.

Compared with Fourier transforms, an advantage of POD is that the POD modes are optimal in a kinetic-energy sense for modeling or reconstructing a set of flow fields. The first POD mode represents the most energetic flow structure while the first Fourier mode represents the structures with the largest length scale; a smaller number of POD modes is sufficient to capture a specified fraction of the kinetic energy of the original flow field compared to any other orthogonal basis. POD has been proposed as a method to define and visualize “coherent structures” in turbulence. The time-varying coefficients which are independent of space can be used to describe the dynamic behavior of dynamically important structures, as well as to measure or quantify the CCV in a piston engine. The POD energy spectrum can be used to characterize the flow’s level of complexity. POD can also be used as a way to make comparisons between experiment and simulation that goes beyond ensemble averaging.

2.5 Key issues to be addressed in the proposed research

In this dissertation, we will address the following two key issues for IC engines:

1. A careful assessment of the capability of LES to provide more accurate results than traditionally used RANS, and to capture the dynamics of turbulence,
especially CCV, will be carried out for two motored engine configurations.

2. POD will be evaluated as a method to analyze the complex in-cylinder turbulence flows. In particular, the potential of POD in analyzing CCV and make objective comparisons between simulation and experiments will be explored.

For the LES part, the behavior of physical models and numerical algorithms will be evaluated for simplified motored engine configurations. The advantages of LES with respect to RANS will be examined for the same configurations. The tradeoff between prediction that can be made more accurately with LES versus the additional computational cost compared to RANS are also discussed for the simplified motored engine. The questions of how to perform LES, and how to interpret LES results for complex geometries with moving boundaries on relative coarse computational mesh, will be explored. The resolution quality of the LES will also be quantified by estimating the fraction of the resolved turbulence kinetic energy (TKE) versus the total TKE. The CCV in trapped mass and in-cylinder pressure will be examined, and the CCV root causes will be explored.

The application of POD in IC engines will be examined and explored. This includes quantification of CCV, the ability to capture the dominant in-cylinder flow structures, and the potential to make objective comparisons between experiment and simulation, thus allowing the valuable information from modern high-fidelity experimental diagnostics to be better brought to bear to improve engines.

The physical interpretations of POD modes and corresponding eigenvalues will be discussed. Two POD variants (phase-dependent POD and phase-invariant POD) will be introduced, and their applications will be discussed. The sensitivity of POD results to variations in parameters will also be discussed.

While the present scope is limited to nonreacting flows, it is expected that these tools eventually will be extended to include spark ignition and turbulent flame propagation for HCSI and SCSI engines.
3.1 Large-eddy simulation

As discussed in Chapter 1, in LES one solves equations that govern the evolution of the large, energy-containing scales (larger than the filter width $\Delta$) and models the effects of unresolved scales on the resolved ones using SFS models. Because the small scales tend to be more universal, LES offer the promise of more accuracy with greater generality. In general, the filter width $\Delta$ should be smaller than the size of the energy-containing eddies. Ideally, $\Delta$ should lie in the inertial subrange. Further details can be found in [97], for example.

3.1.1 Governing equations

The starting point is the instantaneous Navier-Stokes equations:

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j},$$

(3.1)

where $\rho$ is the density, $u_i$ is the velocity component in the $i$-direction, $p$ is the pressure, and $\sigma_{ij}$ is the viscous stress tensor written as:

$$\sigma_{ij} = 2\mu S_{ij} - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij},$$

(3.2)
where $S_{ij}$ is the rate-of-strain:

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad (3.3)$$

and $\delta_{ij}$ is the Kronecker delta function:

$$\begin{cases} 
\delta_{ij} = 1, (i = j), \\
\delta_{ij} = 0, (i \neq j).
\end{cases} \quad (3.4)$$

A spatial filter is applied, and each quantity is decomposed into the sum of a spatially filtered contribution (denoted using an overbar) and a fluctuation about the spatially filtered value (denoted using a double prime). For example,

$$u_i = \bar{u}_i + u_i'' \quad (3.5)$$

The resulting filtered Navier-Stokes equations can be written as:

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j + \bar{p} \delta_{ij}) = \frac{\partial}{\partial x_j} (\tilde{\sigma}_{ij} + \tau_{SFS,ij}), \quad (3.6)$$

where ‘$\sim$’ denotes a density-weighted (Favre) filtered value:

$$\tilde{u}_i \equiv \frac{\bar{\rho} u_i}{\bar{\rho}}. \quad (3.7)$$

The filtered viscous stresses are written as:

$$\tilde{\sigma}_{ij} = 2 \mu \tilde{S}_{ij} - \frac{2}{3} \mu \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij}, \quad (3.8)$$

where $\tilde{S}_{ij}$ is the resolved rate-of-strain:

$$\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right). \quad (3.9)$$

The quantity $\tau_{SFS,ij} = \bar{\rho} (\tilde{u}_i \tilde{u}_j - \tilde{u}_i u_j)$ is an apparent SFS stress [97, 98, 99]. Here the SFS stress is modeled using eddy-viscosity type closures, which assume a linear relationship between the SFS stresses and the resolved rate-of-strain $\tilde{S}_{ij}$.
where $k_{SFS}$ is the SFS turbulent kinetic energy defined as:

$$\bar{\rho}k_{SFS} = -\frac{1}{2}\tau_{SFS, kk}, \quad (3.11)$$

and $\mu_{SFS}$ is an apparent SFS turbulent viscosity.

### 3.1.2 Subfilter-scale models

Many SFS models have been proposed to model the influence of unresolved (SFS) motions on resolved scales. Two SFS models are considered here: a Smagorinsky SFS model and a one-equation SFS model.

#### 3.1.2.1 Smagorinsky model

The Smagorinsky model is the most commonly used SFS model [40]. It is derived from a local equilibrium assumption: the production and dissipation of SFS turbulent kinetic energy are equal. It can be written in the following form [40]:

$$\mu_{SFS} = \bar{\rho}C_s \Delta \frac{2}{3} \parallel \widetilde{S} \parallel, \quad (3.12)$$

where $\parallel \widetilde{S} \parallel = (\widetilde{S}_{ij}\widetilde{S}_{ij})^{1/2}$ is the Frobenius norm of the resolved strain-rate tensor, and $\Delta$ is taken as $V_{cell}^{1/3}$ [100], where $V_{cell}$ is the volume of a computational cell. The baseline value of the model constant $C_s$ is taken to be the square of the classic Smagorinsky constant ($C_s = 0.165^2$) [101, 102] and the values can be adjusted following the recommendations available in the literature for shear flows and free flows [103, 104]. The SFS kinetic energy then is modeled using a closure similar to the one proposed by Yoshizawa [105]:

$$k_{SFS} = 2C I \Delta \sqrt{\parallel \widetilde{S} \parallel}^2. \quad (3.13)$$
The standard value of the model constant $C_I$ is 0.202. The SFS turbulent dissipation rate $\varepsilon_{SFS}$ then can be defined as

$$
\varepsilon_{SFS} = 2C_\varepsilon \frac{k_{SFS}^{3/2}}{\Delta},
$$

(3.14)

where $C_\varepsilon$ can be obtained from equilibrium arguments as

$$
C_\varepsilon = 2C_a C_I^{-3/2}.
$$

(3.15)

### 3.1.2.2 One-equation model

Speziale [106] recommended solving a transport equation for $k_{SFS}$ rather than using a local equilibrium assumption for the SFS kinetic energy. A modeled transport equation for $k_{SFS}$ can be written as

$$
\frac{\partial \overline{\rho} k_{SFS}}{\partial t} + \frac{\partial \overline{\rho} \overline{u}_j k_{SFS}}{\partial x_j} = -\tau_{SFS,ij} \overline{S}_{ij} - C_1 \overline{\rho} \frac{k_{SFS}^{3/2}}{\Delta} + \frac{\partial}{\partial x_j} \left[ C_k \overline{\rho} \Delta k_{SFS}^{1/2} \frac{\partial k_{SFS}}{\partial x_j} \right].
$$

(3.16)

Here the standard value for model constants $C_1$ and $C_k$ are: $C_1 = 1.0$ and $C_k = 0.05$. The turbulent kinetic energy thus obtained is then used as a velocity scale for the SFS viscosity [105, 107, 108]:

$$
\mu_{SFS} = C_k \overline{\rho} \Delta k_{SFS}^{1/2}.
$$

(3.17)

### 3.1.2.3 Wall models

For wall-bounded flows, most turbulence is generated in the near-wall region. It is therefore necessary to resolve the details of the near-wall flow, which requires a fine mesh. A wall model is often used to model the turbulence in the near-wall region to relax the mesh-resolution requirements. Here the near-wall treatment is implemented as a two-step process. In the first step, the wall friction velocity $u_\tau$ is estimated by inverting a third-order Spalding law [109]:

$$
y^+ = u^+ + \frac{1}{E} (e^{\kappa u^+} - 1 - \kappa u^+ - \frac{(\kappa u^+)^2}{2} - \frac{(\kappa u^+)^3}{3})
$$

(3.18)
where $\kappa = 0.417$ is the von Karman constant, and $y^+$ and $u^+$ are obtained from:

$$y^+ = y u_\tau / \nu, \quad (3.19)$$
$$u^+ = u / u_\tau, \quad (3.20)$$
$$u_\tau = (\tau_w / \rho)^{1/2}. \quad (3.21)$$

Here $y$ is the wall-normal distance, $\nu = \mu / \rho$ is the kinematic viscosity, and $\tau_w$ is the wall shear stress. The empirical constant $E$ is equal to 9.00 for a smooth wall. In the second step, the relevant fluxes for momentum, thermal energy and chemical species are computed on the basis of an estimated $u_\tau$. The wall models are active only in those cells that have one or more faces that correspond to a wall, following standard practice.

### 3.1.3 A two-equation RANS turbulence model

It is appropriate to compare the LES results with results from a standard RANS-based turbulence model that typically would be used for IC engines. A two-equation $k - \varepsilon$ model suffices for this purpose. In that case, modeled equations are solved for turbulence kinetic energy, $k$, and the viscous dissipation rate of turbulence kinetic energy, $\varepsilon$. The equations are:

$$
\frac{\partial}{\partial t} (\langle \rho \rangle k) + \frac{\partial}{\partial x_j} (\langle \rho \rangle \hat{u}_j k - (\mu + \mu_t) \frac{\partial k}{\partial x_j}) = \mu_t P - \rho \varepsilon - \frac{2}{3} (\mu_t \frac{\partial \hat{u}_i}{\partial x_i} + \langle \rho \rangle k) \frac{\partial \hat{u}_i}{\partial x_i},
$$

(3.22)

where ‘\(\langle \rangle\)’ denotes an ensemble-averaged value, ‘\(^\wedge\)’ denotes a Favre-averaged value (density-weighted mean), $P$ is the turbulence production rate,

$$P \equiv \widehat{S}_{ij} \frac{\partial \hat{u}_i}{\partial x_j},$$

(3.23)
and,

\[
\frac{\partial}{\partial t}(\langle \rho \rangle \varepsilon) + \frac{\partial}{\partial x_j}[(\langle \rho \rangle \hat{u}_j \varepsilon - (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \frac{\partial \varepsilon}{\partial x_j})] = C_{\varepsilon 1} \frac{\varepsilon}{k} [\mu_t P - \frac{2}{3} (\mu_t \frac{\partial \hat{u}_i}{\partial x_i} + \langle \rho \rangle k) \frac{\partial \hat{u}_i}{\partial x_i}]
\]

\[
- C_{\varepsilon 2} \langle \rho \rangle \frac{\varepsilon^2}{k} + C_{\varepsilon 3} \langle \rho \rangle \varepsilon \frac{\partial \hat{u}_i}{\partial x_i}.
\]

(3.24)

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\varepsilon$</th>
<th>$C_{\varepsilon 1}$</th>
<th>$C_{\varepsilon 2}$</th>
<th>$C_{\varepsilon 3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.0</td>
<td>1.22</td>
<td>1.44</td>
<td>1.92</td>
<td>-0.33</td>
</tr>
</tbody>
</table>

Table 3.1. The constants used in the $k - \varepsilon$ turbulence model.

The turbulence viscosity in the mean momentum equation then is specified as,

\[
\mu_t = \frac{C_\mu \rho k^2}{\varepsilon}.
\]

(3.25)

Here $\sigma_k$, $\sigma_\varepsilon$, $C_\mu$, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and $C_{\varepsilon 3}$ are model constants; standard values are given in Table 3.1 [110, 111, 112]. The mean dilatation term in Equation 3.24 was introduced by El Tahry [112]; there the value $C_{\varepsilon 3} = -1/3$ was deduced analytically with an assumption of local isotropy.
3.2 Proper orthogonal decomposition

The fundamental idea behind POD is to decompose a time-dependent velocity field, \( \mathbf{u}(x, t) \), into a linear combination of \( M \) spatial basis functions (the POD modes, denoted \( \psi^{(k)}(x) \)) and the corresponding time-dependent coefficients (denoted \( a^{(k)}(t) \)):

\[
\mathbf{u}(x, t) = \sum_{k=1}^{M} \left( a^{(k)}(t) \psi^{(k)}(x) \right).
\] (3.26)

In practice, this is done using samples of the velocity field obtained at discrete spatial locations and at discrete instants in time, obtained from experiment or from simulation. In POD, the basis functions are not specified \( a \) priori; rather, they are computed from the velocity field itself. Key properties of POD modes are: the original velocity field can be expressed as a linear combination of POD modes; the POD modes are mutually orthogonal and of unity magnitude (they are an orthonormal basis); and the POD modes are optimal in the sense that a higher fraction of the original flow’s kinetic energy can be captured using fewer POD modes compared to any other orthogonal basis. Details of the theory and method of calculation can be found in [61].

In most applications to turbulent flows, the POD modes have been found using the ‘method of snapshots’ introduced by Sirovich [113]. The method of snapshots is equivalent to the more formal direct method for computing the POD [61, 114] and is computationally less intensive, especially in cases where the number of spatial locations at which the velocity field is sampled is greater than the number of instants in time at which it is sampled. The method of snapshots is the approach that has been adopted here.

A basic algorithm for extracting the POD modes is outlined in the following subsection. Subsequent subsections introduce the modifications to the basic algorithm that are required to deal with flows in piston engines, and other aspects of POD-based analysis that are relevant to the engine application.

3.2.1 Method of snapshots

The starting point is a sequence of \( M \) instantaneous velocity fields, or “snapshots.” Each snapshot consists of one, two or three velocity components at \( N \) discrete
locations in physical space. The spatial locations are arbitrary (e.g., they needn’t correspond to the nodes of a structured mesh), but they must be the same locations for all $M$ snapshots. The POD modes are computed by solving an $M$-by-$M$ eigenvalue-eigenvector problem, followed by some additional linear algebra; the resulting $M$ modes then are ordered by decreasing kinetic energy. The algorithm is as follows.

Let $\mathbf{u}(\mathbf{x}, t)$ denote the velocity (a $D$-dimensional vector; $D=2$ for two-dimensional (2-D) velocity vectors, $D=3$ for three-dimensional (3-D) velocity vectors) at spatial location $\mathbf{x}$ at time $t$. Each snapshot then consists of $D \cdot N$ velocity components at $N$ different spatial locations at a fixed time $t$; there are $M$ such snapshots, each snapshot corresponding to a different time $t$. The notation $\mathbf{u}^{(k)}(\mathbf{x}_n) = \mathbf{u}(\mathbf{x}_n, t_k)$ denotes a velocity vector ($D$ components) at spatial location $\mathbf{x}_n$ at time $t_k$.

The inner product of two snapshots is denoted by $(\mathbf{u}^{(i)}, \mathbf{u}^{(j)})$, and is defined as,

$$
(u^{(i)}, u^{(j)}) \equiv \sum_{n=1}^{N} \left[ \sum_{d=1}^{D} (u_d^{(i)}(\mathbf{x}_n) u_d^{(j)}(\mathbf{x}_n)) \right] = M \cdot C_{ij} ,
$$

where the $M \times M$ matrix $C$ has been introduced. The following equation then is solved for the $M$ eigenvalues $\lambda^{(k)}$ and the $M$ eigenvectors $\mathbf{A}^{(k)}$ ($k = 1, \ldots, M$):

$$
\begin{bmatrix}
C_{11} & \cdots & C_{1M} \\
\vdots & \ddots & \vdots \\
C_{M1} & \cdots & C_{MM}
\end{bmatrix}
\begin{bmatrix}
A_1^{(k)} \\
\vdots \\
A_M^{(k)}
\end{bmatrix}
= \lambda^{(k)}
\begin{bmatrix}
A_1^{(k)} \\
\vdots \\
A_M^{(k)}
\end{bmatrix} .
$$

The $M$ POD modes $\psi^{(k)}(\mathbf{x})$ then are formed as follows:

$$
\psi_d^{(k)}(\mathbf{x}_n) = \sum_{m=1}^{M} (A_m^{(k)} u_d^{(m)}(\mathbf{x}_n)) .
$$

Each POD mode has the same structure ($D \cdot N$ components) as each of the snapshots of the original velocity field, and linear combinations of the modes sometimes have been identified as ‘coherent structures’ in the flow. The time-varying coefficients $a^{(k)}(t)$ are calculated by projecting the POD modes onto the
original snapshots:

$$a^{(k)}(t) = (\mathbf{u}^{(i)}, \psi^{(k)}) = \sum_{n=1}^{N} \left[ \sum_{d=1}^{D} \left( u^{(i)}_d(\mathbf{x}_n) \psi^{(k)}_d(\mathbf{x}_n) \right) \right] ,$$

where the index $i$ plays the role of the temporal index.

An important result is that the coefficients are uncorrelated [61]:

$$\langle a^{(i)} a^{(j)} \rangle = \delta_{ij} \lambda^{(i)} ,$$

where angled brackets denote a mean value. Here the mean would be estimated as an average over the discrete instants in time at which samples are available. Thus the mean of the square of each coefficient is equal to the corresponding eigenvalue, and it can be shown that the magnitude of each eigenvalue is equal to twice the mean kinetic energy in the corresponding POD mode.

It is useful to order the eigenvalues and eigenvectors by decreasing magnitude of the eigenvalues, so that the first POD mode contains the highest kinetic energy, the second mode contains the next highest kinetic energy, and so on. The eigenvalues then can be used to characterize the degree of organization of the flow. A rapid decrease in eigenvalue magnitude with mode number would be a characteristic of a highly organized flow [72], where most of the energy is contained in the first few POD modes. Conversely, a gradual decrease in eigenvalue magnitude with mode number would be a characteristic of a disorganized flow where a large number of modes is required to capture a significant fraction of the flow’s kinetic energy. This will be discussed further in subsequent chapters.

### 3.2.2 Modifications required for flows in piston engines

The standard method of snapshots outlined above can be applied directly to velocity fields that are obtained from multiple engine cycles at a given crank position. This has been called ‘phase-dependent’ POD in the IC-engine context. In phase-dependent POD, the intent is to extract the dominant energy-containing structures for a particular phase. For example, if one is interested in the flow structures at TDC, one selects snapshots at TDC obtained on different engine
cycles as the input for the POD analysis. The first few POD modes (the exact number depending on the degree of organization of the flow) then give a general impression of the flow structure at TDC, and the behavior of the eigenvalues provides insight into the structural complexity of the flow. This process can be repeated for each phase of interest in an engine cycle.

The idea of a ‘phase-invariant’ POD that provides a single set of POD modes that is representative of the flow dynamics over the full engine cycle was introduced in [72]. There phase-invariant POD was used to provide insight into the breakdown of large-scale in-cylinder tumble to generate turbulence near TDC. To the extent that the time-dependent in-cylinder flow through the full engine cycle can be recreated using a small number of POD modes, phase-invariant POD offers the potential for rapid analysis and prediction of the in-cylinder flow structure that might eventually be used in a real-time control system, for example.

Phase-invariant POD starts with snapshots obtained at multiple piston positions. As noted earlier, a fundamental requirement for the method of snapshots is that the velocity data must be provided at the same spatial locations for all snapshots. Three modifications were proposed in [72] to deal with the time-varying geometry. First, a linear spatial transformation was applied so that the velocity components are defined at the same spatial locations (a baseline grid) for all snapshots. Second, a linear velocity transformation was applied to retain the 1-D global dilatation from each snapshot during the spatial transformation. And third, the velocities were rescaled so that each snapshot has the same kinetic energy prior to performing the POD analysis. These transformations have been retained in the present work.

Here the baseline grid is taken to correspond to piston mid-stroke, and a linear spatial transformation is used. With $z$ denoting the spatial coordinate along which the piston moves, $z = 0$ corresponding to the head, and $z$ increasing from the head toward the piston, the spatial mapping can be written as,

$$z' = z \frac{z_{\text{piston ms}}}{z_{\text{piston}}}.$$  \hspace{1cm} (3.32)

Here $z'$ denotes the transformed $z$ coordinate, $z_{\text{piston}}$ denotes the actual piston position for the snapshot, and $z_{\text{piston ms}}$ denotes the piston position at mid-stroke.
This spatial transformation is implicit, as the spatial locations do not appear explicitly in the POD analysis. The \( z \) component of velocity (denoted as \( w \)) is modified using a linear transformation that preserves the global 1-D divergence of the original velocity field:

\[
    w' = w \frac{z_{\text{piston ms}}}{z_{\text{piston}}}.
\] (3.33)

This transformation increases the energy of snapshots that correspond to piston positions \( z_{\text{piston}} < z_{\text{piston ms}} \) (e.g., close to TDC) and decreases the energy of snapshots that correspond to piston positions \( z_{\text{piston}} > z_{\text{piston ms}} \) (e.g., close to BDC). Finally, the velocities are normalized by the square root of the kinetic energy in the snapshot so that each snapshot has the same kinetic energy prior to performing the POD analysis. The reason for this is that POD is an energy-weighted procedure. To obtain modes that are representative of the full engine cycle, it is appropriate to start with equal energies for all phases. Otherwise, the dominant POD modes would always correspond to the intake or exhaust processes when the kinetic energy of the flow is highest.

The transformations that have been adopted for phase-invariant POD appear to be reasonable choices, but they have not been rigorously justified or evaluated. Results obtained with and without the two velocity transformations are compared and discussed in Chapter 5.

### 3.2.3 Flow reconstruction

As discussed earlier, the original flow field \( \mathbf{u}(\mathbf{x}, t) \) can be reconstructed from a linear combination of POD modes \( \psi^{(k)}(\mathbf{x}) \) and the corresponding coefficients \( a^{(k)}(t) \) (Equation 3.26). In the case of phase-invariant POD, the inverse of each of the transformations introduced in the previous subsection must be applied. The original flow can be approximated using a reduced set of POD modes and coefficients, with some loss of fidelity. Because the POD modes are ordered by descending eigenvalue magnitude (decreasing kinetic energy), in cases where most of the kinetic energy is contained in the first few POD modes it is expected that the first few modes should be sufficient to capture the main features of the flow. Examples of flow reconstruction are provided in Chapters 5 and 6.
3.2.4 Comparing POD modes and other velocity fields

It is useful to have a quantitative measure of the degree to which two velocity fields are similar or dissimilar. Such a criterion can be used to compare a velocity field obtained from simulation with a velocity field obtained from experiment, to compare a POD mode with a velocity field obtained from simulation or from experiment, or to compare two POD modes that were obtained using different methods of analysis (e.g., phase-dependent analysis versus phase-invariant analysis). One such criterion is the ‘relevance index’, $f_{u,v}$, that is obtained by projecting one velocity field $u$ onto another velocity field $v$:

$$f_{u,v} = \frac{(u,v)}{\|u\| \|v\|}.$$  \hspace{1cm} (3.34)

Here the numerator is the inner product over the whole domain as defined earlier, and $\| \cdot \|$ denotes the $l^2$ norm: $\|u\| = (u,u)^{1/2}$. In the case of a POD mode, the $l^2$ norm is equal to unity. The value of the relevance index $f_{u,v}$ varies from $-1$ to $+1$; a value of $+1$ means that the two velocity fields are identical, while a value of $-1$ means that they are exactly opposite. The relevance index of Equation 3.34 has been adopted as a quantitative basis for comparing velocity fields in the Results section.

3.2.5 Cycle-to-cycle variations

One motivation for applying POD analysis to in-cylinder flows in piston engines is to develop objective criteria for identifying and quantifying CCV in flow (and eventually, combustion). Here two criteria are proposed for this purpose, and these criteria are applied in Chapters 5 and 6.

The first criterion is the convergence rate of the POD modes. The percentage of energy in each POD mode can be plotted as a function of POD mode number; by construction, this is a non-increasing function. The slope is an indication of the convergence rate of the POD modes, with steeper (more negative) slopes corresponding to more rapid convergence. The cumulative energy in the first $m$ POD modes also can be plotted or tabulated, and this is a non-decreasing function. The number of POD modes required to capture a specified fraction of the flow’s
kinetic energy can then be determined. In general, a small number of POD modes would be required to capture a high fraction in the energy in a highly organized flow, and such a flow would be expected to exhibit low CCV. The converse is true of a less organized flow. A limiting case would be one where the input velocity fields for a given phase (piston position) are all identical. In that case, 100% of the energy would be contained in the first mode, and there are no CCV.

The second criterion is the standard deviation of the POD coefficients $a^{(k)}(t)$. As discussed earlier, the POD coefficients are obtained by projecting the POD modes onto the original velocity fields. For phase-invariant POD, this gives a time-varying coefficient for each mode. In the limit of no CCV, the value of $a^{(k)}(t)$ for a particular mode $k$ would be the same at all times that correspond to the same piston position. The degree of variation of $a^{(k)}(t)$ at a given piston position for different engine cycles is an indication of CCV, and this can be quantified by computing the standard deviation in $a^{(k)}(t)$ at each piston position.

### 3.3 CFD algorithms

A unstructured finite-volume CFD code, STAR-CD version 4 [115, 116], has been used for this study. Central differencing is used for the convective terms in the momentum equations. The PISO algorithm [117, 118] is used for pressure-velocity coupling, which results in a temporal accuracy comparable to a second-order scheme. A zero-equation Smagorinsky [40] model or one-equation SFS turbulence model proposed by Speziale [106] have been used here, and the values of the model constants and numerical parameters are discussed in the following chapters.
A turbulent planar channel flow

Before simulating in-cylinder flows in piston engines, the suitability of the CFD algorithms for LES is explored in a configuration for which many earlier LES studies have been reported using a variety of numerical algorithms and models.

4.1 Geometric configuration and operating conditions

The configuration is a fully-developed, isothermal, incompressible planar turbulent channel flow. A 2-D cross section of the geometry is shown in Figure 4.1. The length of the channel is $L = 2\pi$ (in $x$), the width is $W = \pi$ (in $z$), and the height is $2H = 2$ (in $y$). The dimensions follow those used by Kim, Moin and Moser [119] in their DNS study. Any consistent set of units can be used; here the dimensions are taken to be in meters. The baseline computational mesh is shown in Figure 4.2. The numbers of cells in the $x$, $y$, and $z$ directions are 30, 60 and 50, respectively. The spatial distributions of cells in the streamwise and spanwise directions are uniform, whereas a nonuniform distribution is used in the wall-normal direction with higher resolution near the channel walls. This is achieved by using an expansion ratio of 1.1096, where the expansion ratio is defined as the ratio of the larger cell height $\Delta y$ to the smaller cell height between the adjacent cells along the wall-normal direction. The total number of cells is 90,000.

This relatively coarse LES mesh has been chosen intentionally to assess whether...
reasonable results can be obtained compared to earlier studies where similar numerical methods and mesh sizes have used. Much finer meshes would be required to capture the detailed wall dynamics, for example. In the subsequent engine LES work, comparably coarse meshes will be used by necessity.

The flow is maintained by a pressure drop in the streamwise direction. The pressure force in the streamwise direction is balanced by the shear force at the top and bottom walls of the channel. No-slip boundary conditions are applied at walls, and periodic boundary conditions are applied in both the streamwise (x-) and spanwise (z-) directions. The Smagorinsky model is used as the baseline SFS model. The SIMPLE three-time-level implicit scheme is used for temporal discretization and central differencing is used for spatial discretization. The baseline computational time step is 0.001 s, corresponding to a maximum material Courant
number of 0.0936.

The mean velocity and other mean quantities are functions only of the wall-normal component $y$, and are symmetric about $y = H$. The statistical averaging of flow variables begins after the turbulent flow is fully developed. Our results in the next section shows that the time averaging window of 25 s is sufficient, particularly when further combined with spatial averaging over the homogeneous directions (parallel to the walls). All mean profiles plotted have been extracted in this manner.
4.2 Results

The simulations are run for 50 s, corresponding to approximately 160 flow-through times. The turbulent flow is fully developed in the first 25 s (25,000 time steps), as shown in Figure 4.3, after which the statistical averaging of flow variables begins. Results are normalized using the half channel height \( H \) and the wall friction velocity \( u_\tau \), where

\[
u_\tau = \sqrt{\frac{\tau_w}{\rho}}.
\] (4.1)

Here the density is constant (\( \rho = 1 \text{ kg/m}^3 \)), so that \( u_\tau = 1 \text{ m/s} \).

The Reynolds number \( Re_\tau = \rho u_\tau H/\mu \) is then set by specifying the fluid dynamic viscosity \( \mu \) to be equal to \( Re_\tau^{-1} \text{ Pa-s} \). Results for \( Re_\tau = 395 \) [119] are presented later in this section. DNS studies for this configuration have been reported for \( Re_\tau = 180, 395 \) and 590 [119, 120]. Available data include mean velocity profiles and Reynolds-stress-components. Earlier LES studies using second-order finite-volume methods include [38] (CHAD CFD code, \( Re_\tau = 180 \)), [121] (Fluent CFD code, \( Re_\tau = 186 \)) and [122] (OpenFOAM CFD code, \( Re_\tau = 186 \)).

<table>
<thead>
<tr>
<th>Time Step</th>
<th>( \Delta t = 0.0005 \text{ s} )</th>
<th>( \Delta t = 0.001 \text{ s} )</th>
<th>( \Delta t = 0.01 \text{ s} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Smagorinsky model</td>
<td>( C_s = 0.01 )</td>
<td>( C_s = 0.20 )</td>
<td>( C_s = 0.0 )</td>
</tr>
<tr>
<td>One-equation model</td>
<td>( C_k = 0.2 )</td>
<td>( C_k = 0.02 )</td>
<td></td>
</tr>
<tr>
<td>Number of cells in x- direction</td>
<td>30</td>
<td>40</td>
<td>50</td>
</tr>
<tr>
<td>Number of cells in y- direction</td>
<td>30</td>
<td>60</td>
<td>90</td>
</tr>
<tr>
<td>Number of cells in z- direction</td>
<td>120</td>
<td>60</td>
<td>70</td>
</tr>
<tr>
<td>Location of the first grid</td>
<td>( y^+ = 0.5 )</td>
<td>( y^+ = 1 )</td>
<td>( y^+ = 2 )</td>
</tr>
</tbody>
</table>

| Number of cells in z- direction | 80                                | 60                               | 70                            |
| Location of the first grid | \( y^+ = 4 \)                    | \( y^+ = 8 \)                    | \( y^+ = 13.1 \)            |

Table 4.1. LES run matrix for the swirling case. Values in bold font correspond to the baseline case.

We first show the baseline LES results compared with the DNS data. Then a parametric sensitivity study is performed where a single parameter is varied at a time with all other parameters remaining at their baseline values. Table 4.1 shows the run matrix for the planar channel flow case. The parameters in bold font are
the baseline parameters.

### 4.2.1 Instantaneous quantities and mean quantities

To encourage turbulence to develop, a large perturbation is applied in the initial velocity field. To judge when the flow has reached statistical stationarity so that time averaging can begin, it is useful to monitor the velocity components at selected monitoring locations. Figure 4.3 suggests that the choice 25 s is probably quite conservative, and that averaging could have started much earlier. Examples of

![Figure 4.3](image)

**Figure 4.3.** $y$- and $z$- velocity components (m/s) versus time (s) at $x, y, z = 0.1047$ m, $0.00253$ m, $-1.225$ m.

instantaneous velocity fields are provided in Figure 4.4(a). Figure 4.4(a) shows contours of the instantaneous streamwise velocity component at $t=50$ s. This provides a sense of the magnitude of the resolved instantaneous velocity fluctuations. The peak streamwise velocity magnitude is approximately 24 m/s, compared to the bulk mean velocity of 19.61 m/s. Figure 4.4(b) shows contours of the time-averaged mean streamwise velocity component (averaged over 25 s).
Figure 4.4. Contour plot of the streamwise velocity component (m/s) (a) Instantaneous velocity. (b) Mean velocity.

Figure 4.5. Mean streamwise velocity profile for the baseline case.

Mean velocity and Reynolds-stress profiles for the baseline LES case are compared with DNS data in Figures 4.5 and 4.6. In all cases, only the resolved-scale contributions are shown for LES (no SFS contribution has been added to the LES Reynolds-stress components).

The DNS data have been obtained from Moser, Kim and Mansour [120] at $Re_\tau = 395$. In Figure 4.5, the LES results for $0 < y/H < 0.06$ match the DNS
Figure 4.6. Reynolds-stress-component profiles for the baseline case. (a) Component $\langle u'u' \rangle$. (b) Component $\langle v'v' \rangle$. (c) Component $\langle w'w' \rangle$. (d) Component $\langle u'v' \rangle$.

data reasonably well. For $0.06 < y/H < 0.4$, which is approximately in the buffer region of the turbulent wall-layer, the LES overpredicts somewhat, whereas for $0.4 < y/H < 1.0$, which is approximately in the log region, the LES underpredicts somewhat. Thus in the region of $0.06 < y/H < 0.4$, the slope of the mean velocity profile from LES is smaller than that of the DNS data. In Figure 4.6, the four nonzero components of the Reynolds stresses are plotted. All the values are non-dimensionalised by the friction velocity $u_f$. It can be observed that LES overpredicts the magnitude of the streamwise fluctuations $\langle u'u' \rangle$ at the expense of
the cross-stream fluctuations $\langle v'v' \rangle$ and $\langle w'w' \rangle$. This has been observed in earlier LES studies using similar numerical methods and computational meshes [38, 121, 122].

4.2.2 Sensitivity studies

The sensitivity of LES to key numerical and physical model parameters has been investigated. In each case, a single parameter has been varied with all other parameters remaining at their baseline values. These include the computational time step, the computational mesh and SFS stress model.

The influence of computational time step is examined first. Computed mean velocity and Reynolds-stress-component profiles for different time steps are shown in Figures 4.7 and 4.8, respectively. The baseline time step 0.001 s corresponds to a maximum material Courant number of approximately 0.0936. Further reduction in time step shows little benefit, while results deviate increasingly from the DNS results as $\Delta t$ is increased from the baseline value. This suggests that results become...
insensitive to time step provided that the time step corresponds to a maximum material Courant number of approximately 0.1.

The sensitivity study of other numerical and physical parameters (as shown in Table 4.1) are available but not shown for brevity. Based on these results, it is recommended that the computational time step should correspond to a maximum material Courant number of 0.1 or smaller; better results can be obtained by using finer meshes; care must be taken in the placement of the first grid point.
adjacent to the wall in $y^+$ units, and care should be taken to the choice of SFS models. In summary, for the planar channel flow, there is evidence that reasonable good-quality results can be obtained with careful attention to grid distribution, sufficiently small time step, grid size and SFS stress model.
Chapter 5

A simplified piston-cylinder assembly

The first engine configuration studied in the dissertation is an axisymmetric piston-cylinder assembly with and without swirl. A systematic LES study is carried out for this simplified piston engine. The sensitivity of LES to key numerical and physical model parameters is investigated. POD is then applied on the LES datasets to look into the dynamics of in-cylinder flow, including CCV. The potential of POD as a tool for analyzing the complex in-cylinder turbulent flow is also explored.

The geometry configurations and operating conditions are introduced first in Section 5.1. The comprehensive LES and POD studies are presented in Sections 5.2 and 5.3, respectively. A chapter summary is made in Section 5.4.

5.1 Geometric configuration and operating conditions

5.1.1 Experimental configurations

The axisymmetric piston-cylinder assembly is shown schematically in Figure 5.1; key geometric parameters and operating conditions are summarized in [78]. This is a pancake (flat head and piston) chamber with a 75-mm bore, 60-mm stroke, and 30-mm clearance. The piston moves in simple harmonic motion at a crankshaft rotational speed of $\Omega_{CS} = 200$ r/min, which corresponds to a mean piston speed of $\overline{V_p}=0.4$ m/s. Flow enters the chamber through an annular passage angled at
30 degrees with respect to the cylinder axis through a fixed, open valve. For the swirling cases, swirl vanes are added upstream of the valve around the valve stem. The angle of the valve entry is 30 degrees with respect to the cylinder axis and the width of the parallel section is 4 mm, measured in the radial direction [79, 81]. The working fluid is air, which is treated as an ideal gas. The ambient pressure and temperature are taken to be uniform at 1 atm and 300 K, respectively.

![Diagram of axisymmetric piston-cylinder assembly](image)

**Figure 5.1.** Axisymmetric piston-cylinder assembly [78].

Both swirling and nonswirling cases have been studied in [78, 79, 80, 81] using Laser-Doppler anemometry (LDA). Ensemble- (phase-) averaged radial profiles of mean and RMS velocity components at 10-mm axial increments starting from the head for crank positions of 36°, 90° and 144° after piston TDC are obtained. For nonswirling cases, only the axial velocity component was measured and measurements also were reported at 270° after top-dead-center (aTDC). For the swirling case, mean and RMS profiles of all three velocity components (axial, radial, and tangential) were reported. The number of samples (engine cycles) was 100, and five sets of data were taken to confirm repeatability.

Sources of experimental error include uncertainty in the position of measurement, flow asymmetry, variation in the rotational speed of the engine and the rotating diffraction grating, velocity-gradient broadening, crank-angle broadening and biasing effects due to limited amplifier bandwidth and filter setting. The uncertainties are discussed in detail in [79, 81]; there it was concluded that the
uncertainty in the mean velocity values does not exceed 3 percent, except at the lowest mean velocities and highest RMS levels. Further confirmation was provided by evaluating the net mass flow rates from the measured velocity profiles.

The nonswirling case has been the subject of numerous RANS-based (reviewed in [37]) and LES-based [20, 38, 123] modeling studies. The swirling case is more complex: RANS-based calculations have been performed by El Tahry [124] using three different turbulence models, and no LES results have been reported to date. In the present study, a comprehensive LES investigation is reported for both swirling and nonswirling cases with systematic variations in numerical parameters and physical models.

5.1.2 Numerical methods

5.1.2.1 Computational mesh

The mesh topology is illustrated in Figure 5.2. An unstructured mesh has been used to maintain approximately uniform mesh spacing in the in-cylinder region. All cells are hexahedral, including the region around the valve. The total number of computational cells including the valve region is 168,880 for the coarse mesh shown in Figure 5.2. Two different ways of moving the mesh to accommodate piston motion were explored. The first approach is to deform the mesh without cell removal or addition. In that case, the aspect ratio of in-cylinder cells varies by a factor of three over a cycle. The second approach is to remove and add mesh layers in the cylinder. In that case, the aspect ratios of in-cylinder cells remain constant, except for the layer of cells adjacent to the piston. The number of in-cylinder cells varies by a factor of three over an engine cycle. Both approaches have been implemented in this study, and a comparison of the two approaches is made in Section 5.2.1.1.

A similar mesh size and topology was used in the early LES study of Haworth and Jansen [38]. There the total mesh size was 151,620 cells. This is rather coarse by modern standards. The baseline mesh for the present study contains approximately 1.3 million cells, and corresponds to a factor of two mesh refinement in each direction with respect to the coarse mesh shown in Figure 5.2. A fine mesh of approximately 2.6 million cells (additional factor of two mesh refinement in the
axial direction only) also was tested. The number of cells in the radial direction in the annular valve gap is 8 for the coarse mesh and 16 for the baseline and fine meshes.

5.1.2.2 Initial and boundary conditions and the estimation of mean quantities

For the Imperial College piston-cylinder assembly, the initial pressure and temperature are uniform at 1 atm and 300 K, respectively. The no-slip boundary condition is applied at solid walls, and all walls are adiabatic. There is a large plenum upstream of the valve (not shown in Figure 5.2) so that no inflow-outflow boundary conditions are needed. The volume of the plenum is approximately 50 times larger than that of the in-cylinder region, so that the global pressure and temperature vary less than 2% through each engine cycle.

The computations begin at bottom-dead-center (BDC). For nonswirling cases, the simulations are run through seven engine cycles, and the first two cycles are discarded to avoid contamination by initial conditions. Sensitivity of results to the number of cycles is discussed in Section 5.2.1. In general, one would expect five cycles to be too few to compile converged ensemble-averaged point statistics. However, we take advantage of the statistical axisymmetry of the configuration to extract meaningful averages. At a specified crank-angle position (time) and axial location, radial profiles of velocity are sampled at 20-degree azimuthal increments.
around the cylinder axis, yielding 18 profiles that can be averaged from each engine cycle. The effective number of samples is then 18 times the number of cycles simulated; for five cycles, this is close to the 100 samples that were taken in the experiments. Standard scaling arguments suggest [38] that the turbulence integral length scale at TDC should be equal to a fraction of the clearance height; in the annular jet during induction, the turbulence integral length scale should be proportional to the annulus width. Together, these suggest an upper bound on the turbulence integral scale of approximately 4~5 mm. The 20-degree sampling angle corresponds to an azimuthal separation of at least 4 mm as close as 11 mm to the cylinder axis. At smaller radial distances, the 18 samples may not be statistically independent, yielding increasing statistical uncertainty in the computed averages as we approach the axis of symmetry.

For the swirling case, the simulations were run for ten cycles and the first five cycles were discarded. A rotating body force was added in the momentum equation in the region upstream of intake valve to mimic the effect of swirl vanes. The magnitude of the body force was adjusted to give the correct global level of in-cylinder swirl.

5.2 Variations in physical models and numerical parameters

5.2.1 Nonswirling Imperial College piston-cylinder assembly

We begin by examining the distribution of the turbulence integral length scale $l_0$. A rough estimate can be obtained from a RANS run with the $k-\varepsilon$ turbulence model:

$$l_0 = \frac{C_{\mu}^{0.75} k^{1.5}}{\varepsilon},$$  \hspace{1cm} (5.1)

where $k$, $\varepsilon$ and $C_{\mu}$ have been defined previously.

To guide the selection of mesh resolution (filter size $\Delta$) for LES, it is useful to examine $l_0$ and the ratio $l_0/\Delta$. For this configuration, both $l_0$ and $\Delta$ vary with spatial location and with time. Figures 5.3 and 5.4 show contours of the
Figure 5.3. Contour plot showing the integral length scale $l_0$ for the baseline mesh. (a) 36° aTDC. (b) 144° aTDC.

Figure 5.4. Contour plot showing the ratio $l_0/\Delta$ for the baseline mesh. (a) 36° aTDC. (b) 144° aTDC.
integral length $l_0$ and the ratio $l_0/\Delta$ for a 2-D section through the baseline mesh. In Figure 5.3 it can be seen that, except in the cells immediately adjacent to the wall and some cells close to the valve, the integral length ranges from 0.3 mm to 4.8 mm. The integral length scale close to the annular valve is smaller than at other locations, which means a finer mesh resolution is required in that region. In Figure 5.4 it can be seen for both 36° and 144° aTDC, except in the cells immediately adjacent to the wall and some cells close to the valve, the value of $l_0/\Delta$ exceeds unity. As will be shown later, the $k-\varepsilon$ model does not perform particularly well for this configuration, so these length-scale estimates cannot be taken too seriously. Nevertheless, they provide some qualitative guidance. A more direct approach to establish the suitability of the computational mesh is to examine the sensitivity of statistical quantities of interest to variations in mesh size. This analysis is performed below.

As discussed before, for LES calculations without swirl, seven consecutive cycles are simulated and the first two are discarded. The influence of the averaging window is shown in Figure 5.5; in all cases, the first two cycles have been discarded. Averaging over three cycles gives results that differ little from those obtained by averaging over five cycles. This suggests that five cycles is sufficient (even conservative) to ensure converged statistics. In Figure 5.5 and subsequent figures, each horizontal tick mark (dashed lines) corresponds to one unit of mean piston speed $V_p$. Unless specified otherwise, only the resolved-scale contribution to the RMS values is shown. The contribution of the SFS model to RMS values will be discussed later.

Table 5.1 shows the run matrix for the nonswirling case. The parameters in

![Figure 5.5](image_url)  

Figure 5.5. Computed (lines) and measured (symbols) radial profiles at 36° aTDC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.
bold font are the baseline parameters. We first show the baseline LES results compared with the measured data. We next compare the RANS and baseline LES results using the same mesh and timestep. Then a parametric sensitivity study is performed where a single parameter is varied with all other parameters remaining at their baseline values.

The computed and measured radial profiles of axial mean and RMS velocity with baseline parameters are shown in Figures 5.6 - 5.9. In these figures, only the resolved-scale contribution to the RMS values is shown. Figure 5.6 shows results for three axial stations at 36° aTDC (early on the intake stroke), and Figures 5.7 - 5.9 show the corresponding results for axial stations at 90°, 144°, and 270° aTDC.

<table>
<thead>
<tr>
<th>Time Step</th>
<th>Smagorinsky</th>
<th>SFS model</th>
<th>One-equation</th>
<th>SFS model</th>
<th>Mesh size</th>
<th>Baseline mesh</th>
<th>Fine mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>∆t = 2 CA</td>
<td>C_s = 0.00</td>
<td>C_s = 0.30</td>
<td>C_k = 0.00</td>
<td>C_k = 0.20</td>
<td>Coarse mesh</td>
<td>170 K cells</td>
<td>Baseline mesh</td>
</tr>
<tr>
<td>∆t = 1 CA</td>
<td>C_s = 0.01</td>
<td>C_s = 0.50</td>
<td>C_k = 0.01</td>
<td>C_k = 0.30</td>
<td>1.3 M cells</td>
<td>Fine mesh</td>
<td>2.6 M cells</td>
</tr>
<tr>
<td>∆t = 0.5 CA</td>
<td>C_s = 0.02</td>
<td>C_s = 0.80</td>
<td>C_k = 0.02</td>
<td>C_k = 0.50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>∆t = 0.25 CA</td>
<td>C_s = 0.10</td>
<td>C_s = 1.00</td>
<td>C_k = 0.05</td>
<td>C_k = 0.80</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>∆t = 0.1 CA</td>
<td>C_s = 0.20</td>
<td>C_s = 1.50</td>
<td>C_k = 0.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.1. LES run matrix for the nonswirling case. Values in bold font correspond to the baseline case.

Figure 5.6. Computed (lines) and measured (symbols) radial profiles at 36° aTDC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

In general, computed mean velocity profiles are in good agreement with the experimental profiles at 36°, 144° and 270°. The flow undergoes a transition in structure at approximately 90°, and it is difficult to capture the phasing of the transition precisely. Better agreement between model and measurement can be achieved at 90° with different model parameters, but at the expense of poorer
Figure 5.7. Computed (lines) and measured (symbols) radial profiles at 90° aTDC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

Figure 5.8. Computed (lines) and measured (symbols) radial profiles at 144° aTDC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

agreement at 36° and 144°. Results at 270° are not sensitive to variations in numerical and model parameters and will not be included in the subsequent discussion. The focus will be on the 36° and the 144° results.

The computed RMS profile (resolved-scale fluctuations only) at z= 20 mm at 36° lies below the experimental profiles. At this measurement location, the local RMS velocity is of the same order of magnitude as the local mean velocity. The

Figure 5.9. Computed (lines) and measured (symbols) radial profiles at 270° aTDC for the baseline case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.
contribution of the SFS model will be discussed below.

While the agreement between model and measurement is not perfect, both the mean and RMS computed profiles show better agreement with measurements than has been reported using any RANS-based model \[37, 125\], and the present results are similar to those that have been reported in other LES studies for this configuration \[20, 38, 123\].

### 5.2.1.1 Piston motion

As discussed in Section 5.1.2.1, there are two different ways to accommodate the moving piston. The first approach is to deform the mesh in the axial direction without layer addition or removal; the second approach involves layer addition and removal in the axial direction without deforming the mesh. Mean axial velocity profiles obtained using the two approaches are compared in Figures 5.10 and 5.11 for a coarse-mesh case. For the first approach, the number of cells is approximately 170,000; for the second approach, the number of cells varies from approximately 70,000 to 170,000 with the piston movement. It can be seen that the two approaches produce very similar results. Unless specified otherwise, all the subsequent results are obtained without cell addition and removal.

![Figure 5.10. Computed (lines) and measured (symbols) radial profiles at 36° aTDC for two approaches to accommodate piston motion. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.](image)

### 5.2.1.2 RANS vs LES

Baseline LES results are next compared to the results obtained using a standard \(k - \varepsilon\) RANS turbulence model with the same mesh and timestep. Figure 5.12
Figure 5.11. Computed (lines) and measured (symbols) radial profiles at 144° aTDC for two approaches to accommodate piston motion. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

Figure 5.12. Computed axial velocity at a fixed spatial location for LES (resolved velocity) and RANS (mean velocity).

down shows the instantaneous axial velocity component at a fixed spatial location in the cylinder for both LES and RANS. The location is on the center line of the cylinder, approximately 15 mm below the head. After the first two cycles, the RANS mean velocity trace remains essentially the same for subsequent cycles, while significant CCV are evident for LES. This figure serves to illustrate a key difference between RANS and LES for in-cylinder flows.

LES results with baseline parameters are compared with the RANS results in Figures 5.13 and 5.14. For RANS, \( \langle w'^2 \rangle^{1/2} \) has been estimated as the square root of \( \frac{2}{3}k \), where \( k \) is TKE. At 36° and 144° aTDC, while the RANS-based mean velocity profiles are at least qualitatively similar to the experimental profiles, the RANS turbulence levels are severely underpredicted.
Figure 5.13. Computed (lines) and measured (symbols) radial profiles at 36° aTDC for $k - \varepsilon$ RANS and for the baseline LES case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

Figure 5.14. Computed (lines) and measured (symbols) radial profiles at 144° aTDC for $k - \varepsilon$ RANS and for the baseline LES case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.2.1.3 Sensitivity to grid size

Figures 5.15 and 5.16 explore the sensitivity of LES results to variations in the computational mesh (see Table 5.1). Here the one-equation SFS model with $C_k = 0.3$ and a timestep of 0.1 CAD have been used. In general, the LES results tend to approach the experimental data as the mesh is refined. Results at $z = 20$ mm, 36° aTDC, in particular improve with the refinement of the mesh. Here only the resolved-scale contribution to the RMS velocities is shown.

Establishing the quality of LES results has proven to be difficult. One approach is to consider the resolved-scale and SFS contributions to the TKE. Pope [96] and Klein [126] have introduced single-grid estimators of LES quality by estimating the fraction of the residual (SFS) turbulent kinetic energy in the total kinetic energy. Celik et al. [127] proposed an index of quality for LES based on Richardson extrapolation using multiple meshes. According to Pope [96], a good LES should
resolve at least 80% of the TKE.

The contribution of SFS velocity fluctuations is shown in Figure 5.17(b) for the baseline mesh at 36° aTDC. Here \( \langle w'^2 \rangle_{SFS}^{1/2} \) has been estimated as the square root of \( \frac{2}{3} k_{SFS} \). At most locations, the SFS (model) contribution is small compared to the resolved-scale contribution. At this instant, more than 80% of the TKE is resolved, and a similar conclusion is drawn at the other crankangles (not shown). Figure 5.17 also shows the sensitivities of the resolved and the model contributions to the RMS velocity profiles to variations in the mesh size. Compared to the baseline case in Figure 5.17(b), it can be seen that with the refinement of mesh, the resolved contribution to the RMS velocity increases while the SFS model contribution decreases. The sum of the resolved and model contributions increases somewhat from the baseline mesh to the finest mesh, but the increase is small compared to that from the coarse mesh to the baseline mesh. This suggests that the results on the baseline and fine meshes are at least close to being grid independent, in this sense. Similar results are found at 90° and 144° (not shown).

\[ \text{(a)} \quad \text{(b)} \]

**Figure 5.15.** Computed (lines) and measured (symbols) radial profiles at 36° aTDC for three meshes. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

### 5.2.1.4 Sensitivity to computational timestep

The influence of computational timestep is examined next. Computed axial mean and RMS velocity profiles with different timesteps are shown in Figures 5.18 and 5.19. The baseline timestep of 0.1 CAD corresponds to a maximum material Courant number of approximately 0.033 based on the mean piston speed \( \bar{V}_p \). The results are relatively insensitive to timestep provided that the timestep is sufficiently small (here, less than 0.25 CAD).
Figure 5.16. Computed (lines) and measured (symbols) radial profiles at 144° aTDC for three meshes. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

Figure 5.17. Computed (lines) and measured (symbols) radial profiles of axial RMS velocity at 36° aTDC. (a) Coarse mesh. (b) Baseline mesh. (c) Fine mesh.

Figure 5.18. Computed (lines) and measured (symbols) radial profiles at 36° aTDC for three computational timesteps. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.
5.2.1.5 Sensitivity to SFS models

Figures 5.20 and 5.21 show LES results using the Smagorinsky and the one-equation SFS models with different values of the model constants $C_s$ and $C_k$, respectively. Smaller values of $C_s$ and $C_k$ correspond to smaller apparent turbulence viscosity, and hence to larger resolved-scale RMS velocities (higher resolved turbulence level). A wide range of values of $C_s$ and $C_k$ have been tried (Table 5.1), and the LES results are found to be very sensitive to the SFS model and its constants. No single value of the model constant gives uniformly the best results for all the locations and crankangles. The cases with $C_s = 0.2$ and $C_k = 0.3$ are found to give the best results overall for the Smagorinsky and one-equation models, respectively. The one-equation SFS model with $C_k = 0.3$ gives slightly better results than that of the Smagorinsky SFS model with $C_s = 0.2$ at the locations shown in Figures 5.20 and 5.21. However, at other crankangles, the Smagorinsky
SFS model gives somewhat better results than the one-equation SFS model. The fact that the results are sensitive to variations in the SFS model is encouraging, and suggests that better results might be obtained with more sophisticated SFS models.

Figure 5.21. Computed (lines) and measured (symbols) radial profiles at 144° aTDC with variations in SFS model. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

5.2.2 Swirling Imperial College piston-cylinder assembly

A systematic parametric study also has been performed for the swirling case (Table 5.2). The sensitivities of computed results to variations in physical and numerical parameters are generally similar to those that were observed in the parametric study for the nonswirling case. Hence the comparisons in this section will be limited to mesh sensitivity and a comparison between LES and RANS with a standard $k – \varepsilon$ turbulence model. The one-equation SFS model with $C_k = 0.05$ gives the best results overall, and that is the value used for all LES results that are shown in this section.

<table>
<thead>
<tr>
<th>Time Step</th>
<th>$\Delta t = 1$ CA</th>
<th>$\Delta t = 0.1$ CA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Smagorinsky model</td>
<td>$C_s = 0.02$</td>
<td>$C_s = 0.20$</td>
</tr>
<tr>
<td><strong>One-equation model</strong></td>
<td>$C_k = 0.02$</td>
<td>$C'_k = 0.05$</td>
</tr>
<tr>
<td>Mesh size</td>
<td>Coarse mesh</td>
<td><strong>Baseline mesh</strong></td>
</tr>
<tr>
<td></td>
<td>170,000 nodes</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.2. LES run matrix for the swirling case.

Figures 5.22 - 5.30 show the computed and measured mean and resolved-scale RMS profiles of three velocity components at 36°, 90° and 144° aTDC. Because this
is the first LES study to be reported for this configuration, LES results are shown for all crankangles at which measurements are available, and for all measurement stations and all three velocity components. For RANS, the RMS velocity profiles have been estimated as the square root of $\frac{2}{3}k$, where $k$ is the TKE.

In general, the LES results are in at least as good agreement with experiment.
as for the nonswirling cases reported in Section 5.2.1, and arguably are even better here. For example, the computed and measured axial mean and RMS velocity profiles at 36° and 144° are in better agreement compared to their counterparts for the nonswirling configurations. The LES results again show a significant improvement over the RANS results with \( k - \varepsilon \) turbulence model, especially for the RMS velocity profiles.

![Figure 5.25.](image1.png)

**Figure 5.25.** Computed (lines) and measured (symbols) radial profiles at 90° aTDC for the swirling case. (a) Mean azimuthal velocity profiles. (b) Azimuthal RMS velocity profiles.

![Figure 5.26.](image2.png)

**Figure 5.26.** Computed (lines) and measured (symbols) radial profiles at 90° aTDC for the swirling case. (a) Mean radial velocity profiles. (b) Radial RMS velocity profiles.

There are important differences in flow structure between the swirling and nonswirling cases; these have been discussed in detail in [79] and [81]. The swirl is far from being solid-body in nature, except close to the cylinder axis (Figures 5.22(a), 5.25(a) and 5.28(a)). Compared to the nonswirling case, the mean flow in the configuration with swirl exhibits an elongated main vortex that reaches close to the piston, and a different pattern of secondary vortices. Strong anisotropy is evident in the Reynolds stresses for the swirling case (compare...
Figure 5.27. Computed (lines) and measured (symbols) radial profiles at 90° aTDC for the swirling case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.

Figures 5.22(b) 5.23(b) and 5.24(b), for example), and the LES captures this quite naturally.

Some discrepancies remain between LES results and experiments, especially at 90°. But overall, these are quite satisfactory results, given the simplicity of the models that have been used and the complexity of this flow.

Figure 5.28. Computed (lines) and measured (symbols) radial profiles at 144° aTDC for the swirling case. (a) Mean azimuthal velocity profiles. (b) Azimuthal RMS velocity profiles.
Figure 5.29. Computed (lines) and measured (symbols) radial profiles at 144° aTDC for the swirling case. (a) Mean radial velocity profiles. (b) Radial RMS velocity profiles.

Figure 5.30. Computed (lines) and measured (symbols) radial profiles at 144° aTDC for the swirling case. (a) Mean axial velocity profiles. (b) Axial RMS velocity profiles.
5.3 POD analysis

A comprehensive LES study has been carried out above for both the swirling and the nonswirling cases, including systematic variations in numerical parameters and physical models. In order to perform POD analysis, more engine cycles of LES data are obtained for the baseline-mesh case (approximately 1.3 M cells) and coarse-mesh case (168,880 cells) with baseline parameters.

The computations begin at BDC. For the nonswirling case, the simulations were run through 52 engine cycles for the coarse mesh or 32 cycles for the baseline mesh; the first two cycles are discarded to avoid contamination by initial conditions. For the swirling case, the simulations were run for 35 cycles for both coarse and baseline meshes, and the first five cycles are discarded. The POD analysis shows that 30 consecutive cycles of LES data after discarding the first two or five cycles are sufficient to give reasonably converged POD results.

The ‘raw’ data for POD analysis are instantaneous cell-centered velocities (interpreted as spatially filtered velocities in LES) on unstructured 3-D meshes. These are saved at time increments that correspond to one CAD of rotation, so that up to 360 snapshots are available per engine cycle. The raw data can be used directly for POD analysis, or velocities can first be interpolated onto a (usually) coarser mesh prior to POD analysis. The effect of interpolation is also explored.

The results are organized as follows. In the first two subsections, results from phase-dependent POD and phase-invariant POD are presented, respectively. These include parametric studies with variations in how the POD analysis is performed (e.g., 2-D versus 3-D POD, subtracting versus not subtracting the ensemble average prior to performing the POD, use of raw versus interpolated velocity data, etc.). Flow reconstruction from POD modes is discussed next. This is followed by POD-based analysis of CCV. Up to this point, the focus is in the nonswirling case. In the final subsection, results for the swirling case are shown and differences between the swirling and nonswirling cases are highlighted. Unless stated otherwise, all results correspond to the baseline-mesh LES. Results obtained using the coarse mesh have been found to be essentially the same, in all cases.
5.3.1 Phase-dependent POD

We begin with an example that illustrates the behavior of the POD eigenvalues and the insight that those provide into the behavior of in-cylinder flow. Here phase-dependent POD has been performed for 360 phases (one per CAD of rotation) using data from the LES over 30 consecutive engine cycles for a 2-D cutting plane that contains the cylinder axis. There are 18,893 velocity vectors in the cutting plane, and minimum interpolation is necessary to obtain the node values from the cell-centered values. As discussed earlier, each eigenvalue gives the kinetic energy in the corresponding POD mode, and the modes are ordered by decreasing eigenvalue magnitude. The percentage of the total kinetic energy in the first mode, in the first three modes, and in the first five modes is plotted as a function of crank angle in Figure 5.31. The fraction of the energy in the first mode varies from a low of approximately 0.19 at TDC (0 and 360 CAD) to a high of approximately 0.83 at 30° aTDC. Similar trends are evident for the sums of the energies in the first three modes and the first five modes. At 30° aTDC, 83.3% of the energy resides in the first mode, and more than 90% resides in the first three modes. This high concentration of energy in the first few POD modes indicates a highly organized flow with small CCV. In general, well-organized flow is evident at mid-stroke on intake and exhaust. In contrast, the percentage of the energy contained in the first few modes is lower near TDC and BDC (180 CAD). This implies that the input flow fields for those phases vary considerably from cycle to cycle, and the flow is relatively disorganized. These observations are qualitatively consistent with those made by Fogleman [72, 73]. There the flow was observed to be highly organized during intake with a large fraction of the kinetic energy in the first few modes, and to be less organized near TDC and BDC.

The results at 30° aTDC (organized flow) and at TDC (disorganized flow) are next examined more closely. A larger fraction of the flow's kinetic energy is contained in a smaller number of modes for the more organized flow at 30° aTDC (Figure 5.32(a)) compared to the less organized flow at TDC (Figure 5.32(b)). Moreover, it can be seen that fewer snapshots (engine cycles) are required to obtain converged statistics at 30° aTDC. The same analysis has been performed for the coarse-mesh LES datasets using up to 50 snapshots per phase, and similar results have been found (not shown).
Figure 5.31. Fractions of kinetic energy in the first few modes from 2-D phase-dependent POD analysis for the nonswirling case for a cutting plane that contains the cylinder axis.

Figure 5.32. Fraction of kinetic energy versus mode number and number of snapshots from 2-D phase-dependent POD analysis for the nonswirling case for a cutting plane that contains the cylinder axis. (a) 30° aTDC. (b) TDC.

Figure 5.33 shows the first three POD modes and normalized (by its kinetic energy) ensemble average velocity vectors at 30° aTDC. In this and subsequent vector figures, a subset of the vectors (here one one out of every four) is plotted, for clarity, and the cylinder axis is shown in the center as a plotting artifact, because of the polar mesh. The first mode corresponds to the most energetic structures, and is similar in appearance to an annular intake jet. The first mode also strongly resembles the normalized ensemble average velocity field; the relevance index between the two is 0.998 (Equation 3.34). It is important to note that in principle,
Figure 5.33. Phase-dependent 2-D POD modes and normalized ensemble average velocity vectors for a cutting plane that contains the cylinder axis at 30° aTDC for the nonswirling case. (a) Mode 1. (b) Mode 2. (c) Mode 3. (d) Normalized ensemble average.

the first mode need not correspond to the ensemble average. Significant departures from axisymmetry are evident for the second and third modes.

The corresponding POD modes and ensemble average velocities at TDC are shown in Figure 5.34. In this case, the first mode differs significantly from the ensemble average in appearance, and the relevance index between them is 0.302. In general, it is found that for phases where a large fraction of the kinetic energy is captured in a small number of POD modes, the structure of the first mode is similar to that of the ensemble average velocity; for phases where a large number of modes is required to capture most of the kinetic energy, the first mode can be quite different from the ensemble average.

One can subtract the phase ensemble average velocity from each snapshot prior to performing the POD analysis, and that is explored next. Figure 5.35 shows the first two modes for the fluctuating velocity field for two phases, 30° aTDC and TDC. By comparing the modes for the fluctuating velocity field in Figure 5.35 with the modes for the original velocity field in Figure 5.33 at 30° aTDC, it can be seen that the first mode for the velocity fluctuations (Figure 5.35(a)) is very similar
Figure 5.34. Phase-dependent 2-D POD modes and normalized ensemble average velocity vectors for a cutting plane that contains the cylinder axis at TDC for the nonswirling case. (a) Mode 1. (b) Mode 2. (c) Mode 3. (d) Normalized ensemble average.

to the second mode for the original flow (Figure 5.33(b)); the relevance index between them is 0.973. Moreover, for 30° aTDC, the $n$-th ($n = 1, 2, ..., 29$) mode for the velocity fluctuations is similar to the $(n+1)$-th ($n = 1, \ldots, 30$) mode for the original flow, although the two may have opposite signs. Recall that for this phase, the first mode of the original velocity field is very close to the ensemble average (Figure 5.33); (the relevance index between them is 0.941), so that the subsequent modes essentially represent the turbulent fluctuations about the ensemble average. The differences between the $n$-th ($n = 1, 2$) mode of the velocity fluctuations and the $(n+1)$-th mode of the original flow are plotted in Figure 5.36. It can be seen that the differences are small (Figures 5.36(a) and 5.36(c)). If we then normalize the differences by their kinetic energy as shown in Figures 5.36(b) and 5.36(d), it can be seen that the structures are similar to those in the ensemble average velocity field in Figure 5.33(d).

The results for phases where the flow is less organized are quite different. The $n$-th ($n = 1, 2, ..., 29$) mode of the velocity fluctuations differs considerably from the $(n+1)$-th ($n = 1, 2, \ldots, 30$) mode of the original flow at TDC (Figures 5.34 and 5.35); the relevance index between them is 0.327. For this phase, the first
Figure 5.35. Phase-dependent 2-D POD modes for the fluctuating velocity field for a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1, $30^\circ$ aTDC. (b) Mode 2, $30^\circ$ aTDC. (c) Mode 1, TDC. (d) Mode 2, TDC.

mode of the original flow is different from the ensemble average velocity, and the second mode of the original flow does not represent the fluctuations with respect to the ensemble average.

We next explore the influence of data interpolation on the computed POD modes. Interpolation is required prior to performing 2-D POD for cutting planes that do not correspond to layers of finite-volume cells, and is expedient for 3-D POD to reduce the computational effort required to perform the analysis. A 3-D example is shown in Figure 5.37. There the raw in-cylinder velocity data have been interpolated onto a polar-cylindrical mesh of 320,000 grid points prior to performing the analysis for the ‘interpolated data’ case. The eigenvalues extracted using the raw velocity data are essentially the same as those extracted using the interpolated velocity data, and the same is true for the POD modes, with relevance index 0.982 (not shown). This is expected to be the case as long as the interpolation mesh remains sufficiently fine to capture the large-scale flow structures that contain most of the flow’s kinetic energy, and that dominate the first few POD modes.

3-D POD analysis has been performed for all phases using interpolated velocity data; the eigenvalue distributions for two phases are shown in Figure 5.38. The
Figure 5.36. Differences between the velocity-fluctuation-based POD modes and the original-flow POD modes, from phase-dependent 2-D POD for a cutting plane that contains the cylinder axis for the nonswirling case. (a) Figure 5.35(a) − Figure 5.33(b). (b) Normalized Figure 5.36(a). (c) Figure 5.35(b)+Figure 5.33(c). (d) Normalized Figure 5.36(c).

qualitative behavior is similar to that observed for the 2-D POD analysis in Figure 5.32.

The first two 3-D POD modes on two different cutting planes are shown in Figures 5.39 - 5.42. Figures 5.39 and 5.41 show the modes on the same cutting plane on the earlier 2-D examples, and the structures are similar to those in the corresponding 2-D POD modes for this plane, with relevance indices 0.876 and 0.884 for the first and second POD modes, respectively. Figures 5.40 and 5.42 show 3-D modes on a cutting plane normal to the cylinder axis, 10 mm below the head. An advantage of 3-D POD is that a single analysis provides much more information than a large number of 2-D POD analysis for multiple cutting planes.

5.3.2 Phase-invariant POD

Phase-invariant POD allows snapshots from multiple phases (piston positions) to be used as input. For the nonswirling case, there are 30 cycles of LES data for the baseline mesh and 50 cycles for the coarse mesh, and data have been saved at
Figure 5.37. Comparison of eigenvalues obtained using raw versus interpolated velocity data from phase-dependent 3-D POD at 90° aTDC for the nonswirling case.

Figure 5.38. Fraction of kinetic energy versus mode number and number of snapshots from 3-D phase-dependent POD analysis for the nonswirling case. (a) 30° aTDC. (b) TDC.

intervals of one-CAD (360 per cycle). Thus 10,800 input snapshots are available for the baseline mesh and 18,000 are available for the coarse mesh.

Figure 5.43 shows eigenvalue distributions for the first 15 modes from the nonswirling datasets on a cutting plane that contains the cylinder axis (2-D POD analysis) with variations in the number of cycles and in the number of phases per cycle. In Figure 5.43(a), up to 10,800 input snapshots are included; well-converged POD results are obtained with 20 cycles of data. The same conclusion is drawn for the coarse mesh (not shown). For this phase-invariant 2-D POD, over 30% of the kinetic energy resides in the first mode, and the first five modes
account for more than 60% of the kinetic energy. There is essentially no change in
the computed eigenvalues when as few as 30 phases per cycle are included in the
analysis (Figure 5.43(b)); in all cases, the phases are equally spaced in CAD. This
suggests that using all 360 phases corresponds to significant oversampling for this
configuration.

The first two modes corresponding to Figure 5.43 (with all 10,800 snapshots
used) are shown in Figure 5.44. The first mode appears to correspond to the
exhaust stroke, since the flow is exiting the cylinder. However, it is important to
keep in mind that POD is an energy-based procedure. The velocity field that is
obtained by multiplying all components of a POD mode by $-1$ is an equally valid
Figure 5.41. Phase-dependent 3-D POD modes for a cutting plane that contains the cylinder axis at TDC for the nonswirling case. (a) Mode 1. (b) Mode 2.

Figure 5.42. Phase-dependent 3-D POD modes for a cutting plane normal to the cylinder axis ($z = 10$ mm) at TDC for the nonswirling case. (a) Mode 1. (b) Mode 2.

POD mode that has the same energy; the ambiguity in reconstructing the original velocity field is resolved by the sign of the coefficient. Therefore, it is better to interpret the first mode here as representing the intake and/or exhaust processes.

2-D phase-dependent POD modes for a cutting plane that contains the cylinder axis are shown in Figure 5.45 at mid-stroke on intake ($90^\circ$ aTDC) and on exhaust ($270^\circ$ aTDC). By comparing these phase-dependent modes with the phase-invariant modes in Figure 5.44(a), it can be seen that the first mode of the phase-dependent POD at $270^\circ$ aTDC is very similar to the first mode of the phase-invariant POD with relevance index 0.781, while the relevance index between the first mode of the phase-dependent POD at $90^\circ$ aTDC and the the first mode of the phase-invariant POD is -0.273 An important difference between the two is that
Figure 5.43. Fractions of kinetic energy in the first 15 modes from 2-D phase-invariant POD analysis for the nonswirling case for a cutting plane that contains the cylinder axis. (a) Data from all 360 phases used, with variations in the number of cycles. (b) Data from all 30 cycles used, with variations in the number of phases.

Figure 5.44. Phase-invariant 2-D POD modes for a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1. (b) Mode 2.

the phase-invariant POD mode represents all phases simultaneously. Therefore, the comparison to modes from a particular phase in phase-dependent POD is somewhat arbitrary. Here the comparison at mid-stroke was motivated by the observations that were made from Figure 5.44.

3-D phase-invariant POD results for the nonswirling case are shown in Figures 5.46 - 5.48. The eigenvalue (or kinetic energy) distribution is shown in Figure 5.46. It can be seen that 20 cycles of data are sufficient for converged
Figure 5.45. Phase-dependent 2-D POD modes for a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1, 90° aTDC. (b) Mode 1, 270° aTDC.

Figure 5.46. Fraction of kinetic energy versus mode number and number of cycles from 3-D phase-invariant POD for the nonswirling case. All phases have been included.

POD results, and this is consistent with what was shown earlier for a 2-D example (Figure 5.43). The first mode contains approximately 30% of the kinetic energy; this is slightly lower than for the 2-D example.

Figures 5.47 and 5.48 show 3-D phase-invariant modes on two different cutting planes. The structures of the 3-D modes on the cutting plane that contains the cylinder axis is similar to those of the corresponding 2-D modes in Figure 5.44.

The effects of the two velocity transformations that have been used for phase-invariant POD in piston engines are explored in Figure 5.49. The POD modes obtained without the dilatation correction (Figures 5.49(a) and 5.49(b)) remain
Figure 5.47. Phase-invariant 3-D POD modes on a cutting plane that contains the cylinder axis for the nonswirling case. (a) Mode 1. (b) Mode 2.

Figure 5.48. Phase-invariant 3-D POD modes on a cutting plane normal to the cylinder axis ($z = 10\,\text{mm}$) for the nonswirling case. (a) Mode 1. (b) Mode 2.

essentially the same as those obtained with the correction (Figure 5.44). The relevance index between them is 0.807 and 0.821 for the first and second mode, respectively. However, the dilatation correction may have greater effect at high engine speeds. In contrast, the POD modes obtained without the kinetic energy normalization (Figures 5.49(c) and 5.49(d)) are significantly different from those obtained with kinetic energy normalization (Figure 5.44). The relevance index is 0.422 and 0.129 for the first and second mode, respectively. This is to be expected,
since POD is an energy-weighted method.

5.3.3 Flow reconstruction from POD modes

As discussed earlier, the original velocity field can be reconstructed using a linear combination of POD modes and the corresponding coefficients. The reconstruction is exact if all POD modes are used, and is an approximation if a subset of modes is used. Here we examine the fidelity of the flow reconstruction for the snapshot at TDC of the third cycle using different numbers of POD modes. A graphic example is provided in Figure 5.50 for the nonswirling case. There contours of the instantaneous $z$ velocity component ($w$) are shown at TDC of the third cycle for the original flow and for velocity fields reconstructed at the same instant using
different numbers of POD modes. It is clear that the fidelity improves as the number of modes increases.

Figure 5.50. Reconstruction of the instantaneous velocity field (velocity component \( w \)) at TDC of the third cycle using different numbers of 2-D phase-dependent POD modes for the nonswirling case on a cutting plane that contains the cylinder axis. (a) First three modes. (b) First five modes. (c) First ten modes. (d) Original flow.

<table>
<thead>
<tr>
<th>Crank angle</th>
<th>First mode</th>
<th>First 3 modes</th>
<th>First 10 modes</th>
<th>All 30 modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>TDC</td>
<td>0.454</td>
<td>0.566</td>
<td>0.792</td>
<td>1.000</td>
</tr>
<tr>
<td>30° aTDC</td>
<td>0.943</td>
<td>0.970</td>
<td>0.979</td>
<td>1.000</td>
</tr>
<tr>
<td>90° aTDC</td>
<td>0.917</td>
<td>0.938</td>
<td>0.962</td>
<td>1.000</td>
</tr>
<tr>
<td>BDC</td>
<td>0.692</td>
<td>0.718</td>
<td>0.892</td>
<td>1.000</td>
</tr>
<tr>
<td>270° aTDC</td>
<td>0.906</td>
<td>0.911</td>
<td>0.924</td>
<td>1.000</td>
</tr>
<tr>
<td>330° aTDC</td>
<td>0.858</td>
<td>0.870</td>
<td>0.943</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Table 5.3. Relevance index between reconstructed velocity fields (using 2-D phase-dependent POD modes) and the original velocity field of the third cycle for the nonswirling case on a cutting plane that contains the cylinder axis.

Quantitative comparisons of reconstructed and original velocity fields for the nonswirling case are provided in Table 5.3 (phase-dependent POD, 2-D case) and Table 5.4 (phase-invariant POD, 3-D case) for several phases (piston positions). There the relevance index is used as the quantitative measure of the degree to which
<table>
<thead>
<tr>
<th>Crank angle</th>
<th>First 3 mode</th>
<th>First 10 modes</th>
<th>First 30 modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>TDC</td>
<td>0.593</td>
<td>0.757</td>
<td>0.971</td>
</tr>
<tr>
<td>30° aTDC</td>
<td>0.754</td>
<td>0.873</td>
<td>0.925</td>
</tr>
<tr>
<td>60° aTDC</td>
<td>0.928</td>
<td>0.937</td>
<td>0.955</td>
</tr>
<tr>
<td>90° aTDC</td>
<td>0.911</td>
<td>0.929</td>
<td>0.943</td>
</tr>
<tr>
<td>120° aTDC</td>
<td>0.897</td>
<td>0.912</td>
<td>0.932</td>
</tr>
<tr>
<td>150° aTDC</td>
<td>0.766</td>
<td>0.801</td>
<td>0.920</td>
</tr>
<tr>
<td>BDC</td>
<td>0.679</td>
<td>0.776</td>
<td>0.874</td>
</tr>
<tr>
<td>210° aTDC</td>
<td>0.621</td>
<td>0.791</td>
<td>0.918</td>
</tr>
<tr>
<td>240° aTDC</td>
<td>0.718</td>
<td>0.812</td>
<td>0.949</td>
</tr>
<tr>
<td>270° aTDC</td>
<td>0.804</td>
<td>0.862</td>
<td>0.943</td>
</tr>
<tr>
<td>300° aTDC</td>
<td>0.816</td>
<td>0.899</td>
<td>0.944</td>
</tr>
<tr>
<td>330° aTDC</td>
<td>0.734</td>
<td>0.889</td>
<td>0.941</td>
</tr>
</tbody>
</table>

Table 5.4. Relevance index between reconstructed velocity fields (using 3-D phase-invariant POD modes) and the original velocity field of the third cycle for the nonswirling case.

two velocity fields are similar (index magnitude close to unity) or dissimilar (index magnitude close to zero). It can be seen that different numbers of POD modes are required to reproduce the original velocity field to the same level of fidelity for different phases. For example, for the phase-dependent 2-D POD case in Table 5.3, at TDC and BDC (relatively disorganized flow) more modes are required compared to mid-stroke on intake and exhaust. A single POD mode represents the flow quite well at 30° aTDC, where the flow is well organized and CCV is small.

The ability to reconstruct a time-dependent velocity field using a small number of POD modes is an important feature of POD analysis. In the case of 3-D phase-invariant POD, a small number of modes may be sufficient to capture the most important dynamic features of the time-dependent flow over multiple engine cycles. To the extent that the time-dependent in-cylinder flow can be recreated using a small number of POD modes, phase-invariant POD offers the potential for rapid analysis and prediction of in-cylinder flows that might eventually be used for real-time control.
5.3.4 Cycle-to-cycle variations

Two criteria were proposed earlier to quantify CCV. The first criterion is the slope of the eigenvalue-versus-mode-number plot from phase-dependent POD, or equivalently, the fraction of the kinetic energy contained in the first few POD modes. This has been discussed in the context of the results that have already been presented. For example, in Figure 5.31 it was shown that a higher fraction of the kinetic energy is captured in the first few POD modes at mid-stroke compared to TDC or BDC, and this suggests that CCV are smaller during mid-stroke.

The second criterion is the standard deviation of the phase-invariant POD coefficients. Each coefficient is obtained by projecting the corresponding POD mode onto the original velocity field. The time-varying coefficient then gives the contribution of that POD mode at each phase and for each cycle. Figure 5.51(a) shows the coefficients of the first three POD modes as functions of phase over 30 consecutive engine cycles, from 2-D phase-invariant POD for the nonswirling case for a cutting plane that contains the cylinder axis. The spread in the coefficient values over the 30 engine cycles is greatest near TDC and BDC, and is smaller at mid-stroke during intake and exhaust. The magnitude of the spread is quantified by computing the standard deviation in the coefficient value at each phase over the 30 engine cycles. This criterion confirms directly that CCV are higher near TDC and BDC when the flow is relatively disorganized, and are lower at mid-stroke on intake and exhaust when the flow is more organized.

5.3.5 Swirling flow

A systematic POD analysis also has been performed for the swirling case. Here a subset of the results is presented, with emphasis on the results that show how POD captures important differences between the nonswirling flow and the swirling flow.

Figure 5.52 shows the percentage of the total kinetic energy in the first mode, in the first three modes, and in the first five modes as functions of crank angle for 2-D phase-dependent POD for a cutting plane that contains the cylinder axis. The corresponding data for the nonswirling case are shown in Figure 5.31. The general trends are similar for the swirling and the nonswirling cases. One difference is that
Figure 5.51. Time-varying coefficients from 2-D phase-invariant POD for the nonswirling case for a cutting plane that contains the cylinder axis. (a) Coefficients of the first three POD modes versus phase for 30 engine cycles. (b) Standard deviation of the coefficients over 30 engine cycles versus phase.

for the swirling case, the flow is more organized at TDC by virtue of the large-scale coherent swirl. The swirling flow shows the least organization at BDC, while the nonswirling flow shows the least organization at TDC.

The fraction of kinetic energy versus mode number and number of snapshots from 2-D phase-dependent POD analysis for the swirling case on a cutting plane
Figure 5.52. Fractions of kinetic energy in the first few modes from 2-D phase-dependent POD analysis for the swirling case for a cutting plane that contains the cylinder axis.

Figure 5.53. Fraction of kinetic energy versus mode number and number of snapshots from 2-D phase-dependent POD analysis for the swirling case for a cutting plane that contains the cylinder axis. (a) 30° aTDC. (b) TDC.

that contains the cylinder axis is plotted in Figure 5.53 for two phases. The corresponding figure for the nonswirling case is Figure 5.32, and the behavior is essentially the same for the swirling and the nonswirling flows.

Figure 5.54 shows the first two modes at 30° aTDC for a cutting plane that contains the cylinder axis. The first mode is very similar in appearance to the first mode for the nonswirling case (Figure 5.33), while the second mode appears quite different. The relevance index between the first modes for the swirling case and the nonswirling case is 0.96, versus 0.43 for the second modes.
Figure 5.54. Phase-dependent 2-D POD modes for a cutting plane that contains the cylinder axis at 30° aTDC for the swirling case. (a) Mode 1. (b) Mode 2.

Figure 5.55. Fraction of kinetic energy versus mode number and number of snapshots from 3-D phase-dependent POD analysis for the swirling case. (a) 30° aTDC. (b) BDC.

Figure 5.55 shows the fraction of kinetic energy versus mode number from 3-D phase-dependent POD at two different phases for the swirling case. There are important differences with respect to the nonswirling case (Figure 5.38; note that the BDC phase is shown here while the TDC phase was shown there). Compared to the nonswirling case, the fraction of kinetic energy in the first few POD modes is higher for the swirling case. At BDC, the first mode for the swirling case represents approximately 50% of the kinetic energy, and fewer cycles are required to obtain converged POD modes compared to the nonswirling case. These are consequences of the more organized nature of the swirling flow.

Figures 5.56 and 5.57 show the 3-D phase-dependent POD modes at 30° aTDC on two cutting planes. These can be compared to Figures 5.39 and 5.40 for the nonswirling case. Here the large-scale swirl is evident in the cutting plane normal
Figure 5.56. Phase-dependent 3-D POD modes for a cutting plane that contains the cylinder axis at 30° aTDC for the swirling case. (a) Mode 1. (b) Mode 2.

Figure 5.57. Phase-dependent 3-D POD modes on cutting plane normal to the cylinder axis \((z = 10 \text{ mm})\) at 30° aTDC for the swirling case. (a) Mode 1. (b) Mode 2.

to the cylinder axis.

Two- and 3-D phase-invariant POD results for the swirling case are shown in Figures 5.58 - 5.62. Figure 5.58 shows the fractions of energy in the first 15 modes from 2-D and 3-D POD analysis. The corresponding information for the 2-D nonswirling case is in Figure 5.43. A larger fraction of the kinetic energy is captured in the first 3-D mode compared to the first 2-D mode, and 20 engine cycles are more than sufficient to give converged POD modes in both cases.

Phase-invariant POD modes are plotted in Figures 5.59 - 5.61. These are similar to the corresponding modes for the nonswirling case (Figures 5.44, 5.47 and 5.48), with the exception of the coherent large-scale swirl that is evident here in cutting
Figure 5.58. Fractions of kinetic energy in the first 15 modes from phase-invariant POD analysis for the swirling case, with variations in the number of engine cycles considered. (a) 2-D POD for a cutting plane that contains the cylinder axis. (b) 3-D POD.

Figure 5.59. Phase-invariant 2-D POD modes for a cutting plane that contains the cylinder axis for the swirling case. (a) Mode 1. (b) Mode 2.

Finally, the time-varying coefficients and their standard deviations from a 2-D time-invariant POD analysis are shown in Figure 5.62. This can be compared to Figure 5.51 for the nonswirling case. As was observed for the nonswirling case, the spread in the coefficients tends to be higher near TDC and BDC compared to mid-stroke. An important difference between the swirling and the nonswirling cases is that the magnitude of the standard deviation for the first mode is much lower at TDC for the swirling case compared to the nonswirling case. The swirling case
Figure 5.60. Phase-invariant 3-D POD modes on a cutting plane that contains the cylinder axis for the swirling case. (a) Mode 1. (b) Mode 2.

Figure 5.61. Phase-invariant 3-D POD modes on a cutting plane normal to the cylinder axis ($z = 10$ mm) for the swirling case. (a) Mode 1. (b) Mode 2.

remains more organized at TDC and exhibits less CCV by virtue of the large-scale coherent swirl.

5.4 Chapter summary

LES has been performed for an axisymmetric piston-cylinder assembly with and without swirl. While several earlier LES studies have been published for the
Figure 5.62. Time-varying coefficients from 2-D phase-invariant POD for the swirling case. (a) Coefficients of the first three POD modes versus phase for 30 engine cycles. (b) Standard deviation of the coefficients over 30 engine cycles versus phase.

configuration without swirl, these are the first LES results to be reported for the configuration with swirl. For the meshes that have been used in this study, more than 80% of the TKE is resolved, and the amount that is resolved increases as the mesh is refined. The sum of the resolved and modeled contributions to the TKE approaches grid independence for the meshes that have been used in this study. The sensitivity of LES to key numerical and physical model parameters has been
investigated. Results are especially sensitive to mesh and to the SFS turbulence model. Satisfactory results can be obtained using simple viscosity-based SFS turbulence models, although there is room for improvement. No single model gives uniformly best agreement between model and measurements at all measurement stations and crank angles. The strong sensitivity of computed mean and RMS velocity profiles to variations in the SFS turbulence model is an encouraging result. This suggests that better results might be obtained using more advanced models, such as dynamic models and/or non-dissipative models [128]. Such models will be explored in future work.

A systematic and comprehensive study of POD analysis for in-cylinder flow has been performed using datasets obtained from LES for a piston-cylinder assembly with and without swirl. Parametric studies have been performed to explore different possibilities in how the POD analysis is performed. These include comparisons of phase-dependent versus phase-invariant POD, two-dimensional versus three-dimensional POD, results obtained with versus without interpolation prior to POD analysis, results obtained with versus without velocity transformations for phase-invariant POD, and results obtained with versus without subtraction of the ensemble average prior to POD analysis. Flow reconstruction using a small number of POD modes has been demonstrated, POD-based approaches to quantify cycle-to-cycle flow variations have been proposed and tested, and the ability of POD to identify differences between flows with and without large-scale coherent swirl has been shown.

Key findings include the following.

- The degree of flow organization varies over the engine cycle, and this is captured in the POD analysis.

- For phases where a small number of POD modes is sufficient to capture a large fraction of the flow’s kinetic energy, the first POD mode strongly resembles the ensemble average. The first POD mode can differ significantly from the ensemble average for phases where a large number of POD modes is required to capture a significant fraction of the flow’s kinetic energy.

- The dilatation correction that has been used in phase-invariant POD has only a small influence on the results for low engine speeds; it may be more
important at higher engine speeds. Kinetic energy normalization is essential to obtain sensible results with phase-invariant POD.

• Cycle-to-cycle flow variations can be quantified using the standard deviation over engine cycles of the POD coefficient in phase-invariant POD analysis.

• POD analysis can discern the differences between in-cylinder flows that are or are not characterized by large-scale coherent motions.

The results reported here can provide guidance to other researchers who apply POD to analyze PIV and LES data for flows in real engines, and who seek to make quantitative comparisons between experimental measurement and simulation data using POD. To the extent that the time-dependent in-cylinder flow through the full engine cycle can be recreated using a small number of POD modes, phase-invariant POD offers the potential for rapid analysis and prediction of the in-cylinder flow structure that might eventually be used in a real-time control system, for example.
A motored two-valve, four-stroke-cycle engine

A systematic LES study and a comprehensive POD analysis for a simplified engine-like configuration without valve movement or compression were carried out in the last chapter. In this chapter, we extend the simulations and analysis to a real (but still relatively simple) two-valve engine. The geometric configuration and operation conditions are introduced first. This includes experimental measurements and numerical methods. The results are discussed next.

6.1 Geometric configuration and operating conditions

The geometric configuration for the TCC engine is illustrated in Figures 6.1 and 6.2, and closeups of the port-and-cylinder region can be seen in Figures 6.4 and 6.5. Key parameters are summarized in Table 6.1 [19, 82, 129]. This is a two-valve, four-stroke-cycle engine with a pancake-shaped combustion chamber and a central spark plug. It has a 92-mm bore, 86-mm stroke and a 234.95-mm connecting rod. The clearance at TDC is 9.6 mm, resulting in a 10:1 compression ratio. The piston moves at a crank shaft rotational speed of $\Omega_{CS} = 800$ r/min. There is a large plenum upstream of the intake valve and downstream of the exhaust valve. The intake/exhaust valve profiles are shown in Figure 6.3.
An industry-standard 1-D engine simulation tool, GT-Power [130], has been used to develop a detailed flow model for the engine. This model has been used to prescribe boundary conditions for the CFD, and LES results are compared with those from the 1-D model in Section 6.2.1.

![Computational domain for LES of the TCC engine](image)

### Table 6.1. Parameters for the TCC engine [82].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal compression ratio</td>
<td>10:1</td>
</tr>
<tr>
<td>Bore (mm)</td>
<td>92.00</td>
</tr>
<tr>
<td>Stroke (mm)</td>
<td>86.00</td>
</tr>
<tr>
<td>Connecting rod length (mm)</td>
<td>234.95</td>
</tr>
<tr>
<td>Engine speed (r/min)</td>
<td>800</td>
</tr>
</tbody>
</table>

**6.1.1 Experimental measurements**

PIV studies of the TCC engine have been performed by Reuss [28, 19] and Funk *et al.* [82]. Reuss [28, 19] studied the CCV of the large-scale velocity structures
Figure 6.2. Schematic of the experimental configuration for the TCC engine [28].

with high- and low-swirl in-cylinder flows. Funk et al. [82] studied the Reynolds-decomposed turbulence properties such as kinetic energy, length scales and dissipation rate with high- and low-swirl in-cylinder flows. The earlier studies focused on velocity fields on cutting planes parallel to the piston. For the present work, the PIV measurements are in the cutting plane that contains the cylinder axis and valves (Figure 6.5). The PIV measurements are performed by seeding the intake air with approximately 0.5 mm silicone oil droplets. A sheet of laser light is passed through the quartz ring, and a high-speed camera is used to image the 2-D velocity fields at specified phases (crank positions). Images are taken on 3,000 consecutive cycles. More details of the experiments can be found in [28, 19, 82].
6.1.2 Numerical method

The first RANS simulations of the TCC engine were carried out by Kuo and Reuss [129] using KIVA. The purpose was to evaluate the swirl- and tumble-generating capability of the engine’s intake system. Cases with shrouded valves were studied, with variations in intake-manifold absolute pressure and shroud orientation. It was found that the standard $k - \varepsilon$ turbulence model underpredicted the swirl and tumble ratios, and failed to capture the structure of the mean and RMS velocity fields.

Haworth [20] performed the first LES for the same configuration to study the CCV, using a relative coarse mesh. The computational power available at that time limited the mesh size and number of engine cycles that could be simulated. Nevertheless, the computed velocity magnitudes were comparable to the measured values, and the computations exhibited evident CCV.

6.1.2.1 Computational mesh

The computational domain includes the in-cylinder region, ports, runners, and plenums, as shown in Figure 6.1. The port-and-cylinder mesh topology for the TCC engine is shown in Figure 6.4. The unstructured hexahedral mesh is generated using es-ice [131]. Non-aligned interfaces are applied in the extrusion layer close
to the boundary layer. During the piston movement, in-cylinder cell layers are deleted and added in the axial direction without changing the mesh topology. The deletion layer occurs at a fixed number of layers above the highest bottom face, and is a complete cylinder cell layer. Similar treatments are also applied for the valve movements.

The mesh has approximately 700,000 cells including the plenums at BDC, and approximately 500,000 cells at TDC; most of the in-cylinder cells range between 1 mm and 1.2 mm. This relatively coarse mesh has been used to facilitate runs through large numbers of consecutive engine cycles. The mesh size in the vicinity of the spark-plug and valves (approximately 0.4 mm cells) is somewhat smaller in size to better capture those geometric features. A good prediction of velocity and turbulence in the vicinity of the spark-plug tip will be required for subsequent simulations of ignition and combustion. The computational time step is 0.1 CAD through most of the engine cycle, although somewhat smaller time steps are used
Figure 6.5. The cutting plane that contains the cylinder axis and the two valve stems.

during valve opening/closing events. As discussed in [20, 38, 39, 132], earlier in-cylinder LES studies showed that approximately 80% of the TKE is captured for meshes comparable to those that have been used here. A relatively large number (70) of consecutive cycles is run, and POD analysis is performed on these data to explore the convergence with number of cycles and other aspects of interest. In particular, we seek to establish the extent to which conclusions that were drawn from the simplified engine configuration in Chapter 5 and [75] carry over to a more realistic engine configuration.

6.1.2.2 Initial and boundary conditions and the estimation of mean quantities

The working fluid is air, which is treated as an ideal gas, and the initial temperature in the cylinder and plenums is 318.16 K. The initial pressure in the cylinder and outlet plenum is 101,500 Pa, and 95,000 Pa in the inlet plenum. No-slip boundary conditions with wall functions are applied at solid walls, and the wall temperature is fixed at 318.16 K during the computation. Time-varying pressure and temperature
boundary condition are applied at the plenum inlets/outlets (locations 2 and 5 on Figure 6.1). These boundary conditions are obtained from the 1-D simulation results using GT-Power, without any CCV.

The computation begins at TDC of the intake stroke. The simulations are run through 70 consecutive engine cycles, and the first ten cycles are discarded to avoid contamination by initial conditions. Flow fields are saved at every CAD. Mean quantities then are estimated by ensemble-averaging the resolved-scale computed quantities over 60 engine cycles. Sensitivity of results to the number of cycles is discussed in the Results section below; 60 cycles is sufficient to obtain converged mean and RMS velocity fields, and lower-order POD modes. The 3-D flow field data size is 35 GB per engine cycle.

6.1.2.3 Postprocessing

Global in-cylinder quantities such as in-cylinder mass, mean pressure and temperature are calculated as a function of crank angle, and these are compared with 1-D GT-Power results. Dependent variables such as pressure and temperature at selected monitoring points are also compared with 1-D GT-Power results; the locations of monitoring points are shown in Figure 6.1.

The raw data obtained directly from the CFD simulations are instantaneous cell-centered quantities (resolved fields) on the unstructured mesh. Interpolation is required prior to performing 2-D averaging and POD analysis for cutting planes that do not correspond to layers of finite-volume cells; interpolation is also necessary for 3-D POD analysis to reduce the computational cost [75]. The influence of data interpolation on the computed POD modes has been explored on a subset of the engine cycles. Our results show that the POD modes are independent of the interpolation, as long as the mesh is sufficiently fine to capture the large-scale flow structures that contain most of the flow’s kinetic energy. In this study, for the 2-D cutting plane including the valves and axis (the cutting plane that is of most interest here, Figure 6.5), a uniform mesh of 4,500 grid points is used. For 3-D POD analysis, a polar-cylindrical mesh of 36,000 grid points is used. It has been confirmed that both meshes are fine enough to give converged POD results.
6.2 Results

The results are organized as follows. In the first subsection, the global in-cylinder quantities and monitoring-point histories are presented. Ensemble-averaged quantities (mean and RMS velocities) are discussed in Section 6.2.2. POD analysis is presented in Section 6.2.3; this is the principal emphasis in this chapter. Special attention is paid to the velocity magnitude of the spark-plug gap in Section 6.2.4, which will be important for subsequent simulations that include ignition and flame propagation.

6.2.1 Global in-cylinder quantities and monitoring points

We begin by examining the in-cylinder global quantities for 60 consecutive simulated cycles. In Figures 6.6 and 6.7, the in-cylinder pressure and mass for 60 cycles are plotted as functions of crank angle. The GT-Power result for in-cylinder pressure (which corresponds to an ensemble-averaged value) is shown in Figure 6.6. The global quantities vary from one engine cycle to another, and this is one indication of CCV. CCV are not evident in Figures 6.6 and 6.7, but can be seen in the zoomed-in views in Figures 6.8 and 6.9. The CCV can be quantified by calculating the RMS, as shown in Figures 6.10 and 6.11. This demonstrates that
the CCV of the in-cylinder global quantities which are not accessible from RANS can be captured by using LES. Although the CCV magnitude is relatively small for this motored engine configuration, we expect to see greater CCV in the case of combustion in the same engine, which will be the next step of our study.

We further normalized the RMS of in-cylinder pressure and in-cylinder mass by their mean values at the same crank angles, as shown in Figures 6.12 and 6.13. For the in-cylinder pressure, the maximum absolute CCV occurs at 360° aTDC.
(TDC compression); the maximum relative CCV is approximately 1% of the mean value, and occurs between $360^\circ$ aTDC and $480^\circ$ aTDC, which corresponds to the expansion stroke; the minimum relative CCV is approximately 0.1% of the mean value, and occurs during the exhaust stroke. For the in-cylinder mass, the maximum CCV occurs when the valves are open ($\sim 0.5\%$ of the mean value), and the minimum CCV occurs when the valves are closed ($\sim 0.1\%$ of the mean value).

In addition to global quantities, CCV are also evident at the monitoring locations. The pressure histories at five locations over five cycles are compared with GT-Power results at the same locations in Figure 6.14. The monitoring locations are shown in Figure 6.1. It can be seen that the LES results generally match the GT-Power results, and CCV are evident in the LES. Similar results are obtained for temperature (not shown). Compared with the GT-Power results, the LES at the intake/exhaust plenums (Figures 6.14(a) and 6.14(b)) and intake port (Figure 6.14(c)) shows similar frequencies and oscillation amplitudes. At the exhaust port (Figure 6.14(d)), the LES simulation shows smaller high-frequency oscillation magnitude.

The trapped mass, peak in-cylinder pressure and temperature for 70 cycles are shown in Figure 6.15. It can be seen in Figure 6.15(a) that the trapped mass quickly converges to a cyclic steady state after a relatively low value in the first
Figure 6.14. Pressure histories for five cycles at five monitoring points (Figure 6.1). (a) Intake plenum inlet. (b) Exhaust plenum outlet. (c) Intake port. (d) Exhaust port. (e) In-cylinder.
Figure 6.15. (a) Trapped mass versus cycle number. (b) Peak in-cylinder pressure versus cycle number. (c) Peak in-cylinder temperature versus cycle number.

cycle. The trapped mass then fluctuates with a magnitude of approximately 1 mg, which corresponds to 0.2% of the mean value, with a pattern that repeats over a period of three to four cycles.

For the in-cylinder pressure and temperature (Figures 6.15(b) and 6.15(c)), there is a drop after about 26 cycles, after which they settle into a cyclic steady state. The magnitudes of the drop are approximately 1% of the mean values for both in-cylinder pressure and temperature. The reason for this drop has been
traced to the initial- and boundary-condition specification. The time-averaged pressure and temperature that are imposed at the intake plenum entrance are slightly lower than the initial conditions (pressure 95,000 Pa, and temperature 318.45 K) in the cylinder and intake plenum. The intake plenum volume is approximately 26 times the engine displacement. So after 26 cycles, all of the initial plenum gas is pumped out, and the in-cylinder pressure and temperature drop accordingly. These small thermodynamic variations do not affect the mean and RMS velocities or POD modes, as will be shown in Sections 6.2.2 and 6.2.3, respectively. However, this serves to underscore the importance of initial and boundary condition specification in multiple-cycle LES: a large number of cycles may be needed to reach a cyclic steady in-cylinder thermodynamic state.

![Figure 6.16](image)

**Figure 6.16.** Instantaneous in-cylinder mass versus instantaneous intake-port pressure. (a) 118° aTDC. (b) 180° aTDC.

Figure 6.15 also suggests that acoustic dynamics in the intake and/or exhaust system may govern the observed CCV in global in-cylinder quantities. This is explored further in Figures 6.16 and 6.17. Scatter plots of in-cylinder mass versus intake-port pressure (location 3 in Figure 6.1) are plotted for two phases in Figure 6.16.

The phase 118° aTDC corresponds to the maximum intake valve lift, while the phase 180° aTDC corresponds to BDC. There is a strong correlation between instantaneous in-cylinder mass and instantaneous intake-port pressure, with higher intake-port pressure corresponding to higher in-cylinder mass. Similar correlations
Figure 6.17. Trapped mass versus mean intake port pressure while the intake valve is open.

are found for other phases when the intake valve is open. A scatter plot of trapped mass (in-cylinder mass at compression TDC when intake/exhaust valves are closed) versus the average intake-port pressure over the time when the intake valve is open is shown in Figure 6.17. It is clear that higher average intake-port pressure corresponds to higher trapped mass. These results confirm that the acoustic dynamics of the intake system control the observed CCV in trapped mass.

### 6.2.2 Ensemble-averaged velocity fields

In this study, we focus on two phases where initial PIV data have been taken: 100° aTDC (close to maximum intake-valve lift) and 300° aTDC (during compression). Figure 6.18 shows the ensemble-averaged velocity vectors and RMS of velocity magnitude on the plane that contains the cylinder axis and valves (Figure 6.5) for LES and PIV. The PIV measurements are on the same cutting plane, but have a smaller field of view (V. Sick, D. L. Reuss and P. Abraham, personal communication, December, 2011). For LES RMS velocity fields, only the contributions of the resolved velocity fluctuations are shown. In this and subsequent vector figures for LES, a subset of the vectors (here one out of every four) is plotted for clarity.

At 100° aTDC (Figures 6.18(a) and 6.18(b)), which corresponds to the intake stroke, there is a strong intake jet from the inlet valve. Two vortex structures are generated close the center of the domain because of the strong intake jet. There
Figure 6.18. Ensemble-averaged 2-D velocity vectors and contours of RMS velocity magnitude on a cutting plane that contains the cylinder axis from LES and PIV. (a) Mean 2-D velocity vectors at 100° aTDC from LES. (b) Mean 2-D velocity vectors at 100° aTDC from PIV. (c) RMS velocity magnitude at 100° aTDC from LES. (d) RMS velocity magnitude at 100° aTDC from PIV. (e) Mean 2-D velocity vectors at 300° aTDC from LES. (f) Mean 2-D velocity vectors at 300° aTDC from PIV. (g) RMS velocity magnitude at 300° aTDC from LES. (h) RMS velocity magnitude at 300° aTDC from PIV. (PIV data courtesy of V. Sick, D. L. Reuss and P. Abraham, personal communication, December, 2011)
is another vortex structure close to the piston and the cylinder wall under the intake valve, which is generated by the inlet jet along the cylinder wall. The RMS velocity magnitude (Figures 6.18(c) and 6.18(d)) is high in the intake jet.

At 300° aTDC (Figures 6.18(e) and 6.18(f)), which corresponds to the compression stroke, the piston is moving upward at a relatively high speed, so the lower part of the domain is dominated by the piston motion. There is a vortex structure close to the center of the domain. Tumble introduced by the intake stroke is compressed during the compression, and breaks up later near TDC. The maximum RMS velocity is close to the vortex center, and the magnitude is smaller than that at 100° aTDC.

By comparing Figure 6.18(a) with Figure 6.18(b), we can see that at 100° aTDC, although the intake jet and vortex structures are similar in both LES and PIV, there are still discrepancies for the mean flow structures, especially close to the end of intake jet penetration, below the intake-jet vortex. The relevance index between the LES and PIV mean velocity fields is 0.569 (based on the smaller PIV window size). The LES and PIV RMS velocity are comparable in magnitude, but quite different in spatial structure. Here the LES SFS velocity fluctuations have not been considered.

At 300° aTDC (Figures 6.18(e) and 6.18(f)), the LES and PIV mean velocity fields show better agreement than at 100° aTDC; the relevance index is 0.955. For both LES and PIV, the flow structures at this crank angle are more uniform with smaller mean velocity gradients, and there are fewer difficulties in both LES and PIV. To better capture the flow structures at 100° aTDC, further mesh refinement close to the intake valve might be helpful for the LES; for PIV, it might be necessary to carefully account for the spatial resolution and dynamic range of velocities that can be captured. It is emphasized that these are preliminarily PIV measurements; postprocessing and analysis are ongoing. Future work will focus on more comprehensive comparisons between LES and PIV.

We next explore the influence of the choice of the subset of cycles (the ‘averaging window’) that is used on the LES mean and RMS velocities. Results for seven averaging windows are compared in Table 6.2. There ‘A’ corresponds to the 60-cycle averages that have been shown so far. The mean and RMS velocities vary little for 40, 50 or 60 cycles, while deviations begin to appear when only 30 cycles
Table 6.2. Relevance indices between mean and RMS velocities with different averaging windows. **A**: Average over the last 60 cycles (11th – 70th cycle), **B**: Average over the last 50 cycles (21st – 70th cycle), **C**: Average over the last 40 cycles (31st – 70th cycle), **D**: Average over the last 30 cycles (41st – 70th cycle), **E**: Average over the first 50 cycles (11th – 60th cycle), **F**: Average over the first 40 cycles (11th – 50th cycle), **G**: Average over the first 30 cycles (11th – 40th cycle).

are considered. The results suggest that 60 consecutive cycles of LES data (after discarding the first 10 cycles, 11th – 70th cycle) is sufficient to give converged results for the mean and RMS velocities for 100° aTDC and 300° aTDC, while 30 cycles is too few.

The influence of the 1% drop in peak in-cylinder pressure and temperature discussed earlier is also investigated by comparing the mean and RMS velocities obtained from the first 50 cycles (11th – 60th cycle), the first 40 cycles (11th – 50th cycle) and the first 30 cycles (11th – 40th cycle) with those from the last 50 cycles (21st – 70th cycle), the last 40 cycles (31st – 70th cycle) and the last 30 cycles (41st – 70th cycle), respectively. The relevance indices in Table 6.2 suggest that this small pressure drop has negligible influence on the mean and RMS velocity fields, as long as a sufficient large number of cycles is considered.

### 6.2.3 POD analysis

The POD analysis is organized as follows. In the first two subsections, results from phase-dependent POD and phase-invariant POD are presented, respectively. These include parametric studies with variations in how the POD analysis is performed (e.g., 2-D versus 3-D POD, subtracting versus not subtracting the ensemble average prior to performing the POD, use of all phases versus a subset of phases, etc.).
Flow reconstruction from POD modes is discussed in the final subsection.

### 6.2.3.1 Phase-dependent POD

![Normalized Eigenvalues vs Crank Angle](image.png)

**Figure 6.19.** Fraction of kinetic energy in the first few modes from 2-D phase-dependent POD analysis for a cutting plane that contains the cylinder axis.

Here 2-D phase-dependent POD has been performed for 720 phases (one per crank angle) on a cutting plane that contains the cylinder axis using 60 cycles of LES data. As discussed above, a series of POD modes and the corresponding eigenvalues are obtained from the POD analysis. The eigenvalues are normalized such that each normalized eigenvalue gives the fraction of kinetic energy in the corresponding POD mode. The modes are ordered by decreasing eigenvalue magnitude, so that the first mode contains the most kinetic energy. Figure 6.19 shows the first three normalized eigenvalues as a function of crank angle. The fraction of the energy in the first mode varies from a low of approximately 0.28 at TDC to a high of approximately 0.98 at 510° aTDC when the exhaust valve opens.

The high concentration of kinetic energy in the first mode indicates a highly organized flow with small CCV. In general, well-organized flow is evident at mid-stroke, especially at valve-opening events, when a strong intake or exhaust jet dominates the flow. In contrast, the percentage of the kinetic energy contained in the first mode is lower near TDC. This implies that the input flow fields for those phases vary considerably from cycle to cycle, and the flow is relatively disorganized. This might due to the fact that the large-scale structures introduced by the intake
or exhaust jets are dissipated into smaller structures, which make the flow more stochastic and disorganized. Similar conclusions were drawn in [72, 73], where the tumble breakdown process in a simplified engine was studied using a similar method.

<table>
<thead>
<tr>
<th>Mode 1 at 100° aTDC</th>
<th>Mode 2 at 100° aTDC</th>
<th>Mode 3 at 100° aTDC</th>
<th>Mode 4 at 100° aTDC</th>
<th>Mode 5 at 100° aTDC</th>
<th>Mode 1 at 300° aTDC</th>
<th>Mode 2 at 300° aTDC</th>
<th>Mode 3 at 300° aTDC</th>
<th>Mode 4 at 300° aTDC</th>
<th>Mode 5 at 300° aTDC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.996</td>
<td>0.978</td>
<td>0.451</td>
<td>0.894</td>
<td>0.236</td>
<td>0.999</td>
<td>0.994</td>
<td>0.930</td>
<td>0.928</td>
<td>0.967</td>
</tr>
<tr>
<td>0.975</td>
<td>0.648</td>
<td>0.055</td>
<td>0.086</td>
<td>0.538</td>
<td>0.997</td>
<td>0.955</td>
<td>0.871</td>
<td>0.689</td>
<td>0.862</td>
</tr>
<tr>
<td>0.955</td>
<td>0.958</td>
<td>0.388</td>
<td>0.351</td>
<td>0.142</td>
<td>0.999</td>
<td>0.964</td>
<td>0.843</td>
<td>0.866</td>
<td>0.850</td>
</tr>
<tr>
<td>0.973</td>
<td>0.597</td>
<td>0.191</td>
<td>0.663</td>
<td>0.652</td>
<td>0.993</td>
<td>0.857</td>
<td>0.859</td>
<td>0.663</td>
<td>0.568</td>
</tr>
</tbody>
</table>

Table 6.3. Relevance indices between POD modes obtained using different numbers of input snapshots. **A**: Input the last 60 cycles (11th – 70th cycle), **B**: Input the last 50 cycles (21st – 70th cycle), **C**: Input the last 40 cycles (31st – 70th cycle), **D**: Input the first 50 cycles (11th – 60th cycle), **E**: Input the first 40 cycles (11th – 50th cycle).
Figure 6.21. Phase-dependent 2-D POD modes and normalized ensemble-average velocity vectors for a cutting plane that contains the cylinder axis at 100° aTDC. (a) Mode 1. (b) Mode 2. (c) Mode 3. (d) Normalized ensemble average.

The results at 100° aTDC and 300° aTDC are next examined more closely. More than 70% of the flow kinetic energy is contained in a small number of modes for both phases (Figure 6.20). POD results obtained using different numbers of input snapshots (engine cycles) are shown to study convergence. For the kinetic energy content, it can be seen that at 100° aTDC and 300°TDC, 60 input snapshots give converged statistics for the energy content of at least the first two POD modes. However, for higher-order modes, more input snapshots may be required. POD modes obtained using different numbers of input snapshots are compared by calculating the relevance indices between them (Table 6.3). We first consider the modes at 300° aTDC. From the relevance indices in Table 6.3, it can be seen that fewer cycles are required to converge lower-order modes compared to higher-order modes. For example, based on a relevance index criterion of 0.90 (say), 50 cycles
are required to converge the first five modes (A VS B) while 40 cycles are sufficient for Mode 1 and 2 (A VS C).

The effect of the in-cylinder pressure/temperature drop after the first 26 cycles on the POD mode structures is investigated by comparing the POD modes obtained from the first 50 cycles versus the last 50 cycles (B VS D), and the first 40 cycles versus the last 40 cycles (C VS E). As shown in Table 6.3, the in-cylinder pressure/temperature drop has a relatively small influence on the lowest-order POD modes (Mode 1 and Mode 2 for B VS D and C VS E). The relatively low value of the relevance index for the higher-order POD modes (Mode 4 and Mode 5 for B VS D and C VS E) might because the number of input snapshots is not sufficient for convergence, rather than because of the in-cylinder pressure/temperature drop. Similar conclusions can be drawn for 100° aTDC.

![Figure 6.22](image)

**Figure 6.22.** Phase-dependent 2-D POD modes and normalized ensemble-average velocity vectors for a cutting plane that contains the cylinder axis at 300° aTDC. (a) Mode 1. (b) Mode 2. (c) Mode 3. (d) Normalized ensemble average.

Figure 6.21 shows the first three POD modes and normalized (by its kinetic energy) ensemble-averaged velocity vectors at 100° aTDC. As shown in Figure 6.21, the first mode corresponds to the most energetic structures, and is similar in appearance to an intake jet. The first mode also strongly resembles the normalized ensemble-averaged velocity field; the relevance index between the two is 0.999. It is important to note that in principle, the first mode need not correspond to the ensemble average [75]. The second and third modes represent the structures of
the most energetic velocity fluctuations with respect to the lower modes. The corresponding POD modes and normalized ensemble-averaged velocity vectors at 300° TDC are shown in Figure 6.22.

![Figure 6.22](image)

Figure 6.22. The most energetic velocity fluctuations with respect to the lower modes.

![Figure 6.23](image)

Figure 6.23. Phase-dependent 2-D POD modes for the fluctuating velocity field on a cutting plane that contains the cylinder axis. (a) Mode 1, 100° aTDC. (b) Mode 2, 100° aTDC. (c) Mode 1, 300° aTDC. (d) Mode 2, 300° aTDC.

One can subtract the ensemble-averaged mean velocity from each snapshot prior to performing the POD analysis, as was done in [75]. Figure 6.23 shows the first two modes for the fluctuating velocity field for the phases 100° aTDC and 300° aTDC. By comparing the modes for the fluctuating velocity field (Figure 6.23) with the modes for the original velocity field (Figure 6.21) at 100° aTDC, it can be seen that the first mode for the velocity fluctuations (Figure 6.23(a)) is similar to the second mode for the original flow (Figure 6.21(b)); the relevance index between them is 0.994. The second mode for the velocity fluctuations (Figure 6.23(b)) is similar to the third mode for the original flow (Figure 6.21(c)); the corresponding relevance index is 0.978. In general, it is of interest to compare the \( n \)-th \( (n = 1, 2, ..., 59) \) mode for the velocity fluctuations with the \( (n+1) \)-th \( (n = 1, 2, ..., 59) \) mode for the original flow, to determine the extent to which this pattern holds. The relevance
Table 6.4. Relevance index between the \( n \)-th mode for velocity fluctuations and the \((n + 1)\)-th mode for the original flow.

<table>
<thead>
<tr>
<th>Fluctuations</th>
<th>Original</th>
<th>Relevance index</th>
</tr>
</thead>
<tbody>
<tr>
<td>100° aTDC</td>
<td>7(^{th})</td>
<td>9(^{th})</td>
</tr>
<tr>
<td>100° aTDC</td>
<td>8(^{th})</td>
<td>8(^{th})</td>
</tr>
<tr>
<td>100° aTDC</td>
<td>13(^{th})</td>
<td>15(^{th})</td>
</tr>
<tr>
<td>100° aTDC</td>
<td>14(^{th})</td>
<td>14(^{th})</td>
</tr>
<tr>
<td>300° aTDC</td>
<td>8(^{th})</td>
<td>8(^{th})</td>
</tr>
<tr>
<td>300° aTDC</td>
<td>9(^{th})</td>
<td>9(^{th})</td>
</tr>
<tr>
<td>300° aTDC</td>
<td>10(^{th})</td>
<td>10(^{th})</td>
</tr>
<tr>
<td>300° aTDC</td>
<td>11(^{th})</td>
<td>11(^{th})</td>
</tr>
</tbody>
</table>

Table 6.5. Relevance indices between modes for velocity fluctuations and the original flow.

indices for the first 20 pairs \( (n = 1, 2, \ldots, 20) \) are shown in Table 6.4. At 100° aTDC, with the exception of \( n = 7, 8, 13 \) and 14, the \( n \)-th mode for the velocity fluctuations strongly resembles the \((n + 1)\)-th mode for the original flow with (relevance index greater than 0.9). The four exceptions also provide insight, however. For example, we find that the 7\(^{th}\) mode for the velocity fluctuations resembles the 9\(^{th}\) mode for the original flow (relevance index 0.789, Table 6.5), and the 8\(^{th}\) mode for the velocity fluctuations resembles the 8\(^{th}\) mode for the original flow (relevance index 0.841). Similar matches are found for \( n = 13, 14 \) (Table 6.5). The reason for this behavior is as follows. The POD modes are ordered by decreasing kinetic energy
magnitude, and for higher-order modes, the difference in kinetic energy between adjacent modes is small. In some cases, modes can switch order when the analysis is done based on the original velocity field versus the fluctuating velocity field. Similar behavior is seen at 300° aTDC (Table 6.4 and 6.5).

Three-dimensional phase-dependent POD also has been performed for all phases; the energy contents for 100° aTDC and 300° aTDC are shown in Figure 6.24. The first two 3-D POD modes for the two phases are shown in Figure 6.25. Compared to the 2-D POD modes, 3-D POD modes give more information. The general behavior is similar to what has been discussed up to this point for 2-D phase-dependent POD.

6.2.3.2 Phase-invariant POD

Phase-invariant POD uses snapshots from multiple phases as input. In this study, there are as many as 60 cycles of LES data at intervals of one crank-angle degree (720 per cycle) used as input snapshots in the phase-invariant POD analysis.

Figure 6.26 shows normalized eigenvalues for the first 10 modes from the 2-D phase-invariant POD on a cutting plane that contains the cylinder axis with variations in the number of cycles and number of phases per cycle. In Figure 6.26(a), up to 60 cycles of input snapshots are included and well-converged POD results
Figure 6.25. Velocity vectors and contours (axial velocity component $w$) of phase-dependent 3-D POD modes. (a) Mode 1, 100° aTDC. (b) Mode 2, 100° aTDC. (c) Mode 1, 300° aTDC. (d) Mode 2, 300° aTDC.

are obtained with 30 cycles. That is, the POD modes obtained using 30 cycles are almost identical to those obtained using 60 cycles. The relevance indices between 30- and 60-cycle results for the first three POD modes are 0.999, 0.991 and 0.987, respectively. For this phase-invariant 2-D POD, approximately 25% of the kinetic energy resides in the first mode, and the first five modes account for more than 60% of the kinetic energy. There is essentially no change in the computed eigenvalues of the lowest-order modes when as few as 24 phases per cycle (one sample every 30 crank angles) are included in the analysis, as shown in Figure 6.26(b). The same trend can be found for the mode structures. For example, the relevance indices for the first three POD modes obtained using 24 phases per cycle versus 720 phases per cycle are 0.995, 0.981 and 0.957, respectively. This is a somewhat surprising finding.
Figure 6.26. Fractions of kinetic energy in the first 10 modes from 2-D phase-invariant POD analysis for a cutting plane that contains the cylinder axis. (a) Data from all 720 phases used, with variations in the number of cycles. (b) Data from all 60 cycles used, with variations in the number of phases.

Figure 6.27. Phase-invariant 2-D POD modes for a cutting plane that contains the cylinder axis. (a) Mode 1. (b) Mode 2. (c) Mode 3.
Figure 6.28. Time-varying coefficients from 2-D phase-invariant POD for a cutting plane that contains the cylinder axis. (a) Coefficients of the first three POD modes versus phase for 60 engine cycles. (b) RMS of the coefficients over 60 engine cycles versus phase.

for a realistic engine configuration with moving piston and valves undergoing full four-stroke motored cycles. In all cases, the phases are equally spaced in CAD. This suggests that using all 720 phases corresponds to significant oversampling for this configuration.

The first three modes corresponding to Figure 6.26(a) (with all 43,200 snapshots used) are shown in Figure 6.27. As discussed before, the goal of phase-invariant POD is to construct a series of common basis functions that can represent all of
the phases. There is no clear relationship between the mode structures and the flow at any particular instant in the engine cycle, although some hints of the valve flows can be seen in Figure 6.27.

Figure 6.28(a) shows the coefficients of the first three POD modes as functions of phase over 60 consecutive engine cycles, from 2-D phase-invariant POD for a cutting plane that contains the cylinder axis. The spread in the coefficient values over the 60 engine cycles is greater near TDC, and is smaller at mid-stroke, especially as the intake and exhaust valves open. The magnitude of the spread is quantified by computing the standard deviation in the coefficient values at each phase over the 60 engine cycles in Figure 6.28(b). This criterion confirms directly that CCV are higher near TDC when the flow is relatively disorganized, and are lower at mid-stroke when the flow is more organized. This is consistent with the previous phase-dependent POD results in Figure 6.19. Phase-invariant 3-D POD has also been performed, and similar results have been obtained (not shown).

![Figure 6.28](image)

Figure 6.28. Coefficients of the first three POD modes as functions of phase over 60 consecutive engine cycles, from 2-D phase-invariant POD for a cutting plane that contains the cylinder axis.

Instead of applying phase-invariant POD to a full engine cycle, one can also
Figure 6.30. Time-varying coefficients from 2-D phase-invariant POD for a cutting plane that contains the cylinder axis for intake and compression strokes only. (a) Coefficients of the first three POD modes versus phase for 60 engine cycles. (b) RMS of the coefficients over 60 engine cycles versus phase.

use part of an engine cycle as input snapshots. Fogleman [72, 73] applied phase-invariant POD on the intake and compression strokes of a simplified engine. Moreau et al. [76] applied a similar method to study the tumble breakdown process during the compression stroke in a square cylinder. Here the phase-invariant POD has been performed for the intake and compression strokes of the TCC engine; 60 cycles of LES data at intervals of one crank-angle degree (360 per cycle) are used as input snapshots. The first three POD modes are shown in Figure 6.29,
and the coefficients of the first three POD modes as functions of phase over 60 consecutive engine cycles are shown in Figure 6.30. Figures 6.29 and 6.30 (modes based on intake and compression stokes only) can be compared with Figures 6.27 and 6.28 (modes based on full 720-degree cycle). The structure of the first mode in Figure 6.29 appears to correspond to a large-scale tumble-like motion, while the second mode resembles an intake jet.

The first three POD coefficients are shown in Figure 6.30(a). It can be seen that from 20° aTDC to 120° aTDC, the coefficients of the second POD mode are greater than the other two. This suggests that the second POD mode dominates the intake stroke. The coefficients of the first POD mode begin to decrease after 120° aTDC, while the other two POD coefficients begin to increase. This suggests that energy is transferred from the intake-jet structures to the other POD structures. Similarly, from 160° aTDC to 300° aTDC, the coefficients of the first mode are greater than those of the other two, which means the tumble structures are dominant during these phases. The tumble vortex is compressed until it breaks down at approximately 300° aTDC, and the POD coefficients of the first mode begin to decrease after this point. This suggests that the tumble vortex breaks down, and energy is transferred into more complex smaller-scale structures (higher-order modes).

From the above analysis of the POD modes and corresponding coefficients, one can infer how energy is transferred from one structure to another. In this way, phase-invariant POD can be used as a tool to analyze the dynamic behavior of in-cylinder flows. The interpretation seems to be more clear when the analysis is based on the intake and compression strokes only, as the dynamics of the expansion and exhaust are quite different.

As discussed earlier, the spread of the coefficients in Figure 6.30(a) represents the CCV, and one can quantify CCV by calculating the RMS of the coefficients as shown in Figure 6.30(b). From the RMS of the POD coefficients, one can infer which structures contribute most to the CCV at different phases. As shown in Figure 6.30(b), the third mode appears to contribute more to the CCV than the intake jet and tumble structures.
6.2.3.3 Flow reconstruction from POD modes

The original velocity field can be reconstructed using a linear combination of POD modes and the corresponding coefficients. The reconstruction is exact if all POD modes are used, and is an approximation if a subset of modes is used. It is of interest to explore how many POD modes are required to reconstruct the original velocity field to a specified precision. Here two examples are shown.

![Figure 6.31](image)

**Figure 6.31.** Reconstruction of the instantaneous velocity field (velocity component $w$) at $100^\circ$ aTDC of the eleventh cycle using different numbers of 2-D phase-dependent POD modes on a cutting plane that contains the cylinder axis. (a) First 10 modes. (b) First 30 modes. (c) All modes. (d) Original flow field.

The first example is 2-D phase-dependent POD at $100^\circ$ aTDC of the eleventh cycle (Figure 6.31). There 2-D velocity vectors and contours of the instantaneous axial velocity component ($w$) are shown for the original flow and for velocity fields reconstructed at the same instant using different numbers of POD modes. It can
<table>
<thead>
<tr>
<th>Crank angle</th>
<th>First 3 modes</th>
<th>First 10 modes</th>
<th>First 30 modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>60° aTDC</td>
<td>0.821</td>
<td>0.916</td>
<td>0.935</td>
</tr>
<tr>
<td>120° aTDC</td>
<td>0.777</td>
<td>0.887</td>
<td>0.903</td>
</tr>
<tr>
<td>180° aTDC</td>
<td>0.809</td>
<td>0.902</td>
<td>0.921</td>
</tr>
<tr>
<td>240° aTDC</td>
<td>0.852</td>
<td>0.917</td>
<td>0.942</td>
</tr>
<tr>
<td>300° aTDC</td>
<td>0.824</td>
<td>0.912</td>
<td>0.933</td>
</tr>
<tr>
<td>360° aTDC</td>
<td>0.534</td>
<td>0.782</td>
<td>0.818</td>
</tr>
<tr>
<td>420° aTDC</td>
<td>0.817</td>
<td>0.891</td>
<td>0.925</td>
</tr>
<tr>
<td>480° aTDC</td>
<td>0.781</td>
<td>0.889</td>
<td>0.902</td>
</tr>
<tr>
<td>540° aTDC</td>
<td>0.870</td>
<td>0.960</td>
<td>0.970</td>
</tr>
<tr>
<td>600° aTDC</td>
<td>0.849</td>
<td>0.919</td>
<td>0.937</td>
</tr>
<tr>
<td>660° aTDC</td>
<td>0.854</td>
<td>0.920</td>
<td>0.944</td>
</tr>
<tr>
<td>720° aTDC</td>
<td>0.573</td>
<td>0.804</td>
<td>0.830</td>
</tr>
</tbody>
</table>

Table 6.6. Relevance index between reconstructed velocity fields (using 3-D phase-invariant POD modes) and the original velocity field of the eleventh cycle.

be seen that the fidelity improves as more modes are used. The relevance indices between the original flow and the recreated flow using 60 modes, 30 modes and 10 modes are 1.000, 0.966 and 0.868, respectively.

The second case is 3-D phase-invariant POD (over full four-stroke cycles) of the eleventh cycle. Table 6.6 shows the relevance index between the original flow and the reconstructed flow using different numbers of POD modes at several phases. It can be seen that the fidelity improves as more POD modes are included. Also, different numbers of POD modes are required to reproduce the original velocity field to the same level of fidelity for different phases. More modes are required at TDC (relatively disorganized flow) compared to mid-stroke on intake and exhaust (relatively organized flow).

The ability to reconstruct a time-dependent velocity field using a small number of POD modes is an important feature of POD analysis. In the case of 3-D phase-invariant POD, a small number of modes may be sufficient to capture the most important dynamic features of the time-dependent flow over multiple engine cycles. To the extent that the time-dependent in-cylinder flow can be recreated using a small number of POD modes, phase-invariant POD offers the potential for rapid analysis and prediction of in-cylinder flows that might eventually be used for real-time control.
6.2.4 Velocity at spark-plug gap

Finally, the velocity magnitude at the spark-plug gap is studied (Figure 6.32). There the mean and RMS velocities are plotted as functions of crank-angle degree. The velocity magnitude at the spark-plug gap is very important for ignition (at approximately 20 - 30° before TDC) and subsequent flame propagation. It is clear from Figure 6.32 that the velocity magnitude reaches a maximum at 30° aTDC and 520° aTDC, corresponding to intake- and exhaust-valve opening events. The RMS velocity has a similar trend. At 20° before TDC, the mean velocity magnitude is approximately 2 m/s and the RMS velocity is approximately 1 m/s. The mean piston speed for this engine speed is 2.29 m/s.

![Figure 6.32. Ensemble-averaged velocity magnitude and RMS velocity at the spark-plug gap.](image)

6.3 Chapter summary

LES is increasingly being used as a tool for advanced IC-engine development. It is expected to be more accurate compared to RANS, and has the ability to capture the CCV of in-cylinder flow that limit the performance, emissions, and fuel consumption of modern engines. Here, LES has been performed for a motored two-valve piston engine, and CCV of both global and local quantities are evident. The ensemble mean and RMS velocities at two phases have been discussed in detail, and some comparisons with PIV measurements have been made.
Extensive POD analysis has been performed on the LES data. Parametric studies have been performed to explore convergence of POD modes and several POD variants, including comparisons of phase-dependent versus phase-invariant POD, 2-D versus 3-D POD, the effects of subtracting the ensemble mean prior to POD analysis, and phase-invariant POD analysis over full four-strokes cycles versus over intake and compression strokes only. In general, it has been found that the conclusions that were drawn for a simple piston-cylinder assembly without moving valves or compression [75] carry over to this more realistic engine configuration. This is a very welcome finding.

The salient conclusions are as follows.

- A large number of consecutive cycles may be required to reach a thermodynamic cyclic steady state (depending on the specification of initial conditions), but small variations in the thermodynamic state have little influence on the in-cylinder flow dynamics.

- LES captures CCV in global and local quantities. The acoustic characteristics of the intake systems are largely responsible for the CCV in trapped mass that are found in the simulations.

- POD analysis can be performed before or after subtracting the ensemble mean velocity. The primary difference is a shifting of the POD modes by one, although some mode reordering is also found.

- Initial comparisons of the ensemble mean and RMS velocities between LES and PIV show promising agreement in the mean velocity field and significant differences in RMS velocity fields. It is expected that explicit accounting for the PIV spatial resolution and dynamic range will be required to make careful quantitative comparisons between LES and PIV.

- The degree of flow organization varies over the engine cycle. The flow is relatively disorganized at TDC, and is more organized at the mid-stroke, especially during valve-opening events, when a strong intake/exhaust jet is introduced.
• A small number of POD modes is sufficient to capture a large fraction of the flow’s kinetic energy for organized phases, and the first POD mode strongly resembles the ensemble average at most phases.

• Sixty or fewer input snapshots are sufficient to produce converged mean and RMS velocity fields and lower-order phase-dependent POD modes at 100° aTDC and 300° aTDC. However, more input snapshots are needed to converge higher-order POD modes.

• There is little change in the lower-order phase-invariant POD modes when as few as 24 phases per cycle (30° between samples) are used. This suggests that relatively large time intervals between samples may be sufficient to capture the key in-cylinder flow dynamics using PIV, for example.

• Time-dependent in-cylinder flow through the full engine cycle can be reconstructed using a relatively small number of POD modes for both phase-dependent and phase-invariant POD.

• Insight into CCV and in-cylinder flow dynamics can be obtained through analysis of phase-invariant POD modes.
Conclusions and Future Work

7.1 Summary and principal conclusions

Significant progress has been made in IC-engine design since the introduction of high-resolution optical diagnostics (e.g., PIV) and numerical models (e.g., LES) near end of the last century. The potential for further improvements in thermal efficiency (lower fuel consumption), robust operation, and reduced emissions demand closer scrutiny of the in-cylinder aero-thermal-chemical processes, such as the CCV. In-cylinder turbulent flow for each individual cycle varies significantly from the ensemble mean, which is usually the design target for optimal performance. Consequently, engines are significantly less efficient than they could be due to the fact that the combustion process initiates from different conditions on every cycle.

Multiple-cycle LES can capture CCV, and better captures complex in-cylinder flow dynamics and turbulence compared to RANS. POD can be used as tool to analyze the complex in-cylinder turbulence, and provides an objective basis for quantitative comparisons between LES and PIV beyond ensemble averaging. In this study, motored LES has been performed for a simplified piston-cylinder assembly with and without swirl (Imperial College engine) and a more realistic two-valve, four-stroke-cycle engine (TCC engine). A systematic parametric study has been carried out for the simplified engine to study the influence of numerical and physical parameters on LES results. A comprehensive POD analysis for in-cylinder flow then has been performed using datasets obtained from LES for the two engine configurations. Parametric studies were performed to explore convergence of
POD modes and several POD variants, including comparisons of phase-dependent versus phase-invariant POD, 2-D versus 3-D POD, the effects of subtracting the ensemble mean prior to POD analysis, and phase-invariant POD analysis over full four-strokes cycles versus over intake and compression strokes only. Detailed conclusions for each engine configuration can be found in the corresponding chapter summaries. The main conclusions include:

- LES provides more accurate in-cylinder turbulent flow results than RANS using comparable computational meshes, especially for the RMS profiles in the Imperial College engine. Because less empiricism is involved in LES, LES provides better predictive capability than RANS.

- LES has significant advantage over RANS in predicting CCV and more detailed flow structures, which are very important for IC engines. In LES, all quantities are spatially-filtered, so that large-scale dynamics are explicitly captured. For the class of of turbulence models that has been used here, the principal difference between LES and RANS is the lower dissipation in the LES turbulence model. For the real engine configuration (TCC engine), LES captures CCV in global and local quantities. It is found that the acoustic characteristics of the intake systems are largely responsible for the computed CCV in trapped mass.

- For the simplified engine configuration (Imperial College engine) at moderate Reynolds numbers, a mesh refinement analysis was carried out by performing LES on three meshes (coarse mesh, baseline mesh, and fine mesh). More than 80% of the TKE is resolved for the coarse mesh, and the amount that is resolved increases as the mesh is refined. The sum of the resolved and modeled contributions to the TKE approaches grid independence for the meshes used in this study.

- In principle, the first POD mode, which corresponds to the most energetic structures does not necessarily resemble the ensemble-averaged mean velocity field. Nevertheless, in the cases that have been examined here, the first POD mode essentially corresponds to the ensemble-averaged mean velocity. Moreover, the principal difference between performing POD analysis on the
original velocity fields versus on velocity fields from which the ensemble average has been subtracted is to shift the lower-order POD modes by one; some reordering of modes also has been found. The extent to which these findings can be generalized remains to be established.

- A large number of consecutive cycles is required to obtain converged LES results, and the required number of engine cycles varies for different engine configurations and phases. For a real geometry engine configuration (TCC engine), 40 cycles are sufficient to obtain converged mean and RMS velocities and low-order POD modes for the two phases discussed in the dissertation; for the axisymmetric engine configuration (Imperial College engine), fewer engine cycles are required by taking advantage of averaging over the homogeneous direction.

- A large number of cycles may be needed to reach a cyclic steady, in-cylinder, thermodynamic state, depending on the initial and boundary condition specification, even when the first several cycles are disregard to avoid contamination by initial conditions. However, small variations in the thermodynamic state have little influence on the in-cylinder flow dynamics.

- The sensitivity of LES to key numerical and physical model parameters has been investigated for the simplified engine (Imperial College engine). Results are sensitive to time step, mesh, and SFS turbulence model. Satisfactory results can be obtained using simple viscosity-based SFS turbulence models, although there is room for improvement. The strong sensitivity of computed mean and RMS velocity profiles to variations in the SFS turbulence model is an encouraging result. This suggests that better results might be obtained using more advanced models.

- For the TCC engine where PIV measurements are being made, initial comparisons of the ensemble mean and RMS velocities show promising agreement in the mean velocity field. Significant differences in RMS velocity fields are observed. It is expected that explicit accounting for the PIV spatial resolution and dynamic range will be required to make careful quantitative comparisons between LES and PIV.
• Phase-dependent POD can be used as a tool to extract the most energetic structures of in-cylinder flows. By performing phase-dependent POD on different sources of data, such as LES versus PIV, or LES from different codes, one can make objective comparisons that go beyond ensemble averaging.

• The energy content of phase-dependent POD modes is an indicator of the flow’s level of organization. The in-cylinder flow is ‘organized’ with smaller CCV for phases where a small number of POD modes is sufficient to capture a large fraction of the flow’s kinetic energy, and the first mode resembles the ensemble average. The in-cylinder flow is ‘disorganized’ with greater CCV for phases where a large number of POD modes is required to capture a significant fraction of the flow’s kinetic energy, and the first POD mode can differ significantly from the ensemble average. By performing phase-dependent POD at all the engine phases, it is seen that the degree of in-cylinder flow’s organization varies over an engine cycle. The flow is relatively disorganized at TDC, and is more organized at the mid-stroke, especially during valve-opening events (for the TCC engine only), when a strong intake/exhaust jet is introduced.

• Different numbers of input snapshots are required for converged POD results depending on the engine configuration and phases. In general, the real-geometry engine configuration (TCC engine) required more input snapshots for converged POD result than the simplified engine configuration (Imperial College engine). Also, the number of engine cycles required to extract converged POD modes increases with mode number, and varies with phase (piston position). Convergence can be quantified by projection of velocity fields.

• There is little change in the lower-order phase-invariant POD modes when as few as 24 phases per cycle (30 °) are used. This suggests that relatively large time intervals between samples may be sufficient to capture the key in-cylinder flow dynamics using PIV, for example.

• Complex 3-D time-dependent in-cylinder flow through the full engine cycle can be reconstructed using a relatively small number of POD modes for both
phase-dependent and phase-invariant POD. This bodes well for the concept of using POD modes as a basis for simulation of in-cylinder flows.

- Quantification of CCV and insight into in-cylinder flow dynamics can be extracted through analysis of phase-invariant POD modes and coefficients. The physical interpretation can be clear when the analysis is limited to a portion of the engine cycle, such as intake and compression stroke in the TCC engine.

7.2 Future Work

Future work includes:

- For the TCC engine, more detailed analysis of CCV (e.g., to look for adjacent-cycle correlations and to identify correlations between in-cylinder flow and intake-system acoustic dynamics).

- Quantitative comparisons with PIV data or results from other LES codes and further data mining (e.g., applying filter or transfer functions implied by PIV to the LES velocity data prior to analysis).

- Extend the LES and the POD analysis to homogeneous spark ignition and turbulent flame propagation.

- Explore more advanced LES turbulence models, such as dynamic models and/or non-dissipative models [128].


Kai Liu was born in Jingzhou, Hubei province, China in 1981. He received his bachelor’s degree and master’s degree from Beijing University of Aeronautics and Astronautics, China, in 2003 and 2006, respectively. He joined the professor Daniel Haworth’s research group at the Pennsylvania State University in Fall 2006 as a graduate research assistant. He worked on numerical modeling of turbulence and combustion with focus on Large-eddy simulation of in-cylinder flows in internal combustion engines.