MODELING OF AIR MOTION IN OTOSAN NHDD ENGINE USING 3D CFD CODE KIVA3V

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OTOSAN NHDD MOTORUNDA 3-BOYUTLU SAD PROGRAMI KIVA3V YARDIMI YLA HAVA HAREKETLERİNİN MODELLENMESİ

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Prof. Dr. Orhan DENİZ (Y.T.Ü.)

MAYIS 2004
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April, 2004

Fatih Deniz GENÇ
CONTENTS

ABBREVIATIONS vi
LIST OF TABLES vii
LIST OF FIGURES viii
LIST OF SYMBOLS xi
ÖZET xiii
SUMMARY xv

1. INTRODUCTION 1

2. OTOSAN NHDD ENGINE 4

3. BASICS OF ENGINE MODELING BASED on KIVA3V 7
   3.1 The Focus 7
       3.1.1. Explicit Scheme 7
       3.1.2. Implicit Scheme 8
       3.1.3. Crank-Nicholson Scheme 8
   3.2. KIVA Fundamentals 8

4. PHYSICAL BASICS 13
   4.1 Combustion Fundamentals 13
   4.2. Chemical Equilibrium 14
   4.3. Dissociation 14
   4.4. A Model for Combustion of Hydrocarbon Fuels 15
   4.5. Combustion Kinetics and Sensitivity Analyses 18

5. ENGINE MODELING OVERVIEW 19
   5.1 General 19
   5.2 Zonal Models 20
   5.3 Dimensional Models 22

6. TURBULENCE 24
   6.1 General 24
   6.2 Spectral Description of Turbulence 25
   6.3 Modeling Turbulence 28
       6.3.1 Direct Numerical Solution 28
       6.3.2 The Standard k-ε Model 28
       6.3.3 The RNG Version of k-ε Model 30
   6.4 Turbulent Combustion 31
       6.4.1 Basic Definitions for Turbulent Combustion 31
       6.4.2 Turbulent Combustion Models 32
       6.4.3 Partially Stirred Reactor Model 32

7. MATHEMATICAL BASICS 37
   7.1 General 37
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.2 Basic Equations</td>
<td>38</td>
</tr>
<tr>
<td>7.2.1 Conservation of mass</td>
<td>38</td>
</tr>
<tr>
<td>7.2.2 Conservation of energy</td>
<td>39</td>
</tr>
<tr>
<td>7.2.3 Conservation of momentum (x-Direction)</td>
<td>39</td>
</tr>
<tr>
<td>7.3 Discretization</td>
<td>40</td>
</tr>
<tr>
<td>7.3.1 Discretization Using the Finite-Difference Method</td>
<td>40</td>
</tr>
<tr>
<td>7.3.2 Discretization Using the Finite-Volume Method</td>
<td>41</td>
</tr>
<tr>
<td>7.4 Assembly of Discrete System and Application of Boundary Conditions</td>
<td>42</td>
</tr>
<tr>
<td>7.5 Solution of Discrete System</td>
<td>43</td>
</tr>
<tr>
<td>7.6 Grid Convergence</td>
<td>44</td>
</tr>
<tr>
<td>7.7 Dealing with Non-linearity</td>
<td>45</td>
</tr>
<tr>
<td>7.8 Direct and Iterative Solvers</td>
<td>47</td>
</tr>
<tr>
<td>7.9 Iterative Convergence</td>
<td>48</td>
</tr>
<tr>
<td>7.10 Numerical Stability</td>
<td>51</td>
</tr>
<tr>
<td>8. A STUDY OF SWIRL SIMULATION IN A DI ENGINE FROM LITERATURE</td>
<td>54</td>
</tr>
<tr>
<td>8.1 Overview of the Study</td>
<td>55</td>
</tr>
<tr>
<td>8.2 Swirl Ratio</td>
<td>57</td>
</tr>
<tr>
<td>8.3 Results of the Study</td>
<td>62</td>
</tr>
<tr>
<td>9. GOVERNING EQUATIONS</td>
<td>63</td>
</tr>
<tr>
<td>9.1 Fluid Phase Equations</td>
<td>63</td>
</tr>
<tr>
<td>9.1.1 Continuity Equation</td>
<td>64</td>
</tr>
<tr>
<td>9.1.2 Momentum Equation</td>
<td>64</td>
</tr>
<tr>
<td>9.1.3 Energy Equation</td>
<td>66</td>
</tr>
<tr>
<td>9.2 State Equations</td>
<td>66</td>
</tr>
<tr>
<td>9.3 Chemical Reactions</td>
<td>67</td>
</tr>
<tr>
<td>9.3.1 Kinetic Reaction (Slow)</td>
<td>67</td>
</tr>
<tr>
<td>9.3.2 Equilibrium Reaction (Fast)</td>
<td>68</td>
</tr>
<tr>
<td>9.4 The Spray Droplets Model Equations</td>
<td>69</td>
</tr>
<tr>
<td>10. NUMERICAL SCHEME</td>
<td>74</td>
</tr>
<tr>
<td>10.1 Temporal Differencing</td>
<td>75</td>
</tr>
<tr>
<td>10.1.1 Phase A</td>
<td>75</td>
</tr>
<tr>
<td>10.1.2 Phase B</td>
<td>75</td>
</tr>
<tr>
<td>10.1.3 Phase C</td>
<td>76</td>
</tr>
<tr>
<td>10.2 Spatial Differencing</td>
<td>76</td>
</tr>
<tr>
<td>10.3 Control Volumes</td>
<td>77</td>
</tr>
<tr>
<td>10.4 Boundary Conditions</td>
<td>78</td>
</tr>
<tr>
<td>10.4.1 Physical Boundary Conditions</td>
<td>78</td>
</tr>
<tr>
<td>10.4.2 Boundary Conditions for the Spray Equation</td>
<td>81</td>
</tr>
<tr>
<td>10.4.3 Numerical Boundary Conditions</td>
<td>81</td>
</tr>
<tr>
<td>11. STRUCTURE OF COMPUTER CODE AND SIMULATIONS</td>
<td>82</td>
</tr>
<tr>
<td>11.1 Generation of Bowl Profile Using Analytic Functions</td>
<td>83</td>
</tr>
<tr>
<td>11.2 Mesh Structure</td>
<td>84</td>
</tr>
<tr>
<td>11.3 Experimental Values</td>
<td>86</td>
</tr>
<tr>
<td>11.4 Cold Flow Simulations: Grid Dependence</td>
<td>88</td>
</tr>
<tr>
<td>11.4.1 Effect of Wall Temperatures</td>
<td>93</td>
</tr>
</tbody>
</table>
## ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D</td>
<td>Three Dimension</td>
</tr>
<tr>
<td>ALE</td>
<td>Arbitrary Lagrangian Eulerian</td>
</tr>
<tr>
<td>BDC</td>
<td>Bottom Dead Center</td>
</tr>
<tr>
<td>CA</td>
<td>Crank Angle</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Lewy</td>
</tr>
<tr>
<td>DI</td>
<td>Direct Injection</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>FDM</td>
<td>Finite Difference Method</td>
</tr>
<tr>
<td>LRR</td>
<td>Launder-Reece-Rodi</td>
</tr>
<tr>
<td>ODE</td>
<td>Ordinary Differential Equation</td>
</tr>
<tr>
<td>PaSR</td>
<td>Partially Stirred Reactor</td>
</tr>
<tr>
<td>PDC</td>
<td>Partial Donor Cell</td>
</tr>
<tr>
<td>PDF</td>
<td>Probability Distribution Function</td>
</tr>
<tr>
<td>PGS</td>
<td>Pressure Gradient Scaling</td>
</tr>
<tr>
<td>QSOU</td>
<td>Quasi-Second-Order-Upwind</td>
</tr>
<tr>
<td>RMS</td>
<td>Root Mean Square</td>
</tr>
<tr>
<td>RNG</td>
<td>ReNormalization Group</td>
</tr>
<tr>
<td>RPM</td>
<td>Revolution per Minute</td>
</tr>
<tr>
<td>SGS</td>
<td>Sub-Grid Scale</td>
</tr>
<tr>
<td>SI</td>
<td>Spark Ignition</td>
</tr>
<tr>
<td>SSG</td>
<td>Speziale-Sarkar-Gatski</td>
</tr>
<tr>
<td>TDC</td>
<td>Top Dead Center</td>
</tr>
</tbody>
</table>
LIST OF TABLES

Table 2.1. Specifications of OTOSAN-NHDD engine ........................................ 5
Table 6.1. The constants for standard and RNG k-ε models ............................. 31
Table 8.1. Engine parameters used .................................................................. 55
Table 8.2. Description of cases considered ..................................................... 57
Table 10.1. Three phases overview including the sub-routines used ............... 76
Table 10.2. Boundary conditions in KIVA3V .................................................. 79
Table 11.1 Ford OTOSAN experimental data (Part 1) ...................................... 87
Table 11.2 Ford OTOSAN experimental data (Part 2) ...................................... 88
Table 11.3. The parameters needed for IPREP and ITAPE5 ............................. 88
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page No</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 2.1</td>
<td>OTOSAN-NHDD engine</td>
<td>4</td>
</tr>
<tr>
<td>Figure 2.2</td>
<td>The piston geometry of OTOSAN-NHDD engine</td>
<td>6</td>
</tr>
<tr>
<td>Figure 5.1</td>
<td>Types of engine modeling</td>
<td>20</td>
</tr>
<tr>
<td>Figure 5.2</td>
<td>The types of meshes which available in KIVA</td>
<td>23</td>
</tr>
<tr>
<td>Figure 6.1</td>
<td>Energy spectrum for turbulent flow</td>
<td>26</td>
</tr>
<tr>
<td>Figure 6.2</td>
<td>Schematic illustration of the PaSR model</td>
<td>32</td>
</tr>
<tr>
<td>Figure 6.3</td>
<td>Reaction / mixture step calculation</td>
<td>33</td>
</tr>
<tr>
<td>Figure 7.1</td>
<td>Discretization of a domain</td>
<td>37</td>
</tr>
<tr>
<td>Figure 7.2</td>
<td>Illustration of discretization via FDM</td>
<td>40</td>
</tr>
<tr>
<td>Figure 7.3</td>
<td>Rectangular cell</td>
<td>42</td>
</tr>
<tr>
<td>Figure 7.4</td>
<td>Comparison of numerical and exact solutions</td>
<td>44</td>
</tr>
<tr>
<td>Figure 7.5</td>
<td>Comparison of three numerical solutions and the exact solution</td>
<td>45</td>
</tr>
<tr>
<td>Figure 7.6</td>
<td>Convergence versus # of iterations</td>
<td>50</td>
</tr>
<tr>
<td>Figure 7.7</td>
<td>Exact solution and solutions after 2, 4, 6 iterations</td>
<td>50</td>
</tr>
<tr>
<td>Figure 8.1</td>
<td>Schematic of engine and computational mesh</td>
<td>56</td>
</tr>
<tr>
<td>Figure 8.2</td>
<td>Conventional valve with a shroud</td>
<td>57</td>
</tr>
<tr>
<td>Figure 8.3</td>
<td>Velocity vector plots show the flow through (a) un-shrouded valve, and (b) shrouded valve</td>
<td>58</td>
</tr>
<tr>
<td>Figure 8.4</td>
<td>Swirl ratio versus crank angle</td>
<td>59</td>
</tr>
<tr>
<td>Figure 8.5</td>
<td>Velocity vectors shown in a horizontal plane at a crank angle of 375 degrees for (a) un-shrouded valve case, and (b) shrouded valve case</td>
<td>60</td>
</tr>
<tr>
<td>Figure 8.6</td>
<td>Velocity vectors shown in a horizontal plane at a crank angle of 455 degrees for; (a) un-shrouded valve case, (b) shrouded valve case</td>
<td>61</td>
</tr>
<tr>
<td>Figure 8.7</td>
<td>Computational mesh shown with the half-size intake system</td>
<td>61</td>
</tr>
<tr>
<td>Figure 10.1</td>
<td>Typical cell layout in KIVA3V</td>
<td>74</td>
</tr>
<tr>
<td>Figure 10.2</td>
<td>A typical momentum cell</td>
<td>77</td>
</tr>
<tr>
<td>Figure 10.3</td>
<td>A typical N-V-C-o-C-F cell</td>
<td>78</td>
</tr>
<tr>
<td>Figure 10.4</td>
<td>Mass averaged case for periodic boundary condition</td>
<td>80</td>
</tr>
<tr>
<td>Figure 11.1</td>
<td>Summary of how KIVA3V works</td>
<td>82</td>
</tr>
<tr>
<td>Figure 11.2</td>
<td>Schematic view of NHDD engine piston bowl profile</td>
<td>84</td>
</tr>
<tr>
<td>Figure 11.3</td>
<td>Mesh 1; generated by ICEM-CFD, ncells= 21795 nverts= 24320, in left figure piston is about 42 degrees after BDC and in right figure piston is 2 degrees after TDC</td>
<td>85</td>
</tr>
<tr>
<td>Figure 11.4</td>
<td>Mesh 2; generated by ICEM-CFD, ncells= 32146 nverts= 35513, in left figure piston is about 42 degrees after BDC and in right figure piston is 2 degrees after TDC</td>
<td>85</td>
</tr>
<tr>
<td>Figure 11.5</td>
<td>Mesh 3; generated by ICEM-CFD, ncells= 41599 nverts= 45520, in left figure piston is about 42 degrees after BDC and in right figure piston is 2 degrees after TDC</td>
<td>86</td>
</tr>
<tr>
<td>Figure 11.6</td>
<td>Reference pressure values (Ford OTOSAN experimental data)</td>
<td>87</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>11.34</td>
<td>Turbulent viscosity variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3</td>
<td>107</td>
</tr>
<tr>
<td>11.35</td>
<td>Pressure variation in the combustion chamber using k3prep mesh</td>
<td>108</td>
</tr>
<tr>
<td>11.36</td>
<td>Temperature variation in the combustion chamber using k3prep mesh</td>
<td>109</td>
</tr>
<tr>
<td>C.1</td>
<td>Pressure distributions in the combustion chamber at various crank angles</td>
<td>121</td>
</tr>
<tr>
<td>D.1</td>
<td>Temperature distributions in the combustion chamber at various crank angles</td>
<td>125</td>
</tr>
<tr>
<td>E.1</td>
<td>Air motions in the combustion chamber at various crank angles</td>
<td>131</td>
</tr>
<tr>
<td>F.1</td>
<td>Injection characteristic (arbitrary units)</td>
<td>132</td>
</tr>
<tr>
<td>F.2</td>
<td>Spray formation in the combustion chamber at various crank angles</td>
<td>135</td>
</tr>
<tr>
<td>G.1</td>
<td>Injection characteristic (arbitrary units)</td>
<td>136</td>
</tr>
<tr>
<td>G.2</td>
<td>Vapor distribution in the combustion chamber at various crank angles</td>
<td>142</td>
</tr>
</tbody>
</table>
**LIST OF SYMBOLS**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B$</td>
<td>Break-up transition probability function</td>
</tr>
<tr>
<td>$C$</td>
<td>Courant number</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Constant pressure specific heat</td>
</tr>
<tr>
<td>$C_e$</td>
<td>Coefficients for the turbulence model</td>
</tr>
<tr>
<td>$c, c_0, c_i$</td>
<td>Time points for PaSR</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion coefficient</td>
</tr>
<tr>
<td>$e_{ij}$</td>
<td>Deformation of a fluid particle</td>
</tr>
<tr>
<td>$F$</td>
<td>Force</td>
</tr>
<tr>
<td>$\bar{F}^s$</td>
<td>(rate of momentum gain)/(volume) due to spray</td>
</tr>
<tr>
<td>$f(r)$</td>
<td>Probability distribution function</td>
</tr>
<tr>
<td>$\dot{j}_{bu}$</td>
<td>Source due to droplet break-up</td>
</tr>
<tr>
<td>$\dot{j}_{coll}$</td>
<td>Source due to droplet collision</td>
</tr>
<tr>
<td>$g$</td>
<td>Specific body force</td>
</tr>
<tr>
<td>$h_m$</td>
<td>Specific enthalpy</td>
</tr>
<tr>
<td>$I$</td>
<td>Specific internal energy</td>
</tr>
<tr>
<td>$\bar{J}$</td>
<td>Heat flux vector</td>
</tr>
<tr>
<td>$K$</td>
<td>Mean kinetic energy of a flow</td>
</tr>
<tr>
<td>$K$</td>
<td>Thermal conductivity</td>
</tr>
<tr>
<td>$K_e$</td>
<td>Equilibrium constant</td>
</tr>
<tr>
<td>$k$</td>
<td>Turbulent kinetic energy</td>
</tr>
<tr>
<td>$k_b$</td>
<td>Backward reaction rate coefficient</td>
</tr>
<tr>
<td>$k_f$</td>
<td>Forward reaction rate coefficient</td>
</tr>
<tr>
<td>$k(t)$</td>
<td>Total kinetic energy of a flow</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Density of kinetic energy for unit wave-number</td>
</tr>
<tr>
<td>$L(T_d)$</td>
<td>Fuel latent heat of vaporization</td>
</tr>
<tr>
<td>$N$</td>
<td>Number (of sub-cycles)</td>
</tr>
<tr>
<td>$O(\Delta x)$</td>
<td>Truncation error</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$Q_d$</td>
<td>The rate of heat conduction</td>
</tr>
<tr>
<td>$\dot{Q}^c$</td>
<td>Source term due to chemical heat release</td>
</tr>
<tr>
<td>$\dot{Q}^s$</td>
<td>Source term due to spray interactions</td>
</tr>
<tr>
<td>$R_0$</td>
<td>Universal gas constant</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$R_f$</td>
<td>One way equilibrium rate</td>
</tr>
</tbody>
</table>
\( r \) : Droplet radius (equilibrium)
\( r_{52} \) : Sauter mean radius
\( Sh \) : Sherwood number
\( T \) : Temperature
\( T_d \) : Temperature of droplet
\( t \) : Time
\( u \) : Velocity vector
\( W_m \) : Molecular weight of species m
\( Y_m \) : Mass fraction of species m
\( y \) : Distortion from sphericity
\( \nabla \) : Vector operator
\( \epsilon \) : Dissipation rate of turbulent kinetic energy
\( \rho \) : Total mass density
\( \rho_m \) : Mass density of species m
\( \beta \) : Degree of dissociation
\( \phi \) : Equivalence ratio
\( \lambda \) : Air/fuel ratio
\( \ell \) : Velocity scale
\( \sigma \) : Viscous stress tensor
\( \sigma \) : Collision transition probability function
\( \mu \) : Viscosity
OTOSAN NHDD MOTORUNDA 3-BOYUTLU SAD PROGRAMI KİVA3V YARDIMIYLAYA HAVA HAREKETLERİİNİN MODELLENMESİ

ÖZET


Son olarak, hem yakıt tüketimi hem de verim yanma ile ilgili konulardır. Ekonomik ve verimli bir motor için yanma iyileştirilmelidir. Diğer taraftan, SAD (Sayısal Akişkanlar Dinamiği) yanma proseslerinin araştırılmasında ve anlaşılmasında birkaç senedir büyük ölçüde kabul ve rağbet görmüştür.
Bu trend sayesinde çok boyutlu motor modellenmesi popüler hale gelmiştir. Sayısal Akışkanlar Dinamiğinin (SAD) motor modellemede bir dönüm noktası olduğunu ve olacağını aşıkardır. Bu çalışmada odak noktası, bellii bir motordaki (OTOSAN-NHDD) hava hareketlerinin incelenmesi olmuştur. Simülasyonlar 3 boyutlu bir SAD (Sayısal Akışkanlar Dinamiği) programı olan KIVA3V tarafından LINUX (SUSE 8.0) platformunda gerçekleştirilmiştir. Bütün hesaplamalar (hen fiziksel hem de kimyasal) ve grafik çıktılar bu kod kullanılarak yürütülmuş ve oluşturulmuştur. İput dosyaları Taskiran’in dosyalarının modifiye edilmesi suretiyle elde edilmiştir. Odak noktası hava hareketleri olduğunu için, input dosyalarına (iprep ve itape5) yapılan modifikasyonların çoğu daha iyi bir mesh yapısı elde etmek hedefini gütmektedir. Sonuçlar; elde çıkan daha iyi bir program olmamasından dolayı; GMV programını yardımcı ile değerlendirilmiştir. Bazı sonuçlar ayrıca daha iyi bir görsellik elde etmek için dış uygulamalarla (örneğin GifCSP) işlenmiştir. Nümerik sonuçlar denenysel sonuçlarla mukayese edilmiştir.
MODELLING OF AIR MOTION IN OTOSAN NHDD ENGINE USING 3D CFD CODE KIVA3V

SUMMARY

Air motion in an internal combustion engine is one of the most important factors which determine combustion characteristics; thus maximum power output, fuel consumption, exhaust emissions and efficiency of that engine. Actually, these four parameters are not independent from each other. They are all connected together and the problem is the optimization. In order to develop a better performance engine, one needs to know combustion phenomenon and the factors affecting this phenomenon.

To be able to take place in the low tax group (in accordance to “cylinder volume criteria”), the engine manufacturers are trying to increase the maximum power output of small engines. They prefer performance-based designed small engines instead of moderate-performance designed larger engines. This kind of development requires knowledge of combustion.

In recent years, the exhaust emissions limit values are dramatically decreased by related regulations; such as EURO norms. By other words, engine manufacturers are forced to produce engines with lower emission values. There are two possible ways to reduce these emission values. First method dictates that the combustion process should be revised so that the fuel is combusted as efficient as possible and the emissions being given out of the exhaust to atmosphere are only H₂O and CO₂. This is the theoretical case and it is hard to achieve. Also it should be noted that CO₂ itself is a great problem (Greenhouse Effect) for environment. The other method implies trapping exhaust emissions by using a catalytic converter. In either case an improvement to combustion is necessary.

Finally, both fuel consumption and the efficiency are also combustion related topics. To have an economic and efficient, combustion needs to be improved.

On the other hand, CFD (Computational Fluid Dynamics) has been increasingly accepted as an adjunct to experimentation in the design and understanding of practical combustion systems over the past several years. By the help of this trend, popularity of multi-dimensional engine modeling has been increased. It is evident that CFD will be (actually is) a great milestone in engine design. In this study, the main focus is the air motion in a specific engine. (OTOSAN-
The simulations are done via KIVA-3V - a 3D CFD code - on a LINUX platform. (SUSE 8.0) All the calculations (both physical and chemical) and graphical outputs are obtained by the help of this code. The input files are modified versions of Taskiran’s. Since the air motions in the engine are focused, most of the modifications to the input files (iprep and itape5) are done to achieve a better mesh structure. The results are post-processed by GMV due to lack of a better post-processor available. Some results are also visualized via third party programs (GifCSP…) in order to improve present ability. Numerical results are compared to experimental results.
CHAPTER 1

INTRODUCTION

Having high efficiency, and thus low fuel consumption; diesel engines has found a wide spread application area both in transportation devices (ground, air and sea) and industrial plants. Due to the fact that they do not need a homogenous air-fuel mixture, there is no theoretical limit in their bore dimension. A single cylinder may vary in size from 0,1 Lt to 1000 Lt. Manufacturers have been carrying a lot of researches in order to be able to reduce both fuel consumption values and exhaust emissions values for over thirty years. In the last twenty years of this trend, both experimental and numerical studies became very popular and by usage of these new techniques, important improvements to diesel engines have been done.

In general, the air-fuel mixture in diesel engines is formed by injection of high pressure fuel into the combustion chamber at last periods of compression stroke. Due to the injection, atomization occurs; the net surface areas of fuel droplets increase, leading to a fast vaporization and combustion. Parallel to new technologies, the injection pressure may be over 2000 bars in some very new applications. Atomization of the injected fuel into the combustion chamber is a complicated matter in nature. Since it is impossible to measure or know all the parameters affecting this atomization procedure, usually some assumptions are done and the mathematical formulation is based on these assumptions.

Measurements of mixture formation and combustion parameters imply lots of difficulties and their costs are very high. However, experimental method is still the de-facto method in engine development processes.

Numerical methods have a lot of advantages in comparison to “experimental method” but a comprehensive, exact modeling of all complicated physical and chemical procedures are still impossible via today’s technology. This is why numerical methods are preferred and used in academic environments. For today, the best solution is to use numerical methods to reduce the number of experiments in a certain project, decreasing the total cost.
Furthermore, it becomes possible to analyze the variation of some parameters that cannot be measured in experimental procedures.

It can be stated that for diesel engine modeling, zero-dimensional (thermo-dynamical) and multi-dimensional models are appropriate. Although one-dimensional models are suitable for spark ignition engine modeling, they aren't used in compression ignition (diesel) engine modeling.

Thermo-dynamical models are divided into two groups: Single-zone models and multi-zone models. (Two-zone models and three-zone models) This classification is based on the number of regions that is assumed to have separate, uniform thermo-dynamic properties. These regions are expressed in terms of pressure, temperature and mixture composition. A number of empirical expressions are used to evaluate parameters such as ignition delay, combustion, thermal loses, and air motion in combustion chamber but local values cannot be calculated. Also; atomization of injected fuel, the effect of cylinder geometry and penetration of the injected fuel are some topics that lies beyond the scope of this type of analysis.

The term "multi-dimensional model" refers to two-dimensional and three-dimensional models. Flow fields are expressed in terms of time and dimensions and thus; the change in local parameters can be analyzed. Due to the fact that there are two different fluids in the combustion chamber; one in gas phase and the other in liquid phase; the change in the transition from liquid phase to gas phase with respect to time and position affects many flow properties. The motion of fuel droplets, evaporation, combustion and turbulence parameters, the changing positions and concentrations of species requires multi-dimensional engine modeling.

Multi-dimensional models were first used in 1973 with an internal combustion engine model presented by Watkins. In 1979 combustion calculations were done by Bulter. From that date on, the number and the quality of studies increased, many sub-models were developed in order to be used in main models. Parallel to increasing availability of computational resources, formerly “neglected” or unknown parameters were taken into consideration. Today, there are many computer codes such as KIVA, FLUENT, FIRE, STAR-CD that use numerical methods and capable of developing multi-dimensional models. However, it should be kept in mind that these software use approximations for yet unexpressed phenomena and their results are not always true. There are still different
approaches for collision of fuel droplets in a spray, results of this collision, turbulent flow and this kind of actions.

This study covers the analyses of in-cylinder air motion in OTOSAN-NHDD engine and mesh refinement of a previous study prepared by Taskiran. It is thought to be convenient to start with the physical and mathematical background. In the following chapter a swirl generation study is going to be discussed. Then, detailed information about mesh refinement will be given. Next step is to introduce KIVA-3V program structure. Finally, outputs will be evaluated.
CHAPTER 2

OTOSAN NHDD ENGINE

This engine is OTOSAN’s heavy-duty engine having 6 cylinders and producing 270 HP. It is used in certain truck series. Like all the other manufacturers, OTOSAN is preparing for new emission standards. In this manner a project, is decided to be carried out and this thesis study is a part of that project from ITU.

Since 8-nozzle injectors are used in the engine, modeling of a 45° sector will be enough. Also, in this study only the in-cylinder conditions are considered. (Intake and exhaust systems are not analyzed; instead they are represented by initial conditions.

![OTOSAN-NHDD engine](image)

**Figure 2.1.** OTOSAN-NHDD engine

The main specifications of the engine are given Table 2.1. The values given in this table are standard (mass production) values. The engine is used in experiments in laboratories by OTOSAN nowadays. In these experiments it is possible to measure nearly all parameters of choice and change basic properties of the engine. In this study, the most important section of the engine is the piston due to forming the lower boundary of the combustion chamber. Since new generation diesel engines are manufactured as DI (Direct Injection), there is a strong need for some sort of air motion in the cylinder to
provide a reasonable rate of mixture formation. Especially, at low rpms mixture formation is mostly provided by these air motions.

**Table 2.1. Specifications of OTOSAN-NHDD engine**

<table>
<thead>
<tr>
<th>No of cylinders</th>
<th>6</th>
<th>Idle rpm</th>
<th>600 rpm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>112mm</td>
<td>Max. rpm</td>
<td>3150 rpm</td>
</tr>
<tr>
<td>Stroke</td>
<td>124mm</td>
<td>Injection Sys.</td>
<td>Common Rail</td>
</tr>
<tr>
<td>Displacement</td>
<td>7330cm³</td>
<td>Inlet Valve Open</td>
<td>28⁰ BTDC</td>
</tr>
<tr>
<td>Comp. Ratio</td>
<td>17.4</td>
<td>Inlet Valve Close</td>
<td>42⁰ ABDC</td>
</tr>
<tr>
<td>Max. Power</td>
<td>220.7kW (2200 rpm)</td>
<td>Exhaust Valve Open</td>
<td>59⁰ BBDC</td>
</tr>
<tr>
<td>Max. Torque</td>
<td>750Nm (1495 rpm)</td>
<td>Exhaust Valve Close</td>
<td>27⁰ ATDC</td>
</tr>
</tbody>
</table>

Most of these air motions are generated by the upper piston surface geometry. Thus the form of the piston bowl plays a crucial role in engine output parameters. In addition to these air motions, using special valves (skirt valves) and specially formed intake channels provide extra air motions. However these methods lead to an energy loss due to dynamic flow loses, and decrease the volumetric efficiency.

To obtain accuracy in the calculations, the piston bowl geometry is expressed analytically. This will help us in finding enough number of points for numerical simulation to represent the geometrical form. The drawing of piston is obtained from Ford- OTOSAN and is shown in Figure 2.2.
Figure 2.2. The piston geometry of OTOSAN-NHDD engine
CHAPTER 3

BASICS OF ENGINE MODELING BASED on KIVA3V

3.1. The Focus

For some years scientists have been developing comprehensive numerical models to simulate the in-cylinder dynamics of advanced internal combustion engines. In general, these comprehensive models include:

- Spray dynamics
- Fluid flow
- Species transport
- Mixing
- Chemical reactions
- Heat release

These comprehensive models are combined together; forming the main model and this model is embodied in a computer code. (In our case KIVA3V) It is possible for the code to calculate both two-dimensional and three-dimensional situations.

KIVA3V is a computer program which may be used to generate numerical solutions to multi-component chemically reactive fluid flow problems. Again KIVA3V is a time-marching program that solves finite-difference approximations to the governing differential equations. The transient solution is marched out in a sequence of finite time increments called cycles or time steps. Values of the dependent variables on each cycle are calculated from those on the previous cycle. The temporal difference scheme is explicit. In general; to obtain a solution from such a system, there are three choices: Explicit Scheme, Implicit Scheme and Crank-Nicholson Scheme.

3.1.1. Explicit Scheme

The term of interest is considered to be fixed at its value at time($t$).
3.1.2. Implicit Scheme

The term of interest is considered to be fixed at its value at time \((t + \Delta t)\).

3.1.3. Crank-Nicholson Scheme

The term of interest is considered to vary linearly with the time between \((t)\) and \((t + \Delta t)\), which is equivalent to taking a fixed value equivalent to the average of the values at \((t)\) and \((t + \Delta t)\).

3.2. KIVA FUNDAMENTALS

Spatial differences are formed with respect to a generalized three-dimensional finite-difference mesh or grid, which sub-divides the region of interest into a number of small cells or zones. The corners of the cells are called vertices. The positions of the vertices may be arbitrarily specified as functions of time, thereby allowing a Lagrangian, Eulerian, or mixed description. Since the locations of the vertices are arbitrary, the cells are arbitrary hexahedrons. This type of mesh is called an ALE (Arbitrary Lagrangian Eulerian) mesh [1, 2], and is particularly useful for representing curved and/or moving boundary surfaces. The spatial differencing is made conservative wherever possible. The procedure used is to difference the basic equations in integral form, with the volume of a typical cell used as the control volume, and the divergence terms transformed into surface integrals using the divergence theorem. [1, 3, 4]

The effects of turbulence are represented by a generalized sub-grid scale (SGS) turbulence model. (Optional) This model includes a transport equation for the turbulent kinetic energy associated with the sub-grid scale motions. Boundary layer drag and heat transfer are calculated by matching to a modified turbulent law of the wall.

The numbers of species and chemical reactions that can be represented in KIVA3V is arbitrary; they are limited only by computer time and storage considerations. Chemical reactions are treated by a procedure that distinguishes between slow reactions, which proceed kinetically, and fast reactions, which are assumed to be in equilibrium. [5, 6] Chemical rate expressions for the kinetic reactions are evaluated by the same partially implicit procedure used in CONCHAS-SPRAY [7]. The rate coefficients are assumed to be of a generalized Arrhenius form. The equilibrium reactions are treated by a new iterative procedure [6], which is an improvement over that used in CONCHAS-SPRAY.
Evaporating liquid sprays are presented by a discrete-particle technique [8], in which each computational particle represents a number of similar physical droplets. The radius and other attributes of a particle are statistically assigned using a Monte Carlo sampling technique. The particles and fluid interact by exchanging mass, momentum and energy. These interactions are treated by implicit coupling procedures to avoid the prohibitively small time steps that would otherwise often be necessary. Turbulence effects on the droplets are accounted for by adding a fluctuating component to the local mean gas velocity when calculating each particles mass, momentum and energy exchange with the gas. [8] Droplet collisions and coalescence are accounted for, but the spray is otherwise assumed to be thin; volume-displacement [8] and other thick spray effects [9] are neglected.

From geometry point of view, the spatial differencing is based on the ALE method [1, 2], which in three dimensions uses a mesh made up of arbitrary hexahedrons. Spatial difference approximations are constructed by the control-volume or integral-balance approach [1, 3, 4], which largely preserves the local conservation properties of the differential equations.

Together, the cells constitute the mesh with respect to which spatial differences are formed. The vertices need not to be stationary, but may move in an arbitrarily pre-described manner. This capability includes the Lagrangian and Eulerian descriptions as special cases. In the general case, the cells are asymmetrical.

The cells are indexed by integers (i, j, k), which may be regarded as coordinates in logical space. The indices (i, j, k) also label the vertices, with the understanding that vertex (i, j, k) is vertex 4 of cell (i, j, k). The Cartesian coordinates of vertex (i, j, k) are (x_{ijk}, y_{ijk}, z_{ijk}), which in general depend on the time (t).

A generalized mesh of the ALE type provides a great deal of geometrical flexibility. It allows a convenient direct representation of curved and moving boundaries, such a moving cupped piston. In general, the cells need not to be square or rectangle, so a variety of different geometries can be represented by distorting the cells and deactivating other cells to form obstacles.

The turbulence models used in KIVA3V are; standard version of k-ε, RNG (ReNormalization Group) version of k-ε, SSG (Speziale-Sarkar-Gatski) Reynolds-Stress Turbulence Model and Linear LRR (Launer-Reece-Rodi) Re-Stress Model. Turbulence will be discussed in a separate chapter later in detail.
Numerical calculations of compressible flow have a notorious tendency to be inefficient at low Mach numbers because of the wide disparity between the time scales associated with convection and the propagation of sound waves. In explicit schemes, this inefficiency occurs because the time steps needed to satisfy the sound-speed stability condition are much smaller than those needed to satisfy the convective stability condition alone. In implicit schemes, the inefficiency manifests itself in the additional computational labor needed to solve the implicit system of equations on each time step. This solution is usually performed by iterative techniques.

Provided that the Mach number is not too low, there is a third alternative which effectively combines the advantages of explicit and implicit methods while largely avoiding the disadvantages. This method is called "Acoustic Sub-cycling Method" [10], in which all terms in the governing equations that are not associated with sound waves are explicitly advanced with a relatively large time step $\Delta t$ similar to that of an iterative method. The terms associated with acoustic waves (namely the compression terms in the continuity and energy equations and the pressure gradient in the momentum equation) are explicitly advanced using a smaller time step $\Delta t'$ that satisfies the sound-speed stability condition and of which the main time step $\Delta t$ is an integral multiple. This method eliminates much of the inefficiency of a purely explicit scheme while preserving the simplicity and robustness thereof. The sub-cycling plays a role analogous to the iteration in implicit methods, but unlike the latter it has the advantage that it is not open-ended. That is; the number of sub-cycles is fixed by ratio of stability limits and cannot become unreasonably large, as the number of iterations frequently does.

The acoustic sub-cycling method works very well in most internal combustion engine calculations, where the Mach numbers are not unduly low. The primary disadvantage of the method is that it is unsuitable for very low Mach numbers, such as those that occur in an engine cylinder at very low rpm. The problem is simply that the number of sub-cycles ($N = \Delta t / \Delta t'$) tends to infinity as the Mach number tend to zero, and once $N$ exceeds 50 or so an implicit scheme becomes more efficient. To extend the applicability of the method, it is convenient to combine it with the PGS (Pressure Gradient Scaling) method. [11]

Pressure gradient scaling is a method for artificially increasing the Mach number to somewhat larger values while still keeping it small in an absolute sense. This is done by multiplying the pressure gradient in the momentum equation by a time-dependent
scaling factor. This kind of modification has the desired effect of reducing the effective sound speed by a predefined factor. However; at first it may be expected to affect the solution in other ways as well and therefore to be unacceptable. In particular, since the pressure gradient has no way of distinguishing pressure inhomogeneities, one might expect to incur errors in accelerations, and hence in velocities, that are not merely acoustic in character. Fortunately, and perhaps surprisingly, this fear is not well founded. Physically, the saving grace is that the pressure gradients in a low Mach number flow are effectively determined by the velocity field, and not vice versa. The pressure gradients adjust themselves to whatever values are necessary for the velocity field to have the correct divergence. [12, 13]

Within the context of the acoustic sub-cycling method, the PGS method improves numerical efficiency by reducing the number of sub-cycles required. Reduction of the sound speed by a factor, allows \( \delta t \) to be increased by the same factor, and thus the number of sub-cycles is reduced by the same factor. The appropriate value of this factor is automatically selected in an adaptive manner by continually monitoring the magnitude of the pressure inhomogeneities that occur in the calculation. If these inhomogeneities are smaller than a specified tolerance that the user considers "essentially uniform pressure" then the value of the factor is increased. If the pressure inhomogeneities become large enough that the pressure field threatens to become sensibly non-uniform then the factor is decreased.

The acoustic sub-cycling and PGS methods are used in conjunction with a procedure for damping sound waves. The sound waves are not themselves of interest in low Mach number combustion problems, but in some cases they can distract attention from or even conceal other flow features that are of interest, especially in velocity vector plots at a fixed instant of time. This danger is increased by the PGS method, which artificially increases the amplitude of the sound waves in the process of artificially reducing their speed. Implicit schemes frequently contain sufficient intrinsic damping to eliminate unwanted sound waves, but the acoustic sub-cycling method is neutrally stable and has no intrinsic damping of its own. Therefore, an acoustic damping term is needed to be introduced into KIVA3V sub-cycling procedure. The effect of this term is roughly comparable to that provided by the truncation errors in typical implicit schemes.

Finally, the last point necessary to cover in this overview is the spray model. The dynamics of atomized fuel sprays are represented by a Monte Carlo based discrete-
particle technique. [8] The spray is considered to be composed of discrete computational particles, each of which represents a group of droplets of similar physical properties. The distribution function in droplet size, velocity, spray pattern, and temperature produced by the fuel injector is statistically sampled and the resulting Lagrangian particles are followed as they locally interact, and exchange mass, momentum and energy with the gas. The model accounts for turbulence effects [8] and interactions between droplets [9], but other thick spray effects are neglected.

Drop collisions themselves are calculated by a sampling procedure. The collision frequency is calculated and used in determining the probability that a drop in the given particle will undergo a collision with a drop in a nearby particle. Then all drops in the given particle behave in the same manner; they either do or do not collide, and no new computational particles are created. This procedure has proven preferable to a more straightforward alternative whereby the collision frequency is used to determine the probable number of drops in a given particle that will have collisions with drops in another particle; one or more new particles are then created having the properties of the drops resulting from the collisions.

Particles are introduced into the computational mesh in such a way that a specified distribution of drop sizes is obtained. Two distributions are associated with the injection calculation. Occurrence of the drop radius r at injection is governed by the probability distribution \( f(r) \). Another distribution \( g(r) \) is defined in such a way that \( g(r)dr \) is the probability of that a particle has drops with in the range \((r, r + dr)\). These are the basic definitions of the case and the detailed analyses will be given later.
CHAPTER 4

PHYSICAL BASICS

4.1. Combustion Fundamentals

Combustion is a physical and chemical phenomenon during which the chemical energy is released as thermal energy as the result of the reaction between fuel and oxidizer. Fuel may contain many kinds of chemical species that consist of many kinds of chemical elements. More than 90% of fuel used as energy source is based on carbon and hydrogen and more than 90% of oxidizer used in combustion is the oxygen of the ambient air. The common property of the reactions that we may consider as combustion is a net energy release. This heat release is due to the positive difference of the chemical bond energy between the initial species and the final species.

Combustion begins from the initial state (of reactants) and proceeds in time to the final state (of products) via various intermediate reactions and species. However, for the first step, it is more practical to assume the reactions to occur with infinite rate and consider only the reactants and the final products. This approach gives the opportunity to analyze the combustion system in a much easier way, using only the classical conservation laws and the algebraic equations between temperature and species concentrations. But; in applications like modeling today’s advanced internal combustion engines, using this approach is not suitable. Instead, to analyze the real physical combustion process usage of the governing differential equations of time, concentrations and temperature.

The reaction describing the complete combustion of a hydrocarbon fuel molecule is:

\[ C_nH_{2m} + (n + \frac{m}{4})O_2 \rightarrow nCO_2 + \frac{m}{2}H_2O \]  

(4.1)

This means that \((n + (m/4))\) moles of oxygen are required to burn one mole of fuel \(C_nH_{2m}\) completely. This case can be generalized to a more comprehensive situation by defining and substituting more variables into the system such as a more general formula.
for the fuel including all or preferred components like $N$, $S$ etc., air excess coefficient and dissociation rate.

4.2. Chemical Equilibrium

Even if the reactions occur in two directions, i.e. forward and backward, there is always a dominant direction that is determined by the greater velocity at the temperature considered. Chemical equilibrium will be established at the temperature and the concentrations for which forward and backward rates are equal and the concentrations of the products do not change anymore. For example:

$$CO + H_2O \rightleftharpoons H_2 + CO_2$$  \hspace{1cm} (4.2)

When equilibrium is reached for Equation (4.2), the formation rate of products will be equal to the formation rate of the reactants.

$$k_f[CO][H_2O] = k_b[H_2][CO_2] = R_f$$  \hspace{1cm} (4.3)

Here; $R_f$ is called “one way equilibrium rate”, $k_f$ is the ratio of forward rate coefficient and $k_b$ is the backward rate coefficient. Equilibrium constant $K_c$ can be determined as:

$$K_c = \frac{k_f}{k_b} = \frac{[H_2][CO_2]}{[CO][H_2O]}$$  \hspace{1cm} (4.4)

It is also possible to express this equilibrium constant in terms of mole fractions.

4.3. Dissociation

The inversion (or decomposition) of the products molecules to the initial reactant molecules due to the backward reactions is generally called dissociation. Dissociation may be expressed in a simple way for relatively simple reactions. For example, the bi-directional reaction:

$$CO + H_2O \rightleftharpoons H_2 + CO_2$$  \hspace{1cm} (4.5)

may be cast in two reactions (forward and backward) such as:

$$CO + \frac{1}{2} O_2 \rightarrow CO_2$$  \hspace{1cm} (4.6)
\[ \beta CO_2 \rightarrow \beta CO + \frac{1}{2} \beta O_2 \]  
(4.7)

\[ CO + \frac{1}{2} O_2 \rightarrow (1 - \beta)CO_2 + \beta CO + \frac{1}{2} \beta O_2 \]  
(4.8)

\( \beta \): Degree of dissociation

4.4. A Model for Combustion of Hydrocarbon Fuels

Combustion of a hydrocarbon fuel \( C_nH_m \) can be modeled by 12 species as components of the products. These twelve species are selected species which are of most significant importance. (\( \phi < 3 \))

\[ \varepsilon C_nH_m + 0,21O_2 + 0,79N_2 \rightarrow \nu_1 CO_2 + \nu_2 H_2O + \nu_3 N_2 + \nu_4 O_2 + \nu_5 CO + \nu_6 H_2 \]
\[ + \nu_7 H + \nu_8 O + \nu_9 OH + \nu_{10} NO + \nu_{11} N + \nu_{12} NO_2 \]  
(4.9)

\( \phi \): Equivalence ratio \((1/\lambda)\)

\( \varepsilon \): A coefficient to have stoichiometric mixture with given \( n \) and \( m \) (to be calculated)

For 1 mole fuel:

\[ C_nH_m + (n + \frac{m}{4})O_2 + 3,76(n + \frac{m}{4})N_2 \rightarrow nCO_2 + \frac{m}{2} H_2O + 3,76(n + \frac{m}{4})N_2 \]  
(4.10)

For \( \varepsilon \) mole fuel:

\[ \varepsilon C_nH_m + \varepsilon(n + \frac{m}{4})O_2 + \varepsilon 3,76(n + \frac{m}{4})N_2 \rightarrow \varepsilon nCO_2 + \beta \frac{m}{2} H_2O + \varepsilon 3,76(n + \frac{m}{4})N_2 \]  
(4.11)

If Equations (4.9) and (4.11) are compared:

\[ \varepsilon = \frac{0,21}{(n + \frac{m}{4})} \]  
(4.12)

Conservation of the number of the atoms of the elements yields the following equations:

C: \[ \varepsilon \Delta n = N(y_1 + y_2) \]  
(4.13)

H: \[ \varepsilon \Delta m = N(2y_2 + 2y_6 + y_7 + y_9) \]  
(4.14)

O: \[ 0,42 = N(2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10} + 2y_{12}) \]  
(4.15)
N: \[ 1.58 = N(2y_3 + y_{10} + y_{11} + y_{12}) \] (4.16)

Here:

\[ N = \sum_{i=1}^{12} y_i \quad \text{(Total no of moles of products / 1 mole air)} \] (4.17)

\[ y_i = \frac{y_i}{N} \quad \text{(Mole fractions of the species of the products)} \] (4.18)

\[ \sum_{i=1}^{12} y_i = 1 \] (4.19)

Reactions to be considered for the formation of the selected 12 species and the corresponding equilibrium constants in terms of partial pressures:

\[ \frac{1}{2} H_2 \rightarrow H \quad K_1 = \frac{y_1}{y_6^{1/2} p^{1/2}} \] (4.20)

\[ \frac{1}{2} O_2 \rightarrow O \quad K_2 = \frac{y_8}{y_4^{1/2}} p^{1/2} \] (4.21)

\[ \frac{1}{2} O_2 + \frac{1}{2} H_2 \rightarrow OH \quad K_3 = \frac{y_9}{y_4^{1/2} y_6^{1/2}} \] (4.22)

\[ \frac{1}{2} O_2 + \frac{1}{2} N_2 \rightarrow NO \quad K_4 = \frac{y_{10}}{y_4^{1/2} y_3^{1/2}} \] (4.23)

\[ H_2 + \frac{1}{2} O_2 \rightarrow H_2O \quad K_5 = \frac{y_2}{y_4^{1/2} y_6} p^{-1/2} \] (4.24)

\[ CO + \frac{1}{2} O_2 \rightarrow CO_2 \quad K_6 = \frac{y_1}{y_4^{1/2} y_5^{1/2}} p^{-1/2} \] (4.25)

\[ \frac{1}{2} N_2 \rightarrow N \quad K_7 = \frac{y_{11}}{y_3^{1/2}} p^{1/2} \] (4.26)

\[ \frac{1}{2} N_2 + O_2 \rightarrow NO_2 \quad K_8 = \frac{y_{12}}{y_4 y_8} p^{-1/2} \] (4.27)

With:

\[ C_1 = K_1 / p^{1/2} \quad C_2 = K_2 / p^{1/2} \quad C_3 = K_3 \quad C_4 = K_4 \]

\[ C_5 = K_5 / p^{1/2} \quad C_6 = K_6 / p^{1/2} \quad C_7 = K_7 / p^{1/2} \quad C_8 = K_8 / p^{1/2} \]
We obtain from Equation (4.20) to Equation (4.27)

\[ y_7 = C_1 y_6^{1/2} \quad (4.28) \]
\[ y_8 = C_2 y_4^{1/2} \quad (4.29) \]
\[ y_9 = C_3 y_4^{1/2} y_6^{1/2} \quad (4.30) \]
\[ y_{10} = C_4 y_3^{1/2} y_4^{1/2} \quad (4.31) \]
\[ y_2 = C_5 y_4^{1/2} y_6 \quad (4.32) \]
\[ y_1 = C_6 y_4^{1/2} y_5 \quad (4.33) \]
\[ y_{11} = C_7 y_3^{1/2} \quad (4.34) \]
\[ y_{12} = C_8 y_4 y_3^{1/2} \quad (4.35) \]

From Equation (4.13) and Equation (4.14):

\[ 2y_2 + 2y_6 + y_7 + y_9 - \frac{m}{n} (y_1 + y_5) = 0 \quad (4.36) \]

From Equation (4.13) and Equation (4.15):

\[ 2y_1 + y_2 + 2y_4 + y_3 + y_8 + y_9 + y_{10} + 2y_{12} - \frac{0.42}{\varepsilon \Omega n} (y_1 + y_5) = 0 \quad (4.37) \]

From Equation (4.13) and Equation (4.16):

\[ 2y_3 + y_{10} + y_{11} + y_{12} - \frac{1.58}{\varepsilon \Omega n} (y_1 + y_5) = 0 \quad (4.38) \]

From the 12 equations ((4.28 to 4.38) and Equation (4.19)), we can obtain 12 unknown mole fractions (\(y_1\) to \(y_{12}\)). If we rearrange the equations we get 4 equations for 4 unknowns; \(y_3, y_4, y_5, y_6\).

\[ f_1(y_3, y_4, y_5, y_6) = 0 \quad (4.39) \]
\[ f_2(y_3, y_4, y_5, y_6) = 0 \quad (4.40) \]
\[ f_3(y_3, y_4, y_5, y_6) = 0 \quad (4.41) \]
\[ f_4(y_3, y_4, y_5, y_6) = 0 \quad (4.42) \]

We obtain other concentrations; \(y_1, y_2, y_7, y_8, y_9, y_{10}, y_{11}, y_{12}\) from equations (4.20) to (4.27).

The equations (4.39) to (4.42) are non-linear and can be solved iterative techniques like Newton-Raphson iteration. For application the iteration procedure equations (4.39) to (4.42) must be expanded into Taylor series about a known point.
4.5. Combustion Kinetics and Sensitivity Analyses

The chemical reactions occur with a finite rate, in two directions (forward and backward), between initial and final species. Since all chemical reactions occur as a result of the collisions between atoms or molecules in the mixture, many kinds of may be born as a result of the many possible reactions. This means that the final species are not obtained directly from the reactants but through many intermediate reaction steps. The mathematical model of such a multiple component reaction mechanism consist of non-linear, first order, ordinary differential equations (ODE).

Chemical kinetics problem encountered in homogenous, static (for example; system without heat, energy and matter transport) and gas phase systems. Chemical kinetic means here dealing with the time depended concentrations and system properties, such as pressure and temperature due to the finite rate reactions.

Method of sensitivity analyses is to determine what effect the changes (and uncertainties) of input parameters has on solution. Such analyze will provide us a better understanding of the mechanism and the parameters on which we must focus.
CHAPTER 5

ENGINE MODELING OVERVIEW

5.1 General

The modeling of combustion, which goes to the early days of internal combustion engine development in the nineteenth century, is an important problem in most practical combustion systems. This development is the result of research to develop both more realistic approximations for real engine processes, and more accurate methods for calculating the parameters of combustion in an engine. [14] The computer simulations of combustion models of engine processes are now valuable tools for predicting and analyzing engine performance.

The DI engine operates under regimes where compression heating of the charge results in ignition throughout the bulk mixture that is considered highly heterogeneous. To predict the combustion mechanism in the NHDD engine, the approaches for the combustion modeling can be used. These models for combustion can be classified in three main categories: zonal models, one-dimensional models and multi-dimensional models.

As will be discussed in following sections, each method has its own advantages and disadvantages due to the application type. Choosing the modeling type requires knowledge on both physical basics of advanced internal combustion engines and programming techniques necessary for computational job. In general, the more detailed analyses, the larger computational resources. Thus the need for high-technology and expensive computers are proportional to the detail level of the analyses. In Figure 5.1, a brief scheme that classifies engine modeling into branches is given.

Of course, this classification is general. In some cases it can be an advantage to use more than one of these methods as a check tool for the same case. For example a multi-dimensional modeling can be combined with a thermodynamic modeling to ensure the right results.
5.2 Zonal Models

Zonal models are zero-dimensional and generally used in studies of thermodynamic cycle analysis. These models may be divided in three parts: single-zone, two-zone and multi-zone models. In single-zone models, the mixture composition, pressure and the temperature of the combustion chamber are assumed to be uniform. The chemical heat release is either specified (predictive analysis) or calculated from pressure diagrams (heat release analysis). In multi-zone models the mixture in the combustion chamber is divided into two or three regions: unburnt and burnt regions and the quench layer. These models require the specification of the burning velocity and flame front geometry. More detailed information about these modeling will be given in the following sections. By use of these models, it is possible to study the transient behavior of temperature, pressure and concentrations. The combustion chamber regions are assumed as a homogeneous mixture with the same temperature history, mole fraction and mass fraction of species, to compensate the spatial variation of combustion parameters. The pressure is assumed to be the same throughout the combustion chamber at each moment. The advantage of zonal models is that the computation of detailed mechanisms and different phenomena such as flame propagation is possible. [15]

In this approach the combustion in the cylinder is taken globally, cylinder pressure and temperature changes, by the crank angle degree and cylinder volume, are calculated via the thermodynamics first law. The flame propagation ratio is calculated related to the temperature; pressure; mixture concentrations ratios and some other parameters to get the burned fuel amount in unit time from the global combustion model.

In calculations, the effect of kinetic and equilibrium reactions are taken into account chemically.
Single zone models predict only pressure, temperature and fuel concentration in the combustion chamber. These models have many empirical correlations when they are used to predict auto-ignition onset. Single zone models assume that the combustion chamber is a well-stirred reactor with a uniform temperature, pressure and composition. This model is applicable to the most engine applications. Single zone analysis can predict start of combustion with good accuracy if the conditions at the beginning of the compression stroke are known, and therefore can be used to explore ranges of operation for different fuels and conditions. [16] On the other hand, single zone models cannot take into account the effect of temperature or concentration gradients that exist inside the cylinder. The assumption of uniform charge temperature inside the cylinder results in all the mass igniting at the same time when the ignition temperature is exceeded Therefore, a single zone model under predicts the burn duration, and also over predicts both peak cylinder pressure and NO\textsubscript{X}, and it poorly predicts HC and CO emissions, because HC and CO emissions result from cold mass in crevices and boundary layers, which are too cold to burn to completion. A multi-zone model [17] can take better account of temperature gradients inside the cylinder, and therefore can do a much better job at predicting peak cylinder pressure, NO\textsubscript{X} and burn duration, and generates much improved predictions for HC and CO emissions. These benefits are obtained at the cost of a much-increased time for computation compared with a single zone model. Both models are valuable when judiciously applied. Despite its simplicity, it reproduces the overall engine performance trends and gives very good agreement with experimental data, and is therefore often applied in similar simulations.

Two-zone model was used mostly in auto-ignition and knock studies in several studies in the past. A two-zone model was developed for the prediction of the onset of auto-ignition and knock in several engines with different fuels by Karim. [18], [19], [20] The burnt products and unburnt reactants in the cylinder charge assumed as separated zones and generated important performance parameters such as pressure history and power output. A dimensionless knock criterion was developed to provide an indication of the knock intensity. [18] A two-zone model of the whole cycle of an engine for knock prediction is a valuable tool. The effect of methanol admixture on gasoline knocking also was investigated by this approach. It is found that 9% methanol cancels out knocking for the engine.

A simplified two-zone zero-dimensional model for the end gas in an SI engine by applying principles from classical thermodynamics is used by Hajireza. [21] The end-gas
is assumed to be compressed by the progressing flame front and the piston movement in their first model. In the second model, it is assumed that the unburnt gas is affected by both flame front propagation and the piston movement. [22] A zero-dimensional, three-zone model for the investigation of gas behavior in the combustion chamber of SI engines was also developed by them. [23] The first zone is modeled as the zone behind the flame front like the burned gas products, the second zone for unburned gas ahead of the flame front and the third zone for the end gas adjacent to the wall. In the model, flame front velocity, convective heat transfer coefficient and the thickness of the boundary layer is determined by three empirical equations. [15]

5.3 Dimensional Models

Multi-dimensional models contain the real gas-dynamic flow, turbulence, flame propagation and auto-ignition in the combustion chamber and solve these quantities by numerical methods for control volumes. The prediction of the gas inhomogeneity is better with multi-dimensional models. These models need reduced chemical mechanisms and semi-empirical models of multi-dimensional turbulence. Thus, their universality to more complicated flows like one in an engine is doubtful. Furthermore, current computer resources are not enough to combine multi-dimensional models with detailed chemical kinetics calculations in most cases. In this approach the combustion chamber is formed with computational planes and solved for laminar or turbulent flows by the mass, momentum, and energy equations spontaneously with the chemical reactions equations.

In Figure 5.2, the types of computational volumes (meshes) which available in KIVA are given.

One-dimensional models can be used to calculate the inhomogeneity of pressure, temperature, species concentrations and gas flow field. The flame front propagates in one direction normal to the wall surface in the one-dimensional models [24]. A quasi-one-dimensional model for predicting the onset of end-gas auto-ignition is used by Jenkin [25]. It has been coupled with a chemical kinetic model for the low temperature, pre-flame reactions of hydrocarbon fuel and air mixtures. It can predict the onset of auto-ignition without any knowledge of the cylinder pressure history. The model was used also to investigate the effect of the flame propagation rate on the knock onset time.
Figure 5.2. The types of meshes which available in KIVA

Two and three-dimensional models have been developed in last twenty years. A low-temperature kinetics model (Shell auto-ignition model) was integrated by Natarajan and Bracco [26] with a two-dimensional engine model and applied to cool-flames in a stirred reactor, to spatially uniform mixtures in a constant volume bomb and to a rapid compression machine. They found that the auto-ignition chemistry was activated in front of the main flame and auto-ignition occurred in the low-temperature region of the propagating flame.

In recent years, some researchers use both zonal and multi-dimensional models. It is easier to use zonal models for the understanding and the explanation of knock mechanism. However, one- and multi-dimensional models give information about the inhomogeneity of quantities and the properties of the gas in detail. [15]
CHAPTER 6

TURBULENCE

6.1 General

Turbulence modeling is important and challenging task when trying to develop the diesel engines by a sophisticated numerical simulation tool. The spray behavior greatly influences gas motion, gas turbulence and fuel vapor mixing with air in the combustion chamber. Especially in a medium speed diesel engine due to low running speed and small-swirl effect, the spray mainly causes the air motion and turbulence and therefore it plays an important role in the fuel vapor mixing (combustion) and furthers the emissions formation. In a medium speed diesel engine only a small fraction of the fuel vapor burns under the control of chemical kinetics. The combustion occurs mainly due to the turbulent mixing of the fuel vapor [27]. Therefore, in order to get proper behavior of turbulent mixing controlled combustion the proper computation of turbulence quantities such as the turbulent kinetic energy and its dissipation rate is essential.

The fuel vapor mixing with air can be assumed to take place in a process, when the different size of turbulence eddies break-up into smaller ones and finally the smallest scales which cannot anymore break-up will dissipative into heat. Thus there exists a whole spectrum of mixing times. However, multiple time scales are difficult to account for in the case of complex reactions. Normally, only the large-scale eddy break-up times are considered i.e., ratio of the turbulence kinetic energy to its dissipation rate [28].

The standard (STD) k-ε turbulence model is widely used in diesel combustion research. It is a robust 2-equation model and it yields quite reasonable results in the cases of high Reynolds number and high shear stresses flows when its restrictions are taken into consideration [29]. In some cases e.g., flow over the backward facing step or the high velocity spray the STD k-ε model yields too a large turbulent diffusivity (viscosity) and thus an unrealistic flow behavior. Using RNG (ReNormalization Group) methodology of Yakhot and Orzag [30] for the governing equations, the RNG-formulated k-ε model will be produced, in which the model constants have been re-evaluated.
In the latest version of the RNG k-ε model proposed in the literature, an additional term has been added in the epsilon equation [31]. According to Pope [32] the additional term in the epsilon equation is an ad hoc model, not derived from RNG theory. The additional term accounts for the turbulent to mean-strain time scale ratio through modification of the production coefficient. The term changes dynamically with the rate of strain of the turbulence and it is largely responsible for the difference in performance of the standard and RNG models. In consequence of the operation the turbulent diffusivity decreases significantly yielding a more realistic flow behavior in the high shear stresses area. However, some investigators have been found that in the low shear stresses area the diffusivity with the basic form of the RNG model is too large caused unrealistic fuel vapor drifting [33]. In the Han and Reitz study [34] the background of RNG model is described quite well and so does the compressibility influences to the dissipation rate through the velocity dilatation. In small engines the effect of velocity dilatation to the dissipation rate has to be taken into consideration due to relatively high squish flow while in large engines the effect can be omitted.

To understand the case better, it will be useful to underline standard and RNG versions of k-ε model.

6.2 Spectral Description of Turbulence

In general, turbulent motions are variations in fluid properties and velocity due to the decay of large-scale instabilities within the flow. A treatment of turbulence naturally leads to a discussion about statistics of properties of the flow (usually velocity) and their relation to the flow Reynolds number Re.

Properties of turbulent flows:

1- Irregular in both space and time
2- Continuous spectrum in both space and time
3- Large Reynolds number
4- Enhanced dissipation of energy and heat
5- Enhanced mixing and heat transfer
6- Three-dimensional
7- Dominated by vortical motions
8- Intermittent
Turbulent motions often take the form of vortices (or 'eddies'), which in a Eulerian reference frame manifests itself as series of waves. As a result, frequency space is often preferable to describe the physics of turbulent flow. Eulerian reference frame is stationary. Velocities are related to this fixed frame. Lagrangian reference frame moves with a fluid element.

Simplest 'form' of turbulence is isotropic turbulence. That is, the statistics of the flow have no preferred direction. There are many ways to describe turbulence, but the most convenient method is that of an energy spectrum $E(k)$. ($\kappa$: density of kinetic energy for unit wavenumber, sub-factor of $k$)

![Energy spectrum for turbulent flow](image)

**Figure 6.1. Energy spectrum for turbulent flow**

$$k = \frac{1}{2} u't' = \frac{1}{2} R_y(x,0,t) = \int_0^\infty E(\kappa) d\kappa$$  \hspace{1cm} (6.1)

Here:

$$R_y(x,r,t) = u'_i(x,t)u'_j(x+r,t)$$  \hspace{1cm} (6.2)

At this point the main difficulty is to obtain $\kappa$ from the real data. Taylor's approximation implies that turbulence in a time series is reflective of the variability in space ($f \rightarrow k$). That is, fluctuations are not affected by the mean flow, but merely advected.

Kolmogorov (1941) postulated that at length scales much larger than those where viscosity is important and simultaneously much smaller than the source of turbulent energy, the transfer of energy should be "self-similar". As a result, some people have attempted to understand turbulence from analysis of fractals.
Dimensional examination of turbulence quantities can yield interesting results.

\[ [k] = 1/L \]

\[ [\nu] = L2/T \]

\[ [E(k)] = L3/T2 \]

\[ \varepsilon = L2/T3 \]

Knowing that \( E = f(k, \varepsilon, \nu) \) for length scales much smaller than production, we introduce Kolmogorov length and velocity scale:

Velocity scale: \( \theta = (\varepsilon \nu)^{1/4} \) \hspace{1cm} (6.3)

Length scale: \( \eta = \nu^{3/4} / \varepsilon^{1/4} \) \hspace{1cm} (6.4)

Noticing that we have 4 unknown variables and two dimensions (length and time), it is evident that there are two dimensionless groups:

\[ \frac{E(k)}{\theta^2 \eta} \text{ and } k \eta \] \hspace{1cm} (6.5)

Introducing Kolmogorov wavenumber: \( \eta = 1/k_d \) \hspace{1cm} (6.6)

\[ E(k) = \theta^2 \eta \tilde{E}(k \eta) \] \hspace{1cm} (6.7)

In order to remove dependence on \( \nu \) in unknown function, we choose to remove it:

\[ E(k) = \theta^2 \eta(k \eta)^{-5/3} F(k \eta) \] \hspace{1cm} (6.8)

\[ E(k) = \varepsilon^{2/3} k^{-5/3} F(k / k_d) \] \hspace{1cm} (6.9)

\[ F \sim \exp[-\alpha(k / k_d)^{4/3}] \] \hspace{1cm} (6.10)

For wavenumbers \( k \ll k_d \) (i.e., in the ‘inertial sub-range’)

\[ E(k) = C \varepsilon^{2/3} k^{-5/3} \] \hspace{1cm} (6.11)

C is theoretically a universal constant. Its value, however, depends on details not encapsulated in this simplified analysis.
6.3 Modeling Turbulence

6.3.1 Direct Numerical Solution

This kind of turbulence modeling includes solving below equations directly, usually in Fourier space:

\[
\frac{D\bar{u}}{Dt} = \bar{F} - \frac{\nabla p}{\rho} + \nu \nabla^2 \bar{u} \quad (6.12)
\]

\[
\nabla \bar{u} = 0 \quad (6.13)
\]

The problem is that it is necessary to account for energy at all length scales. For instance, the solution of a reasonably small geophysical flow (river plume: \(U = 1\) m/s, \(\Lambda = 1\) km) where \(Re = 10^7\), requires \(10^{20/4} \sim 10^{10}\) solutions of Equations (6.12) and (6.13).

Even teraflop supercomputers (which do not exist at present: teraflop \(\Rightarrow 10^{12}\) floating point operations per second) would require months of computing time to solve a single flow. As a result, DNS is usually useful for flows where \(Re \sim 10^{3}-10^{4}\).

In the case of internal combustion engine modeling complexity increases. Another difficulty not discussed is the assessment of boundary conditions. In natural flows, the boundary conditions are often extremely complex and can present incalculable hazards to numerical estimation.

6.3.2 The Standard \(k-\epsilon\) Model

This model has an approach which uses turbulence theory to describe production and dissipation in terms of other flow parameters. In short, it uses two equations (one for production, another for dissipation) to estimate the eddy viscosity. This model has assumed isotropic turbulence. No natural flow is isotropic, particularly stratified flows. Most of the errors associated with these models are related to this assumption. Eddy viscosity is not a real viscosity, as is a molecular viscosity, but rather an assumption to the Navier-Stokes equations.

It is convenient to derive some basic definitions at this point. Firstly, the mean kinetic energy of the flow is given by:

\[
K = \frac{1}{2}(U^2 + V^2 + W^2) \quad (6.14)
\]

28
And the turbulent kinetic energy is given by:

\[ k = \frac{1}{2}(u'^2 + v'^2 + w'^2) \]  

(6.15)

Thus, total kinetic energy of a turbulent energy:

\[ k(t) = K + k \]  

(6.16)

Deformation of a fluid particle \( e_{ij} \) is:

\[ e_y = E_{yj} + e_{ij}' = \frac{1}{2} \left[ \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right] + \frac{1}{2} \left[ \frac{\partial U_i'}{\partial x_j} + \frac{\partial U_j'}{\partial x_i} \right] \]  

(6.17)

The extended expression for \( K \) is given below.

\[ \frac{\partial (\rho K)}{\partial t} + \nabla (\rho KU) = \nabla (\rho U - 2 \mu U - \rho U' U') - 2 \mu U' E_{yj} + \rho U' U' E_{yj} \]  

(6.18)

And the extended expression for \( k \) is:

\[ \frac{\partial (\rho k)}{\partial t} + \nabla (\rho kU) = \nabla (\rho U - 2 \mu U - \rho U' U') - 2 \mu U' E_{yj} - \rho U' U' E_{yj} \]  

(6.19)

The viscous damping term is given by:

\[ -2 \mu e_{ij}' e_{ij}' = -2 \mu (e_{11}'^2 + e_{22}'^2 + e_{33}'^2 + 2e_{12}'^2 + 2e_{13}'^2 + 2e_{23}'^2) \]  

(6.20)

Damping rate for unit mass is calculated via:

\[ \varepsilon = 2 \mu e_{ij}' e_{ij}' \]  

(6.21)

Turbulent velocity and length scales may be expressed in terms of \( k \) (turbulent kinetic energy) and \( \varepsilon \) (dissipation rate).

Turbulent velocity scale: \( \theta = k^{1/2} \)  

(6.22)

Turbulent length scale: \( \ell = \frac{k^{3/2}}{\varepsilon} \)  

(6.23)

Of course, the model needs initial conditions for the case of interest. Again; the boundary conditions are needed to be specified. For example; for symmetric boundary condition \( \partial k / \partial n = 0 \) and \( \partial \varepsilon / \partial n = 0 \), for free flow \( k=0 \) and \( \varepsilon=0 \), for solid surfaces determination is done with respect to Reynolds number.
In fact, the standard version of k-ε turbulence model is only for incompressible flows. But it was modified for internal combustion engine applications by adding a compressibility term \((\sigma : \nabla u)\) and fuel spray and gas phase interaction term \(\tilde{W}^s\).

The equations that are used in the standard version of k-ε model is given below:

\[
\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho u k) = -\frac{3}{2} \rho k \nabla \cdot u + \sigma : \nabla u + \nabla \left[ \left( \frac{\mu}{Pr_k} \right) \nabla k \right] - \rho \varepsilon + \tilde{W}^s
\]

(6.24)

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho u \varepsilon) = \left( \frac{2}{3} C_{e1} - C_{e3} \right) \rho \varepsilon \nabla \cdot u + \nabla \left[ \left( \frac{\mu}{Pr_\varepsilon} \right) \nabla \varepsilon \right] + \frac{\varepsilon}{k} \left[ C_{e1} \sigma : \nabla u - C_{e2} \rho \varepsilon + C_{e4} \tilde{W}^s \right]
\]

(6.25)

Here \(\sigma : \nabla u = \sigma_{ij} \partial u_i / \partial x_j\) and the constants are given in Table 6.1.

6.3.3 The RNG Version of k-ε Model

The form difference between the RNG and the standard k-ε turbulence models appears in the \(\varepsilon\) equation. The kinetic energy equations are identical. The modified \(\varepsilon\) equation is given as:

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho u \varepsilon) = \left( \frac{2}{3} C_{e1} - C_{e3} \right) \rho \varepsilon \nabla \cdot u + \nabla \left[ \left( \frac{\mu}{Pr_\varepsilon} \right) \nabla \varepsilon \right] + \frac{\varepsilon}{k} \left[ (C_{e1} - C_{e2}) \sigma : \nabla u - C_{e2} \rho \varepsilon + C_{e4} \tilde{W}^s \right]
\]

(6.26)

Here:

\[
C_{e1} = \frac{\eta (1 - \eta / \eta_0)}{1 + \beta \eta^3}, \quad \eta = \frac{S_m k}{\varepsilon}, \quad S_m = (2S_y S_y)^{1/2}
\]

(6.27)

\[
S_y = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad \eta_0 = 4.38, \quad \beta = 0.012
\]

(6.28)

\[
C_{e2} = \frac{-1 + 2C_{e1} - 3m(n-1) + (-1)\delta \sqrt{6C_{e4} C_y \eta}}{3}
\]

(6.29)

\[
m = 0.5, \quad n = 1.3 - 1.4, \quad \delta = \begin{cases} 1 & \nabla u \leq 0 \\ 0 & \nabla u > 0 \end{cases}
\]

30
Table 6.1. The constants for standard and RNG k-ε models

<table>
<thead>
<tr>
<th>Model</th>
<th>$C_\mu$</th>
<th>$C_{s1}$</th>
<th>$C_{s2}$</th>
<th>$C_{s3}$</th>
<th>$Pr_i$</th>
<th>$Pr_e$</th>
<th>$C_\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
<td>-1.0</td>
<td>1.0</td>
<td>1.3</td>
<td>1.5</td>
</tr>
<tr>
<td>RNG</td>
<td>0.0845</td>
<td>1.42</td>
<td>1.68</td>
<td>Eq. (6.29)</td>
<td>0.7194</td>
<td>0.7194</td>
<td>1.5</td>
</tr>
</tbody>
</table>

6.4 Turbulent Combustion

In case of combustion together with turbulence, there are a lot of unknown parameters exclusive of Reynolds stresses. Although these parameters occurring from reactions are molecular in nature; they are largely affected by eddy interactions of different size. To overcome these difficulties, we use some combustion models. Before going into further detail, some basic definitions are given in the following section.

6.4.1 Basic Definitions for Turbulent Combustion

The term “laminar flame speed” refers to dependence only on thermal and chemical properties of the mixture. When it becomes necessary to analyze flow conditions, it is convenient to use “turbulent flame speed” instead of “laminar flame speed”.

The flame surface is assumed to be represented by the time mean value as instantaneous position of the high temperature zone fluctuations. The flame velocity is determined from reactant flow rates measured.

Detailed solution for a flame problem requires usage of much smaller grid sizes than the ones that our current computers can handle. Thus, the parameters of the combustion zone should be evaluated in terms of sub-grid parameters. Depending on the grid size, some parameters like component concentrations and fluid velocities can be determined via grid scale data. However, the “chemical source term”, which will be covered later in detail, is function combustion zone parameters. Therefore it is necessary to find out the relation between the scale parameters and the sub-scale parameters.

31
6.4.2 Turbulent Combustion Models

The Eddy Break-Up model [35] has successfully modeled turbulent combustion. Due to its simplicity and the lack of any other developed models, it is used in most CFD codes. Actually there are other models available such as Flamelet Model, PDF (Probability Density Function), Lagrangian Approach and some modified versions of the Eddy Break-Up model. When it is necessary to use detailed chemistry mechanisms, only the Lagrangian approach is convenient. Flamelet model assumes that the chemical time scale is much smaller than turbulent time scale. Thus, turbulence and chemical reactions are separated via laminar flow approach; solution is tried to be reached in this manner. This approach is not applicable to diesel fuel spray.

Partially Stirred Reactor is an extension of the eddy-break-up model. Application to diesel fuel spray and detailed chemistry mechanisms is suitable.

6.4.3 Partially Stirred Reactor Model

In this model the cell is divided into two zones. All the reactions occur in one of these zones. There is no reaction in the other zone. Due to the mass transfer, mixture ratios are variable in the cell as a whole. The reactive zone is assumed to be well-stirred, thus the reactive zone is homogenous. This assumption avoids a fluctuation in the calculation of chemical source term.

Division of the cell of interest causes the problem of calculation of ratios. Furthermore, the control of mixture formation should be defined. These problems can be overcome by relating the scale data and the sub-scale data.

Reaction mass ratios are defined in the following manner in the beginning and end of a time step. \((c_0 \rightarrow c_1)\)

![Diagram](image)

**Figure 6.2.** Schematic illustration of the PaSR model

32
First, the model uses three different molar concentrations in a time step.

\( c_0 \): initial concentration (at entrance)

\( c \): unknown concentration at the reactive zone (unknown cell components ratio at sub-grid scale)

\( c_1 \): time averaged value of reactor exit concentration

Reactor exit concentration can be calculated via conservation of mass in the following manner.

\[
\begin{align*}
  c_1 &= \kappa^* c + (1 - \kappa^*) c_0 \\
  \kappa^* &: \text{Reacting mixture mass ratio}
\end{align*}
\]  

(6.30)

Equation (6.30) calculates \( c_1 \) by interpolation between \( c_0 \) and \( c \). By examining Figure 6.3 the following results may be obtained.

![Diagram showing Concentration over time](image)

**Figure 6.3. Reaction / mixture step calculation**

All the process is divided into two sub-models, denoted by I and II.

I: initial concentration at the reaction zone. \((c_0 \rightarrow c)\)

II: reacted mixture \((c)\) and unreacted mixture \((c_0)\) creates \( c_1 \) after turbulent mixing.

Since \( c_1 \) is the initial value for the next step, integral time step should be the one between \( c_0 \) and \( c_1 \). \( c \) and \( c_0 \) is mixed in a turbulent manner; so the time step between \( c \)
and $c_1$ should be turbulent characteristic time step ($\tau_{mix}$). Thus total reaction time step should be ($\tau + \tau_{mix}$).

If it is assumed that the slope in Figure 6.3 is equal to the reaction rate at $c$, the following equations can be obtained.

$$\frac{c_1 - c_0}{\tau} = f_m(c)$$  \hspace{1cm} (6.31)

$$\frac{c - c_1}{\tau_{mix}} = f_m(c)$$  \hspace{1cm} (6.32)

$$\frac{c_1 - c_0}{\tau} = \frac{c - c_1}{\tau_{mix}}$$  \hspace{1cm} (6.33)

Using equations (6.31) and (6.32) and (6.30):

$$c_1 = \kappa \cdot c + (1 - \kappa)C_0, \quad \kappa = \frac{\tau}{\tau + \tau_{mix}}$$  \hspace{1cm} (6.34)

is obtained.

In this case, providing the condition that the integral time step is larger than turbulent characteristic time step sufficiently, $\kappa \approx 1$ and gained properties at the reactor exit are only the ones coming out of the reactor. After $\kappa$ is obtained, we need to find the term $c$ which we will use in calculation of $c_1$.

The chemical source term in the continuity equation is:

$$f_m(c) = \sum_{r=1}^{N_r} \left( \theta_m^e - \theta_m^r \right) \left( k_f' \prod_{s=1}^{N_s} c_s^{e_s} - k_b' \prod_{s=1}^{N_s} c_s^{r_s} \right)$$

$$= M \sum_{r=1}^{N_r} \left( \theta_m^e k_f' \prod_{s=1}^{N_s} c_s^{e_s} + \theta_m^r k_b' \prod_{s=1}^{N_s} c_s^{r_s} \right) - M \sum_{r=1}^{N_r} \left( \theta_m^e k_b' \prod_{s=1}^{N_s} c_s^{e_s} + \theta_m^r k_f' \prod_{s=1}^{N_s} c_s^{r_s} \right)$$  \hspace{1cm} (6.35)

$$= \sum_{r=1}^{N_r} (\theta_1^r - \theta_2^r) = \theta_1^r - \theta_2^r$$

Using Taylor expansion and arranging:

$$f_m(c) = f_m(c_1) + \frac{\partial f_m}{\partial c}(c - c_1) + \frac{1}{2} \frac{\partial^2 f_m}{\partial c^2}(c - c_1)^2$$  \hspace{1cm} (6.36)

Assuming $\partial^2 f_m / \partial c^2 = 0$ and the dominant term is $\partial f_m / \partial c$, chemical time is calculated by the following formula:
\[
\frac{1}{\tau_c} = -\frac{\partial f_m}{\partial c_r}
\]  
(6.37)

Thus, Equation (6.36) turns into:

\[
f_m(c) = f_m(c_1) - \frac{c - c_1}{\tau_c}
\]  
(6.38)

Using Equations (6.31) and (6.34):

\[
\frac{c_1 - c_0}{\tau} = f_m(c) = f_m(c_1) - \frac{1}{\tau_c}\left[\frac{c_1}{\kappa} - \frac{1 - \kappa}{\kappa} c_0 \right] - c_1
\]  
(6.39)

\[
\frac{c_1 - c_0}{\tau} = f_m(c) = f_m(c_1) - \frac{1}{\tau_c\kappa} \left( c_1 - \kappa c_1 - (1 - \kappa c_0) \right) = f_m(c_1) - \frac{1 - \kappa}{\tau_c\kappa} (c_1 - c_0)
\]  
(6.40)

\[
\left(\frac{1 + \frac{1 - \kappa}{\tau C\kappa}}{\tau_c\kappa} \right) (c_1 - c_0) = f_m(c_1)
\]  
(6.41)

is obtained. Application of Equation (6.34) yields:

\[
\left(\frac{1 + \frac{1 - \kappa}{\tau C\kappa}}{\tau_c\kappa} \right) (c_1 - c_0) = \frac{1 - \kappa}{\tau_c\kappa} \frac{c_1 - c_0}{\tau_c + \tau_{mix}} = f_m(c_1)
\]  
(6.42)

By defining:

\[
\frac{\tau_c}{\tau_c + \tau_{mix}} = \kappa
\]  
(6.43)

\[
\frac{c_1 - c_0}{\tau} = f_m(c_1)
\]  
(6.44)

Finally Equation (6.45) is reached.

\[
f_m(c) = \kappa f_m(c_1)
\]  
(6.45)

This expression is the chemistry source term relation at sub-grid scale.

In a turbulent medium, usage of a single scale for both small and large eddies is a great simplification. For turbulence time step, there are three choices available according to [36]. With respect to Kolmogorov:

\[
\tau_s \sim (v/\epsilon)^{1/2}
\]  
(6.46)
Taylor time scale:

\[ \tau_i \sim k / \varepsilon \quad (6.47) \]

Averaging Kolmogorov and Taylor scales:

\[ \tau_{kc} \sim \sqrt{\tau_i \tau_k} \quad (6.48) \]

It is stated that the best result is obtained by using Taylor time scale.
CHAPTER 7

MATHEMATICAL BASICS

7.1 General

Today's most common engineering analyses are done using a method which is called CFD (Computational Fluid Dynamics). The strategy of CFD is to replace the continuous problem domain with a discrete domain using a grid. In the continuous domain, each variable is defined at every point in the domain. For instance, the pressure \( p \) in a continuous 1-D domain shown in the figure below would be given as:

\[
p = p(x), \ 0 < x < 1
\]  

(7.1)

In the discrete domain, each flow variable is defined only at the grid points. So, in the discrete domain shown below, the pressure would be defined only at the \( N \) grid points.

\[
p_i = p(x_i); \ i = 1, 2, \ldots, N
\]  

(7.2)

**Figure 7.1. Discretization of a domain**

In a CFD solution, one would directly solve for the relevant flow variables only at the grid points. The values at other locations are determined by interpolating the values at the grid points.

The governing partial differential equations and boundary conditions are defined in terms of the continuous variables such as \( p \) and \( \vec{V} \). One can approximate these, in the discrete domain in terms of the discrete variables \( p_i, \vec{V}_i \) etc. The discrete system is a large set of coupled, algebraic equations in the discrete variables.
Setting up the discrete system and solving it (which is a matrix inversion problem) involves a very large number of repetitive calculations and is done by the digital computer. This idea can be extended to any general problem domain. Below some headlines of CFD are listed.

- Basic Equations
  
  a) Conservation of Mass
  
  b) Conservation of Energy
  
  c) Conservation of Momentum

- Discretization

7.2 Basic Equations

These equations may be different upon the area of interest, but all kinds of thermo-chemical-fluid problems can be solved using below equations. Conservation equations dictate that a quantity (mass, energy, and momentum) cannot be created or destroyed, but is instead moved from one point to another.

7.2.1 Conservation of mass

As an example, one can demonstrate the conservation of mass with the exhaust products inside an engine cylinder. Once the exhaust valve opens, exhaust products flow through the valve into the exhaust manifold. The conservation of mass simply says that if certain amount of exhaust products exits the cylinder, then the mass of exhaust products inside the cylinder must decrease by exactly that certain amount. Equation (7.3) is a typical form of this equation.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0
\]  

(7.3)

While this may seem trivial, it can become increasingly more complex. A slightly more complicated demonstration is when the intake and exhaust valves of an engine cylinder are open at the same time. Air is entering the cylinder and exhaust products are leaving the cylinder. The mass of air and exhaust inside the cylinder continually changes so that mass is always conserved.
7.2.2 Conservation of energy

The conservation of energy equation is used to calculate the temperature field. The first term represents how the energy within the engine cylinder changes with time. The rest of the terms on the left side describe how energy flows through the engine with the fluid. For example, the air flowing through a compressor wheel carries an amount of energy with it.

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial (\rho u e)}{\partial x} + \frac{\partial (\rho v e)}{\partial y} + \frac{\partial (\rho w e)}{\partial z} =$$

$$\frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) - \nabla \cdot \mathbf{S}_h + S_e$$

(7.4)

The right side of the equation describes how energy is conducted through the engine. The final two terms represent radiant energy and then any other sources or sinks of energy within the engine. At any point within the engine, this equation must balance. An important point is that to solve for the temperature field, one must know the velocity field in order.

7.2.3 Conservation of momentum (x-Direction)

The momentum conservation equation is used to calculate the pressure and velocity fields within an engine. The mass conservation equation is integral to solving the momentum conservation equations.

As with the energy and mass conservation equations, the momentum conservation equation ensures that momentum is not created or destroyed. Again, the first term represents the time rate of change of momentum within the engine, and the remaining terms on the left side represent the momentum carried by the fluid through the engine.

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho uu)}{\partial x} + \frac{\partial (\rho uv)}{\partial y} + \frac{\partial (\rho uw)}{\partial z} = -\frac{\partial p}{\partial x}$$

$$\frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} \right) + S_u$$

(7.5)

The right side of the equation describes how momentum is driven by the pressure field, how momentum is transferred through viscous effects, and then any other sources or sinks of momentum within the engine.
The main difference between the momentum conservation equation and the others is that the velocity is vector and actually has three components. Because of this, there are actually three momentum conservation equations. The three are usually referred to as the \( x \)-, \( y \)-, and \( z \)-momentum conservation equations.

### 7.3 Discretization

Discretization is the process where the domain of interest is divided into small volumes. The primary goal is to separate the domain into enough volumes so that the solution is independent of the size and quantity of the volumes.

This is a fairly complex process, and oftentimes the area where analysts make a mistake. If not done properly, then one can get almost any solution desired. We will discuss this topic later in details.

In order to make the discretization phenomenon clear, we will consider two methods here:

- Discretization Using the Finite-Difference Method
- Discretization Using the Finite-Volume Method

#### 7.3.1 Discretization Using the Finite-Difference Method

To keep the details simple, an illustration of fundamental ideas underlying CFD is done by applying them to the following simple 1-D equation:

\[
\frac{du}{dx} + u \cdot u = 0; \quad 0 \leq x \leq 1; \quad u(0) = 1
\]  \hspace{1cm} (7.6)

![Figure 7.2. Illustration of discretization via FDM](image)

We'll first consider the case where \( m = 1 \) when the equation is linear. The situation \( m=2 \), when the equation is non-linear, will be discussed later in details. We'll derive a discrete representation of the above equation with \( m = 1 \) on the above grid:

\[
\left( \frac{du}{dx} \right)_i + u_i = 0
\]  \hspace{1cm} (7.7)
This grid has four equally-spaced grid points with $\Delta x$ being the spacing between successive points. Since the governing equation is valid at any grid point, we have where the subscript $i$ represents the value at grid point $x_i$. In order to get an expression for $(du/dx)_i$ in terms of $u$ at the grid points, we expand $u_{i-1}$ in a Taylor's series:

$$u_{i-1} = u_i - \Delta x \frac{du}{dx} \bigg|_i + O(\Delta x^2)$$

(7.8)

Rearranging the equation above gives:

$$\left(\frac{du}{dx}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)$$

(7.9)

The error in $(du/dx)_i$ due to the neglected terms in the Taylor's series is called the truncation error. Since the truncation error above is $O(\Delta x)$, this discrete representation is termed first-order accurate. Using the rearranged equation in the original equation and excluding higher-order terms in the Taylor's series, we get the following discrete equation:

$$\frac{u_i - u_{i-1}}{\Delta x} + u_i = 0$$

(7.10)

An important point that must be noted here is that we have gone from a differential equation to an algebraic equation.

This method of deriving the discrete equation using Taylor's series expansions is called the finite-difference method. However, most commercial CFD codes use the finite-volume or finite-element methods which are better suited for modeling flow past complex geometries. For example, the FLUENT code uses the finite-volume method whereas ANSYS uses the finite-element method.

### 7.3.2 Discretization Using the Finite-Volume Method

In the finite-volume method, a quadrilateral is commonly referred to as a “cell” and a grid point as a “node”. In 2-D, one could also have triangular cells. In 3-D, cells are usually hexahedrals, tetrahedrals, or prisms. In the finite-volume approach, the integral form of the conservation equations are applied to the control volume defined by a cell to get the discrete equations for the cell. For example, the integral form of the continuity equation was given earlier. For steady, incompressible flow, this equation reduces to:
\int_{\mathcal{S}} \vec{V} \cdot \hat{n} dS = 0 \tag{7.11}

The integration is over the surface \( \mathcal{S} \) of the control volume and \( \hat{n} \) is the outward normal at the surface. Physically, this equation means that the net volume flow into the control volume is zero.

Consider the rectangular cell shown in Figure 7.3.

The velocity at face \( i \) is taken to be \( \vec{V}_i = u_i \hat{i} + v_i \hat{j} \). Applying the mass conservation equation to the control volume defined by the cell gives:

\[-u_1 \Delta y - v_2 \Delta x + u_3 \Delta y + v_4 \Delta x = 0 \tag{7.12}\]

![Figure 7.3. Rectangular cell](image)

This is the discrete form of the continuity equation for the cell. It is equivalent to summing up the net mass flow into the control volume and setting it to zero. So it ensures that the net mass flow into the cell is zero i.e. that mass is conserved for the cell. Usually the values at the cell centers are stored. The face values \( u_1, v_2, \) etc. are obtained by suitably interpolating the cell-center values for adjacent cells.

Similarly, one can obtain discrete equations for the conservation of momentum and energy for the cell. One can readily extend these ideas to any general cell shape in 2-D or 3-D and any conservation equation.

At this point of analyses, it is necessary to assemble the discrete system and apply the boundary conditions. In the following part this stage is discussed.

### 7.4 Assembly of Discrete System and Application of Boundary Conditions

Recall that, the discrete equation that we obtained using the finite-difference method was Equation (7.10). Rearranging, we get:
\[-u_{i-1} + (1 + \Delta x)u_i = 0 \quad (7.13)\]

Applying this equation to the 1-D grid shown earlier at grid points \( i = 2; 3; 4 \) gives

\[-u_1 + (1 + \Delta x)u_2 = 0 \quad (i = 2)\]
\[-u_2 + (1 + \Delta x)u_3 = 0 \quad (i = 3)\]
\[-u_3 + (1 + \Delta x)u_4 = 0 \quad (i = 4)\]  \hspace{1cm} (7.14)

Here it must be noted that; this equation cannot be applied to \( i = 1 \) (the left boundary point) because \( u_{i-1} \) is not defined. Instead, we use the boundary condition to get \( u_1 = 1 \).

The above equations form a system of four simultaneous algebraic equations in terms of unknowns; \( u_1, u_2, u_3 \) and \( u_4 \). It’s convenient to write this system in matrix form:

\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
-1 & 1 + \Delta x & 0 & 0 \\
0 & -1 & 1 + \Delta x & 0 \\
0 & 0 & -1 & 1 + \Delta x
\end{bmatrix}
\begin{bmatrix}
u_1 \\
u_2 \\
u_3 \\
u_4
\end{bmatrix}
= \begin{bmatrix}1 \\
0 \\
0 \\
0
\end{bmatrix}
\]  \hspace{1cm} (7.15)

In a general situation, one would apply the discrete equations to the grid points (or cells in the finite-volume method) in the interior of the domain. For grid points (or cells) at or near the boundary, one would apply a combination of the discrete equations and boundary conditions. In the end, one would obtain a system of simultaneous algebraic equations with the number of equations being equal to the number of independent discrete variables. The process is essentially the same as above with the details being much more complex.

### 7.5 Solution of Discrete System

The discrete system that we got can be easily inverted to obtain the unknowns at the grid points. Solving for \( u_1, u_2, u_3 \) and \( u_4 \) in turn and using \( \Delta x = 1/3 \), we get:

\[u_1 = 1, \; u_2 = 3/4, \; u_3 = 9/16, \; u_4 = 27/64\]  \hspace{1cm} (7.16)

The exact solution for the 1-D example is easily calculated to be:

\[u_{\text{exact}} = \exp(-x)\]  \hspace{1cm} (7.17)

In Figure 7.4, the comparison of the discrete solution obtained on the four-point grid with the exact solution is shown. The error is largest at the right boundary where it is equal to 14.7%.
In a practical CFD application, one would have thousands to millions of unknowns in the discrete system and if one uses, say, a Gaussian elimination procedure naively to invert the matrix, it would be taking the computer forever to perform the calculation.

![Graph showing numerical and exact solutions](image)

**Figure 7.4 Comparison of numerical and exact solutions**

So a lot of work goes into optimizing the matrix inversion in order to minimize the CPU time and memory required. The matrix to be inverted is sparse i.e. most of the entries in it are zeros since the discrete equation at a grid point or cell will contain only quantities from the neighboring points or cells. A CFD code would store only the non-zero values to minimize memory usage. It would also generally use an iterative procedure to invert the matrix; the longer one iterates the closer one gets to the true solution for the matrix inversion.

### 7.6 Grid Convergence

While developing the finite-difference approximation for the 1-D example, we saw that the truncation error in our discrete system is $O(\Delta x)$. So one expects that as the number of grid points is increased and $\Delta x$ is reduced, the error in the numerical solution would decrease and the agreement between the numerical and exact solutions would get better.

Let's consider the effect of increasing the number of grid points $N$ on the numerical solution of the 1-D problem. We'll consider $N = 8$ and $N = 16$ in addition to the $N = 4$ case solved previously. We can easily repeat the assembly and solution steps...
for the discrete system on each of these additional grids. Figure 7.5 compares the results obtained on the three grids with the exact solution. As expected, the numerical error decreases as the number of grid points is increased.

![Graph showing comparison of numerical solutions with exact solution.](image)

**Figure 7.5.** Comparison of three numerical solutions and the exact solution

When the numerical solutions obtained on different grids agree to within a level of tolerance specified by the user, they are referred to as "grid converged" solutions. The concept of grid convergence applies to the finite-volume approach also where the numerical solution, if correct, becomes independent of the grid as the cell size is reduced. It is very important that you investigate the effect of grid resolution on the solution in every CFD problem you solve. A CFD solution cannot be trusted unless you have convinced yourself that the solution is grid converged to an acceptance level of tolerance (which would be problem dependent).

### 7.7 Dealing with Non-linearity

The momentum conservation equation for a fluid is non-linear due to the convection term $(\vec{V} \cdot \nabla) \vec{V}$. Phenomena such as turbulence and chemical reaction introduce additional non-linearity. The highly non-linear nature of the governing equations for a fluid makes it challenging to obtain accurate numerical solutions for complex flows of practical interest.
In previous parts, \( m = 2 \) situation was said to be discussed in later. The effect of non-linearity can be expressed by setting \( m=2 \) in the previous 1-D example.

\[
\frac{du}{dx} + u^2 = 0; \quad 0 \leq x \leq 1; \quad u(0) = 1
\]  

(7.18)

A first-order finite-difference approximation to this equation, analogous to that in Equation (7.10) for \( m = 1 \), is

\[
\frac{u_i - u_{i-1}}{\Delta x} + u_i^2 = 0
\]

(7.19)

This is a non-linear algebraic equation with the \( u_i^2 \) term being the source of the non-linearity.

The strategy that is adopted to deal with non-linearity is to linearize the equations about a guess value of the solution and to iterate until the guess agrees with the solution to a specified tolerance level. Let \( u_{g_i} \) be the guess for \( u_i \). Define:

\[
\Delta u_i = u_i - u_{g_i}
\]

(7.20)

Rearranging and squaring this equation gives:

\[
u_i^2 = u_{g_i}^2 + 2u_{g_i}\Delta u_i + (\Delta u_i)^2
\]

(7.21)

Assuming that \( \Delta u_i \ll u_{g_i} \), we can neglect the \( \Delta u_i^2 \) term to get

\[
u_i^2 \approx u_{g_i}^2 + 2u_{g_i}\Delta u_i = u_{g_i}^2 + 2u_{g_i}(u_i - u_{g_i})
\]

(7.22)

Thus;

\[
u_i^2 \approx 2u_{g_i}u_i - u_{g_i}^2
\]

(7.23)

The finite-difference approximation after linearization becomes:

\[
\frac{u_i - u_{i-1}}{\Delta x} + 2u_{g_i}u_i - u_{g_i}^2 = 0
\]

(7.24)

Since the error due to linearization is \( O(\Delta u^2) \), it tends to zero as \( u \rightarrow u_g \).

In order to calculate the finite-difference approximation, we need to guess values \( u_g \) at the grid points. We start with an initial guess value in the first iteration. For each subsequent iteration, the \( u \) value obtained in the previous iteration is used as the guess value.
Iteration 1: \( u_g^{(1)} \) (Initial guess)

Iteration 2: \( u_g^{(2)} = u_g^{(1)} \)

Iteration \( l \): \( u_g^{(l)} = u_g^{(l-1)} \)

The superscript indicates the iteration level. We continue the iterations until they converge. We'll defer the discussion on how to evaluate convergence until a little later.

This is essentially the process used in CFD codes to linearize the non-linear terms in the conservation equations, with the details varying depending on the code. The important points to remember are that the linearization is performed about a guess and that it is necessary to iterate through successive approximations until the iterations converge.

### 7.8 Direct and Iterative Solvers

We saw that we need to perform iterations to deal with the non-linear terms in the governing equations. We next discuss another factor that makes it necessary to carry out iterations in practical CFD problems. It can be verified that the discrete equation system resulting from the finite-difference approximation in Equation (7.24) on our four-point grid is:

\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
-1 & 1 + 2\Delta x u_{g_i} & 0 & 0 \\
0 & -1 & 1 + 2\Delta x u_{g_i} & 0 \\
0 & 0 & -1 & 1 + 2\Delta x u_{g_i}
\end{bmatrix}
\begin{bmatrix}
u_1 \\
u_2 \\
u_3 \\
u_4
\end{bmatrix}
= 
\begin{bmatrix}
1 \\
\Delta x u_{g_i}^2 \\
\Delta x u_{g_i}^2 \\
\Delta x u_{g_i}^2
\end{bmatrix}
\]

(7.25)

In a practical problem, one would usually have millions of grid points or cells so that each dimension of the above matrix would be of the order of a million (with most of the elements being zeros). Inverting such a matrix directly would take a prohibitively large amount of memory. So instead, the matrix is inverted using an iterative scheme as discussed below. Rearrange the finite-difference approximation in Equation (7.24) at grid point \( i \), so that \( u_i \) is expressed in terms of the values at the neighboring grid points and the guess values:

\[
u_i = \frac{u_{i-1} + \Delta x u_{g_i}^2}{1 + 2\Delta x u_{g_i}}
\]

(7.26)
If a neighboring value at the current iteration level is not available, the guess value is used for it. Let's say that we sweep from right to left on our grid i.e. we update $u_4$, then $u_3$ and finally $u_2$ in each iteration. In the $m^{th}$ iteration, $u_{i-1}^{(j)}$ is not available while updating $u_i^{(j)}$ and so we use the guess value $u_{i-1}^{(j)}$ for it instead:

$$u_i^{(j)} = \frac{u_{i-1}^{(j)} + \Delta x u_{i-1}^{(j)2}}{1 + 2\Delta x u_{i-1}^{(j)}}$$

(7.27)

Since we are using the guess values at neighboring points, we are effectively obtaining only an approximate solution for the matrix inversion in Equation (7.25) during each iteration but in the process have greatly reduced the memory required for the inversion. This tradeoff is good strategy since it doesn't make sense to expend a great deal of resources to do an exact matrix inversion when the matrix elements depend on guess values which are continuously being refined. In an act of cleverness, we have combined the iteration to handle non-linear terms with the iteration for matrix inversion into a single iteration process. Most importantly, as the iterations converge and $u_g \to u$, the approximate solution for the matrix inversion tends towards the exact solution for the inversion since the error introduced by using $u_g$ instead of $u$ in Equation (7.27) also tends to zero.

Thus, iteration serves two purposes:

1. It allows for efficient matrix inversion with greatly reduced memory requirements.
2. It is necessary to solve non-linear equations.

In steady problems, a common and effective strategy used in CFD codes is to solve the unsteady form of the governing equations and "march" the solution in time until the solution converges to a steady value. In this case, each time step is effectively iteration, with the guess value at any time level being given by the solution at the previous time level.

7.9 Iterative Convergence

Recall that as $u_g \to u_3$, the linearization and matrix inversion errors tend to zero. So we continue the iteration process until some selected measure of the difference between $u_g$ and $u$, referred to as the residual, is "small enough".
We could, for instance, define the residual $R$ as the RMS value of the difference between $u$ and $u_g$ on the grid.

$$R = \sqrt{\frac{\sum_{i=1}^{N} (u_i - u_{g_i})^2}{N}}$$  \hspace{1cm} (7.28)

It's useful to scale this residual with the average value of $u$ in the domain. An unscaled residual of, say, 0.01 would be relatively small if the average value of $u$ in the domain is 5000 but would be relatively large if the average value is 0.1. Scaling ensures that the residual is a relative rather than an absolute measure. Scaling the above residual by dividing by the average value of $u$ gives:

$$R = \sqrt{\frac{\sum_{i=1}^{N} (u_i - u_{g_i})^2}{N \sum_{i=1}^{N} u_i}} = \sqrt{\frac{N \sum_{i=1}^{N} (u_i - u_{g_i})^2}{\sum_{i=1}^{N} u_i}}$$  \hspace{1cm} (7.29)

For the non-linear 1-D example, we'll take the initial guess at all grid points to be equal to the value at the left boundary i.e. $u_{g_1}^{(1)} = 1$. In each iteration, we update $u_g$, sweep from right to left on the grid updating, in turn, $u_4$, $u_3$ and $u_2$ using Equation (7.27) and calculate the residual using Equation (7.29). We'll terminate the iterations when the residual falls below $10^{-9}$ (which is referred to as the convergence criterion). This calculation can be implemented to a mathematical tool like MATLAB in a few minutes. The variation of the residual with iterations obtained from MATLAB is shown in Figure 7.6. Note that logarithmic scale is used for the ordinate. The iterative process converges to a level smaller than $10^{-9}$ in just 6 iterations. In more complex problems, a lot more iterations would be necessary for achieving convergence.

The solution after 2, 4 and 6 iterations and the exact solution are shown in Figure 7.7. It can easily be verified that the exact solution is given by:

$$u_{exact} = \frac{1}{x + 1}$$  \hspace{1cm} (7.30)

The solutions for iterations 4 and 6 are indistinguishable on the graph. This is another indication that the solution has converged.
The iterative convergence error, which is order of $10^{-9}$, is swamped out by the truncation error of order $10^{-1}$. So driving the residual down to $10^{-9}$ when the truncation error is of order $10^{-1}$ is a waste of computing resources. In a good calculation, both errors would be of comparable level and less than a tolerance level chosen by the user. The agreement between the numerical and exact solutions should get much better on refining the grid as was the case for $m = 1$.

Different codes use slightly different definitions for the residual. Reading the documentation to understand how the residual is calculated is essential. The convergence criterion necessary for each conservation equation is problem and code
dependent. It's a good idea to start with the default values in the code. One may then have to tweak these values.

7.10 Numerical Stability

In our previous 1-D example, the iterations converged very rapidly with the residual falling below the convergence criterion of $10^{-9}$ in just 6 iterations. In more complex problems, the iterations converge more slowly and in some instances, may even diverge. One would like to know a priori the conditions under which a given numerical scheme converges. This is determined by performing a stability analysis of the numerical scheme. A numerical method is referred to as being stable when the iterative process converges and as being unstable when it diverges. It is not possible to carry out an exact stability analysis for the Euler or Navier-Stokes equations. But a stability analysis of simpler, model equations provides useful insight and approximate conditions for stability. As mentioned earlier, a common strategy used in CFD codes for steady problems is to solve the unsteady equations and march in time until the solution converges to a steady state. A stability analysis is usually performed in the context of time-marching.

While using time-marching to a steady state, we are only interested in accurately obtaining the asymptotic behavior at large times. So we would like to take as large a time-step $\Delta t$ as possible to reach the steady state in the least number of time-steps. There is usually a maximum allowable time-step $\Delta t_{\text{max}}$ beyond which the numerical scheme is unstable. If $\Delta t > \Delta t_{\text{max}}$, the numerical errors will grow exponentially in time causing the solution to diverge from the steady-state result. The value of $\Delta t_{\text{max}}$ depends on the numerical discretization scheme used. There are two classes of numerical schemes, explicit and implicit (which were introduced in Chapter 3), with very different stability characteristics which we'll briefly discuss next.

The difference between explicit and implicit schemes can be most easily illustrated by applying them to the wave equation;

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$  \hspace{1cm} (7.31)

where $c$ is the wave-speed. One possible way to discretize this equation at grid point $i$ and time-level $n$ is
\[ \frac{u_i^n - u_i^{n-1}}{\Delta t} + c \frac{u_i^{n-1} - u_{i-1}^{n-1}}{\Delta x} = O(\Delta t, \Delta x) \]  \tag{7.31}

The crucial thing to note here is that the spatial derivative is evaluated at the \((n-1)\) time-level. Solving for \(u_i^n\) gives:

\[ u_i^n = \left[ 1 - \left( \frac{c\Delta t}{\Delta x} \right) \right] u_i^{n-1} + \left( \frac{c\Delta t}{\Delta x} \right) u_{i-1}^{n-1} \]  \tag{7.32}

This is an explicit expression i.e. the value of \(u_i^n\) at any grid point can be calculated directly from this expression without the need for any matrix inversion. The scheme in Equation (7.31) is known as an explicit scheme. Since \(u_i^n\) at each grid point can be updated independently, these schemes are easy to implement on the computer. On the downside, it turns out that this scheme is stable only when the condition in Equation (7.33) is satisfied.

\[ C = \frac{c\Delta t}{\Delta x} \leq 1 \]  \tag{7.33}

In Equation (7.33), \(C\) is called the Courant number. This condition is referred to as the Courant-Friedrichs-Lewy or CFL condition. While a detailed derivation of the CFL condition through stability analysis is outside the scope of the current discussion, it can seen that the coefficient of \(u_i^{n-1}\) in Equation (7.32) changes sign depending on whether \(C > 1\) or \(C < 1\) leading to very different behavior in the two cases. The CFL condition places a rather severe limitation on \(\Delta t\) max.

In an implicit scheme, the spatial derivative term is evaluated at the \(n\) time-level:

\[ \frac{u_i^n - u_i^{n-1}}{\Delta t} + c \frac{u_i^n - u_{i-1}^n}{\Delta x} = O(\Delta t, \Delta x) \]  \tag{7.34}

In this case, we can’t update \(u_i^n\) at each grid point independently. We instead need to solve a system of algebraic equations in order to calculate the values at all grid points simultaneously. It can be shown that this scheme is unconditionally stable so that the numerical errors will be damped out irrespective of how large the time-step is.

The stability limits discussed above apply specifically to the wave equation. In general, explicit schemes applied to the Euler or Navier-Stokes equations have the same restriction that the Courant number needs to be less than or equal to one. Implicit
schemes are not unconditionally stable for the Euler or Navier-Stokes equations since the non-linearities in the governing equations often limit stability. However, they allow a much larger Courant number than explicit schemes. The specific value of the maximum allowable Courant number is problem dependent.
CHAPTER 8

A STUDY OF SWIRL SIMULATION IN A DI ENGINE FROM LITERATURE

A computational study of a direct-injection (DI) engine intake system using KIVA3V was conducted in [37]. The engine considered had two intake ports designed to generate a swirling motion of the intake charge in the cylinder. To investigate the effect of adding shrouds to the intake valves on swirl, two sets of intake valves were considered; the first set consisted of conventional valves, and the second set of valves had back shrouds to prevent airflow on the backside of the valves. The effect of port diameters on airflow and swirl motion was also investigated. In this case, ports with two different diameters were modeled. In addition, the effect of using one or two intake ports on swirl generation was determined by blocking one of the ports. The results show that higher swirl was generated with a single port and a shrouded valve.

It is well known that in DI engines swirl is needed for proper mixing of fuel and air. This is particularly true in DI diesel engines [38]. Moreover, the efficiency of an engine can be improved by increasing the burn rate of the fuel/air mixture [39, 40]. This can be achieved in two ways; one by designing the combustion chamber in order to reduce contact between the flame and the chamber surface, and two by designing intake systems that impart a swirling motion to the incoming charge.

The swirl ratio and hence the fluid motion can have a significant effect on fuel-air mixing, combustion, heat transfer, and emissions. It has been shown that small, high speed, direct-injection diesel engines require an intake swirl ratio of 10 or higher when operating under part-load conditions [41]. Hence, it is important to design intake systems that can generate high swirl ratios. This can be achieved by using two or four intake ports arranged in a tangential configuration [41], or by using helical ports [41] and/or shrouded intake valves.

However it should be kept in mind that usage of such techniques increase air flow loses thus yields a decrease in the engine efficiency.
This study was conducted to investigate the effect of the intake system design on swirl ratio using the computer code KIVA3V. CFD is becoming more accepted as an adjunct to experimentation in the analysis and design of various engineering systems. Since multi-dimensional modeling of IC engines is less expensive and less time consuming than experimentation, the KIVA3V code was used to study the effects of using: (1) one or two intake ports, (2) shrouded valves, and (3) ports with different diameters, on swirl ratio. The effect of valve timing or boost pressures will be considered in a future study.

### 8.1 Overview of the Study

The computer code KIVA3V was used to model the intake system in a DI engine. A typical intake system with two ports is shown in Figure 8.1. The engine parameters used in this study are listed in Table 8.1. The engine had a bore of 97.5 mm and a stroke of 95.5 mm. It had two intake ports in a flat head, and a re-entrant piston bowl.

The simulations were performed through the intake and compression strokes only. The exhaust system in this engine was not modeled since the exhaust valves were not considered to open. Details of the computational mesh are shown in Figure 8.1. The mesh had about 150,000 cells. Pressure inflow boundaries were imposed at the open ends of the intake runners. The calculations were started at a crank angle of 345 degrees (15 degrees before TDC the beginning of the intake stroke). The air in the cylinder was considered to be quiescent at the beginning of the simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>79.5 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>95.5 mm</td>
</tr>
<tr>
<td>Squish</td>
<td>1.0 mm</td>
</tr>
<tr>
<td>Engine RPM</td>
<td>2000</td>
</tr>
<tr>
<td>Intake Valve Opening</td>
<td>4 degrees AT DC</td>
</tr>
<tr>
<td>Intake Valve Closing</td>
<td>25 degrees ABDC</td>
</tr>
</tbody>
</table>
Six different cases were simulated. Table 8.2 lists these cases with a description of each case. For the cases when shrouded valves were used the code had to be modified to allow specifying shrouds on the backside of the valves. Figure 8.2 is a schematic of a conventional valve with a shroud. Since air can flow around all sides of an un-shrouded valve, the air flowing through the intake port will enter the cylinder in all directions. This behavior could compromise the value of the swirl ratio. Hence, if a shroud is added to the backside of the valve, air will only flow in one direction into the cylinder. It was assumed that this effect could enhance swirl generation. Figure 8.3a shows the flow around an un-shrouded valve, and Figure 8.3b shows the flow around a shrouded valve. It is very clear that the shroud prevents flow from the backside of the shroud.
Table 8.2. Description of cases considered

<table>
<thead>
<tr>
<th>Case#</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Both intake ports open and no shrouds on valves.</td>
</tr>
<tr>
<td>2</td>
<td>Lower port blocked and no shrouds on valves.</td>
</tr>
<tr>
<td>3</td>
<td>Half-size ports and ro shrouds on valves.</td>
</tr>
<tr>
<td>4</td>
<td>Both intake ports open with shrouded valves.</td>
</tr>
<tr>
<td>5</td>
<td>Lower port blocked with shrouded valves.</td>
</tr>
<tr>
<td>6</td>
<td>Half-size ports with shrouded valves.</td>
</tr>
</tbody>
</table>

Figure 8.2. Conventional valve with a shroud

8.2 Swirl Ratio

Values of swirl ratio versus crank angle for the different cases considered were calculated and are plotted in Figure 8.4. The results show that the case with one port and a shrouded valve had the highest swirl ratio. However, the case with the two ports and un-shrouded valves had the lowest swirl ratio. When comparing the cases with the shrouded valves to those with the un-shrouded valves, the swirl ratio was always higher with shrouded valves. This is true, since the shroud prevents the air to flow from the backside of the valve, and forces it to flow on the front side into the cylinder, hence enhancing swirl motion.
Figure 8.3. Velocity vector plots show the flow through (a) un-shrouded valve, and (b) shrouded valve.

Figure 8.5 is a plot of the velocity vectors in a plane perpendicular to the cylinder axis midway between the cylinder head and the piston. The velocity vectors show the effect of adding shrouds to the valves on swirl motion. The plot shows the air to be coming out on the front side of the port with the shrouded valve.
Figure 8.4. Swirl ratio versus crank angle

However, for the case of the un-shrouded valve the air flows from all sides of the valve. In addition, Figure 8.6 shows that swirl motion develops earlier for the shrouded valves case. This explains the higher swirl ratios achieved for all cases with shrouded valves.

The effect of port diameter on swirl ratio was also considered. In this case, ports and runners having diameters equal to one-half the diameters of the original ports and runners were used. The valves and valve seats diameters were kept the same. Figure 8.7 shows the smaller size intake system.

The results in Figure 8.4 show that reducing the port size did not affect the swirl ratio significantly. The swirl ratio was slightly higher at the end of the compression stroke. Considering that the pumping losses will be higher for the smaller size ports, the slight increase in swirl ratio does not justify using them.

In general, the advantage of an application should be greater than its disadvantage. So it can be concluded that usage of smaller size ports is not an efficient solution.
Figure 8.5. Velocity vectors shown in a horizontal plane at a crank angle of 375 degrees for (a) un-shrouded valve case, and (b) shrouded valve case

The last case study involved blocking one port to determine if a single port would generate a higher swirl ratio than with two ports. The results shown in Figure 8.4 indicate that higher swirl ratios were attained when a single port was used. This leads us to conclude that for this intake system using the tangential port only would produce better swirl motion than with two ports. Since the lower port is positioned behind the tangential port, the air flowing from the lower port was partially blocked by the valve in the tangential port. This is true during the early stages of the intake severe with the shrouded valve, since the air flowing out of the lower port impinges on
Figure 8.6. Velocity vectors shown in a horizontal plane at a crank angle of 455 degrees for: (a) Un-shrouded valve case and (b) Shrouded valve case

Figure 8.7. Computational mesh shown with the half-size intake system
the shroud of the tangential port. Figure 8.5b shows the velocity vectors for this case, and it is apparent that the flow was partially blocked by the shroud. Even without the shrouds, the airflow from the lower port collides with air flowing on the backside of the tangential port. This collision between the separate flows coming out from the two ports creates a jet flow towards the center of the cylinder as shown in Figure 8.5a. This jet flow interferes with the swirl motion that is trying to develop in the cylinder, and hence the swirl motion does not develop as quickly as in the one port case. If two ports are to be used in order to improve the volumetric efficiency of the engine, then the ports could be moved apart to prevent flow interference from the ports.

8.3 Results of the Study

Based on the results generated in this study, the following conclusions can be derived:

-Using shrouded intake valves improves swirl generation in the cylinder and results in higher swirl ratios than with un-shrouded valves.

-For the intake system design considered in this study, blocking one port and using the tangential port resulted in higher swirl ratios than when both ports were used. The flow from the lower port was partially blocked by the valve and the flow from the tangential port due to the close placement of the ports to each other. Hence, it is recommended that the two ports be placed further apart from each other.

-Reducing the ports/runners diameter did not result in a significant increase in the swirl ratio. Rather it only caused a slight increase in the swirl ratio. Considering that the pumping losses in the port will increase in the smaller size ports/runners, the slight increase in the swirl ratio does not justify using this approach to increase swirl ratio.
CHAPTER 9

GOVERNING EQUATIONS

In this section, the governing equations that are used in KIVA3V will be introduced briefly. More detailed information and derivation of the formulas can be found in KIVA manuals which are available from www. Before starting, it will be convenient to remember the basic vector expressions like position and velocity vectors and the differential operator. The position vector and the velocity vector are given in Equation (9.1) and Equation (9.2) respectively.

\[ \ddot{x} = x\ddot{i} + y\ddot{j} + z\ddot{k} \]  \hspace{1cm} (9.1)

\[ \ddot{u} = u(x, y, z, t)\ddot{i} + v(x, y, z, t)\ddot{j} + w(x, y, z, t)\ddot{k} \]  \hspace{1cm} (9.2)

Vector differential operator is defined:

\[ \nabla = \ddot{i} \frac{\partial}{\partial x} + \ddot{j} \frac{\partial}{\partial y} + \ddot{k} \frac{\partial}{\partial z} \]  \hspace{1cm} (9.3)

9.1 Fluid Phase Equations

In this section, continuity equation, momentum equation, energy equation and state relation equations are discussed. Discussion will be basic; because as stated before the detailed derivation of expressions lie beyond the scope of this study and can be found in both KIVA manuals and computational fluid dynamics books. In general, fluid phase equations deal with macroscopic properties of quantities like; velocity, pressure, density, temperature and position. The calculation scheme includes an infinitely small fluid element and all the calculations are carried out via this element. The equations are specially fitted to our purpose by implying other model’s effects in terms of “source terms”.
9.1.1 Continuity Equation

The continuity expression used in KIVA3V is given in Equation (9.4).

\[
\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \vec{u}) = \nabla \cdot \left( \rho D \nabla \left( \frac{\rho_m}{\rho} \right) \right) + \dot{\rho}_m^c + \dot{\rho}^s \delta_{m1} 
\]  \tag{9.4}

Here, the first term of the right hand side of the equation is the diffusion term. Other parameters are briefly expressed below.

\( \rho_m \) : Mass density of species \( m \)

\( \rho \) : Total mass density

\( \vec{u} \) : Fluid velocity

\( D \) : Diffusion coefficient (Fick’s law) \( D = \mu/(\rho S_c) \)

\( \dot{\rho}_m^c \) : Source term due to chemistry

\( \dot{\rho}^s \) : Source term due to spray

\( \delta \) : Dirac delta function

Due to the fact that our fuel is represented by a single component, Dirac delta function is limited with subscript “1”. Again it can be noted that summation of Equation (9.4) for all the species gives the continuity equation for the total fluid density.

\[
\sum_m \text{Equation (9.4) yields:}
\]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = \dot{\rho}^s 
\]  \tag{9.5}

It should also be noted that mass fraction of species \( m \) is given as:

\[
\gamma_m = \frac{\rho_m}{\rho} 
\]  \tag{9.6}

9.1.2 Momentum Equation

In general, the forces acting on the fluid element can be divided into two categories: First category includes mass originated forces like gravitational force and electromagnetic forces. Second category covers surface originated forces. Also this second
category can be divided into two groups: Pressure and Viscous forces. Viscous forces include both normal stresses and shear stresses. Taking these points into account, one obtains:

\[
\frac{\partial}{\partial t} (\rho \tilde{u}) + \nabla \cdot (\rho \tilde{u} \tilde{u}) = -\frac{1}{\mathcal{a}^2} \nabla p - A_0 \left( \frac{2}{3} \rho \kappa \right) + \nabla \sigma + \tilde{F}^s + \rho \ddot{g}
\]  

(9.7)

Here:

\( p \): Fluid pressure

\( \mathcal{a} \): A dimensional quantity to be used in conjunction with the PGS (pressure gradient scaling) method for low M flows. It should be remembered that the PGS method should not be used in problems where it is important to calculate acoustic waves accurately like high M flow problems.

\( A_0 \): Turbulence switch. Determines which turbulence model is used: 0.0 for laminar, 1.0 for turbulent case.

\( \tilde{F}^s \): (rate of momentum gain) / (volume) due to spray

\( \ddot{g} \): Specific body force (constant)

\( \sigma \): Viscous stress tensor (Newtonian fluid). Defined as:

\[
\sigma = \mu \left[ \nabla \tilde{u} + (\nabla \tilde{u})^T \right] + \lambda \nabla \cdot \tilde{u}
\]  

(9.8)

\[
\mu = (1.0 - A_0) \rho \nu_0 + \mu_{\text{air}} + A_0 \frac{C_{\mu} \rho \kappa^2}{\varepsilon}
\]  

(9.9)

\[
\lambda = A_2 \mu
\]  

(9.10)

\[
\mu_{\text{air}} = \frac{A_1 T^{3/2}}{T + A_2} \quad \text{Sutherland Formula}
\]  

(9.11)

\( \nu_0 \): An input constant i.e.; \( \nu_0 = \mu / \rho \)

\( A_1 \): Represented by airmu1 i.e.; \( \text{airmu1} = 1.457e - 5 \)

\( A_2 \): Represented by airmu2 i.e.; \( \text{airmu2} = 110.0 \)

\( A_3 \): \(-2/3\) (Stoke's relation)

\( C_{\mu} \): 0.09 Empirical constant (built-in)
\[ I : \text{Unit dyadic (in Equation (9.8))} \]

\[ T : \text{Transpose (superscript in Equation (9.8))} \]

### 9.1.3 Energy Equation

Energy equation is obtained by applying the First Law of Thermodynamics to the selected fluid element. This means that; the total energy change in the fluid element should be equal to the sum of the total heat transfer from/to the fluid element and the total work done by mass and surface forces of the fluid element. If this approach is continued to carry out, the energy equation is obtained like the one in Equation (9.12), including the effects from chemical heat release and spray interactions.

\[
\frac{\partial}{\partial t} (\rho I) + \nabla \cdot (\rho u I) = -p \nabla \cdot \bar{u} + (1 - A_v) \sigma : \nabla \bar{u} - \nabla \cdot \bar{J} + A_v \rho e + \dot{Q} + \dot{Q}' \quad (9.13)
\]

Where:

\[ I : \text{Specific internal energy, exclusive of chemical energy} \]

\[ \dot{Q}' : \text{Source term due to chemical heat release} \]

\[ \dot{Q} : \text{Source term due to spray interactions} \]

\[ \bar{J} : \text{Heat flux vector and is sum of contributions due to heat conduction and enthalpy diffusion. It is given by:} \]

\[
\bar{J} = -K \nabla T - \rho D \sum_m \left[ h_m \nabla \left( \frac{\rho_m}{\rho} \right) \right] \quad (9.14)
\]

In Equation (9.14); \( T \) is the fluid temperature, \( h_m \) is the specific enthalpy of species \( m \), and \( K \) is the thermal conductivity (= \( \mu C_p \))/Pr, Pr is the turbulent Prandtl number and \( C_p \) is the constant pressure specific heat, that is obtained from the equation of state relations, to be discussed later in detail.).

### 9.2 State Equations

The state equations are used to feed other governing equations in terms of variables like pressure, specific internal energy etc. They are listed below.

\[
P = R_v \sum_m \left( \frac{\rho_m}{W_m} \right) \quad (9.15)
\]
\[ I(T) = \sum_m \left[ \left( \frac{\rho_m}{\rho} \right) f_m(T) \right] \]  
(9.16)

\[ C_p(T) = \sum_m \left[ \left( \frac{\rho_m}{\rho} \right) C_{pm}(T) \right] \]  
(9.17)

\[ h_m(T) = I_m(T) + \frac{R_0 T}{W_m} \]  
(9.18)

Here:

\( W_m \) : Molecular weight of species \( m \)

\( R_0 \) : Universal gas constant (8.3143e+7)

\( h_m(T) \) : Specific enthalpy of species \( m \)

### 9.3 Chemical Reactions

In general, a chemical reaction can be expressed like the symbolic one in Equation (9.19).

\[ \sum_m a_{mr} \chi_m \Leftrightarrow \sum_m b_{mr} \chi_m \]  
(9.19)

Here; \( \chi_m \) represents one mole of species \( m \) and, \( a_{mr} \) and \( b_{mr} \) are integer stoichiometric coefficients for (kinetic/equilibrium) reaction \( r \).

#### 9.3.1 Kinetic Reaction (Slow)

The kinetic reaction \( r \) proceeds at a rate of \( \dot{\omega}_r \), given by:

\[ \dot{\omega}_r = k_f \prod_m \left( \frac{\rho_m}{W_m} \right)^{a_{mr}} - k_{br} \prod_m \left( \frac{\rho_m}{W_m} \right)^{b_{mr}} \]  
(9.20)

Here \( k_f \) and \( k_{br} \) are the forward and backward rate coefficients for reaction \( r \) as stated in previous chapters. Also they are assumed to be of a generalized Arrhenius form:

\[ k_f = A_f T^{\delta_f} \exp \left( - \frac{E_f}{T} \right) \]  
(9.21)
\[ k_{br} = A_{br} T^{a'_{br}} \exp \left\{ \frac{E_{br}}{T} \right\} \]  

(9.22)

In Equations (9.21) and (9.22), \( E_p \) and \( E_m \) are activation temperatures (in Kelvin), \( a'_{mr} \) and \( b'_{mr} \) specify the order of the reaction. \( a'_{mr} \) and \( b'_{mr} \) need not to be equal to \( a_{mr} \) and \( b_{mr} \) so that empirical reactions orders can be used. The chemical source term in Equation (9.4) is given by:

\[ \rho^s_m = W_m \sum_r (b_{mr} - a_{mr}) \dot{\omega}_r \]  

(9.23)

Also the chemical heat release term in Equation (9.13) is defined in the following manner:

\[ \dot{Q}^s = \sum_r Q_r \dot{\omega}_r \]  

(9.24)

Here \( Q_r \) is the negative of the heat reaction at absolute zero.

\[ Q_r = \sum_m (a_{mr} - b_{mr}) (\Delta h_r^0)_m \]  

(9.25)

(\( \Delta h_r^0 \)) is the heat of formation of species \( m \) at absolute zero.

**9.3.2 Equilibrium Reaction (Fast)**

The rate of equilibrium reaction \( r, \dot{\omega}_r \), is implicitly determined by the constraint conditions for Phase A species density \( \rho^A_m \).

\[ \prod_m \left( \frac{\rho_m}{W_m} \right)^{(b_{mr} - a_{mr})} = K'_c(T) \]  

(9.26)

Where \( K'_c(T) \), depends only on temperature, is the concentration equilibrium constant for equilibrium reaction \( r \) and is assumed to be of the form given below in Equation (9.27). As it can be noted, the other parameters are constants.
\[ K' = \exp \left( A_r \ln T_{A} + \frac{B_r}{T_{A}} + C_r + D_r T_{A} + E_r T_{A}^2 \right) \]  

\[ T_{A} = \frac{T}{1000 K} \]

Approximate \( \dot{\omega}_r = \frac{\omega_r}{\Delta t} \)

Since \( \rho C_p \Delta T = \sum Q_r \omega_r \), gives \( \rho C_p (\bar{T} - T^n) = \sum Q_r \omega_r \)

Or \( \bar{T} = T^n + \left( \sum Q_r \omega_r \right) / (\rho C_p) \)

Also Equation (9.23) can be approximated as:

\[ \rho_m - \bar{\rho}_m = W_n \sum_r \left( b_m - a_m \right) \dot{\omega}_r \]

### 9.4 The Spray Droplets Model Equations

Interaction of the spray droplets with the medium of the combustion chamber (the fluid phase) includes; oscillations, distortions, break-ups, collisions and coalescences of the droplets. The fuel droplets are represented by so called “parcels”. Of course it is necessary to define a computational element and in this calculation this element is referred as “computational particle”. Each computational particle represents a number of droplets of identical size, velocity and temperature.

In this manner; the mass, momentum and energy exchange between the spray and the surrounding gases should be accounted for. Basically, to be able to carry out such a calculation, one must know the number of droplets in unit volume. This value can only be calculated using a probability scheme. The droplet distribution probability function has ten independent variables and time and is given in Equation (9.28).

\[ f(\vec{x}, \vec{v}, r, T_d, y, \dot{y}, t) d\vec{v} dr dT_d dy dy' \]  

(9.28)

\( \vec{x} \): Three droplet position components

\( \vec{v} \): Three velocity components

\( r \): Equilibrium radius

\( T_d \): Temperature of the droplet

69
\( y \): Distortion from sphericity

\( \dot{y} \): The time rate of change of \( y \)

The expression in Equation (9.28) verbally means that \( f(\ldots) \) is the probable average number of droplets per unit volume at position \( \vec{x} \) and time \( t \) with velocities, radii, temperatures, in the respective interval \( (\vec{v}, \vec{v} + d\vec{v}) \), \( (r, r + dr) \), \( (T_d, T_d + dT_d) \), and the oscillation (displacement) parameters in the intervals \( (y, y + dy) \) and \( (\dot{y}, \dot{y} + d\dot{y}) \).

The time evaluation of \( f \) is obtained by solving a form of the spray equation. (Not solved directly)

\[
\frac{\partial f}{\partial t} + \nabla \cdot (f \vec{v}) + \nabla \cdot (f \vec{F}) + \frac{\partial}{\partial r} (fR) + \frac{\partial}{\partial T_d} (f \dot{F}_d) + \frac{\partial}{\partial y} (f \dot{y}) + \frac{\partial}{\partial \dot{y}} (f \ddot{y}) = \dot{f}_{\text{coll}} + \dot{f}_{\text{bu}} \tag{9.29}
\]

In Equation (9.29); \( \vec{F}, R, \dot{F}_d, \text{and } \dot{y} \) are the time rates of change, following an individual drop, of its velocity, radius, temperature, and oscillation velocity \( \dot{y} \). These functions determine the trajectories of individual droplets. The terms \( \dot{f}_{\text{coll}} \) and \( \dot{f}_{\text{bu}} \) are sources due to droplet collisions and break-ups.

The source terms due to droplet collisions and break-ups are given below; in Equation (9.30) and in Equation (9.31).

\[
\dot{f}_{\text{coll}} = \frac{1}{2} \int \int f(\vec{r}, \vec{v}_1, r_1, T_{d1}, y_1, \dot{y}_1, \ddot{y}_1, t)f(\vec{r}, \vec{v}_2, r_2, T_{d2}, y_2, \dot{y}_2, \ddot{y}_2, t) \pi(r_1 + r_2)^2
\]

\[
|\vec{v}_1 - \vec{v}_2| \left\{ \sigma(\vec{r}, r, T_d, y, \dot{y}, \ddot{y}, r_1, T_{d1}, y_1, \dot{y}_1, \ddot{y}_1, r_2, T_{d2}, y_2, \dot{y}_2) \right.
\]

\[
- \delta(\vec{r} - \vec{r}_1) \delta(r - r_1) \delta(T_d - T_{d1}) \delta(y - y_1) \delta(\dot{y} - \dot{y}_1)
\]

\[
- \delta(\vec{r} - \vec{r}_2) \delta(r - r_2) \delta(T_d - T_{d2}) \delta(y - y_2) \delta(\dot{y} - \dot{y}_2)
\}
\]

\[
d\vec{r}_1 dr_1 dT_{d1} dy_1 d\dot{y}_1 d\ddot{y}_1 d\vec{r}_2 dr_2 dT_{d2} dy_2 d\dot{y}_2 d\ddot{y}_2 \tag{9.30}
\]

The expression for the collision source term in Equation (9.30) includes another function; the collision transition probability function, denoted by \( \sigma \).

\( \sigma \) is defined such that; \( \sigma dv dr dT_d dy d\dot{y} \) is the probable number of drops with properties in the implied intervals that results from a collision between a droplet with subscript 1 and one with subscript 2 properties.

In general, two types of collisions are accounted for in KIVA3V:

70
1- If the collision impact parameter $b$ is less than a critical value $b_{cr}$, then the droplets coalesce.

2- If $b$ exceeds $b_{cr}$, then the droplets maintain their sizes and temperatures but undergo velocity changes.

$$f_{bu} = \int f(\hat{x}, \hat{y}, r_1, T_{d_1}, 1, \hat{y}_1, t)B(\hat{x}, r, T_d, y, \hat{y}, r_1, T_{d_1}, \hat{y}_1, \hat{x}, t)$$
$$d\hat{x} d\hat{y} dT_{d_1} d\hat{y}_1$$ (9.31)

Again; the expression for the break-up source term in Equation (9.31) includes another function; the break-up transition probability function, denoted by $B$.

$B$ is defined such that; $B d\vec{v} d\vec{r} dT_{d_1} dy d\hat{y}$ is the probable number of droplets with properties in the implied intervals that are produced by a collision of a droplet with subscript 1 properties. The meaning of Equation (9.31) is the following: When a droplet's distortion $\gamma$ exceeds unity, it breaks up into a distribution of smaller drops given by $B$. After break-up, the droplet radii are assumed to follow a $\chi$-square distribution:

$$g(r) = \frac{1}{r} e^{-r/\bar{r}}$$ (9.32)

In Equation (9.32), $\bar{r} = r_{52}/3$ and $r_{52}$ is called the Sauter Mean Radius.

The droplet acceleration $\vec{F}$ has contributions due to aerodynamic drag and gravitational force; and is determined by Equation (9.33).

$$\vec{F} = \frac{3}{8} \left( \frac{\rho}{\rho_d} \right) \frac{[\vec{u} + \vec{u}' - \vec{v}]}{r} (\vec{u} + \vec{u}' - \vec{v}) C_D + \vec{g}$$ (9.33)

Here;

$C_D$: Drag coefficient

$\vec{u}$: Gas velocity

$\vec{u}'$: Turbulent gas velocity

$\vec{v}$: Droplet velocity

The rate of droplet radius change $R$ is given by the Frossling correlation in Equation (9.34):
\[ R = -\frac{(\rho D)_{eq}(\tilde{T})}{2\rho_d r} \frac{Y_i^{*} - Y_i}{1 - Y_i^{*}} Sh_d \]  

(9.34)

Where:

\( Sh_d \): Sherwood number for mass transfer

\( Y_i^{*} \): The fuel vapor mass fraction at the droplet's surface

\( Y_i = \frac{\rho_i}{\rho} \)

\((\rho D)_{eq}(\tilde{T})\): Fuel vapor diffusivity in air

The rate of droplet temperature change \( \dot{T}_d \) is determined by the energy balance equation below:

\[ \rho_d \frac{4}{3} \pi r^3 c_i \dot{T}_d - \rho_d 4\pi r^2 RL(T_d) = 4\pi r^2 Q_d \]  

(9.35)

In Equation (9.35); \( c_i \) is liquid fuel specific heat, \( L(T_d) \) is the fuel latent heat of vaporization and \( Q_d \) is the rate of heat conduction to the droplet surface per unit area. (Given by Ranz-Marshall correlation)

Finally, the equation for the acceleration of the droplet distortion parameter \( \ddot{y} \) is expressed like the one in Equation (9.36).

\[ \ddot{y} = \frac{2}{3} \frac{\rho}{\rho_d} \frac{(\ddot{u} + \ddot{u} - \ddot{v})^2}{r^2} \frac{8a(T_d)}{\rho_d r^3} y - \frac{5\mu(T_d)}{\rho_d r^2} \dot{y} \]  

(9.36)

Here:

\( \mu(T_d) \): The viscosity of the liquid

\( a(T_d) \): The liquid surface tension coefficient

With the above quantities determined, the exchange functions \( \dot{\rho}^s, \dot{F}^s, \dot{Q}^s \) and \( \dot{W}^s \) are obtained by summing the rates of change of mass, momentum and energy of all droplets at position \( \ddot{x} \) and time \( t \). Thus one obtains:

\[ \dot{\rho}^s = -\int_{\rho_d} A \pi r^2 R \dot{\nu} d\dot{r} dt dy \]  

(9.37)

\[ \dot{F}^s = -\int_{\rho_d} A \pi r^3 \ddot{F}^s + 4\pi r^2 RV \dot{\nu} d\dot{r} dt dy \]  

(9.38)
\[ \dot{Q}^* = -\int \rho_d \left\{ 4 \pi r^2 \left[ I_1(T_e) + \frac{1}{2} (\tilde{v} - \tilde{u})^2 \right] + \frac{4}{3} \pi r^3 \left[ c_i \tilde{T}_d + \tilde{F}^* \cdot (\tilde{v} - \tilde{u} - \tilde{u}) \right] \right\} \, d\tilde{v} \, d\tilde{u} \, d\tilde{y} \] (9.39)

\[ \dot{W}^* = -\int \rho_d \frac{4}{3} \pi r^3 \tilde{F}^* \cdot u' \, d\tilde{v} \, d\tilde{u} \, d\tilde{y} \] (9.40)

In Equation (9.40), \( \tilde{F}^* \) is given by:

\[ \tilde{F}^* = \tilde{F} - \tilde{g} \] (9.41)
CHAPTER 10

NUMERICAL SCHEME

As stated before, KIVA3V uses arbitrary hexahedrons to divide the main volume into sub-volumes and solves the equations via finite volume method. In Figure 10.1, a typical cell is shown.

![Figure 10.1. Typical cell layout in KIVA3V](image)

The position vector to vertex \((i, j, k)\) is given by:

\[
\vec{x} = x_{yk} \vec{i} + y_{jk} \vec{j} + z_{jk} \vec{k}
\]  

(10.1)

The center of the cell \((i, j, k)\) is defined as the point with coordinates:

\[
x^c_{yk} = \frac{1}{8} \sum_{a=1}^{8} x_a \quad y^c_{jk} = \frac{1}{8} \sum_{a=1}^{8} y_a \quad z^c_{jk} = \frac{1}{8} \sum_{a=1}^{8} z_a
\]  

(10.2)

This is the point where the thermodynamic properties of the cell are located.

\[
Q_{yk} = \mathcal{O}(x^c_{yk}, y^c_{jk}, z^c_{jk})
\]  

(10.3)
10.1 Temporal Differencing

Any quantities ($Q$) partial differential with respect to time is approximated by the 1st order Euler approximation:

$$\frac{\partial Q}{\partial t} = \frac{Q^{n+1} - Q^n}{\Delta t}$$  \hspace{1cm} (10.4)

In Equation (10.4); $\Delta t$ is the time step size and the integer $n$ is the cycle number.

As introduced in early chapters, KIVA3V uses ALE (Arbitrary Lagrangian Eulerian) approach to solve all the equations together belonging to both phases. In this method finite difference equations are solved in two phases: Lagrangian and Eulerian phases. Formation of a new mesh structure via change of crank angle degree occurs in Eulerian phase. The spray and the fluid phase equations are solved in three phases respectively: A, B and C. The three phases are summarized in Table 10.1.

Phase A: (Lagrangian)

Phase B: (Lagrangian, C.V moving with the fluid)

Phase C: (Eulerian, rezone/remap)

10.1.1 Phase A

In this phase; spray droplet collision and oscillation/break-up terms ($\hat{f}_{col}$, $\hat{f}_{bu}$) and, mass and energy source terms due to the chemistry and spray ($\hat{\rho}_s^c$, $\hat{\rho}'$, $\hat{F}^s$, $\hat{Q}^c$ and $\hat{Q}'$) are calculated.

10.1.2 Phase B

In Phase B, KIVA3V solves the governing equations in a coupled, implicit fashion with individual equations solved by the conjugate residual method. In general the procedure is very similar to the SIMPLE scheme. $\Delta t$ is determined on accuracy, not stability. Acoustic mode terms (namely the pressure gradient in the momentum equations and velocity dilatation terms in mass and energy equations), the spray momentum source term, diffusion terms (mass, momentum, energy) and the remaining source terms in $\kappa$ and $\epsilon$ equations are calculated.
10.1.3 Phase C

The flow field is frozen and rezoned or remapped onto a new computational mesh. The connective transport associated with the moving mesh relative to the fluid. Convective terms are calculated by QSOU (Quasi Second Order Upwind) or PDC (Partial Donor Cell) methods. This is accomplished in a sub-cycled, fully explicit fashion. $\Delta t$ is determined based on stability.

Table 10.1. Three phases overview including the sub-routines used

<table>
<thead>
<tr>
<th>Initialization</th>
<th>Read input data</th>
<th>begin.f, rinput.f, setup.f, timstp.f, newcyc.f</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Grid generation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Calculate gas viscosity</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Initialize time step, piston velocity</td>
<td></td>
</tr>
<tr>
<td>Phase A</td>
<td>Spray modeling (fuel injection, drop breakup, collision, evaporation...)</td>
<td>inject.f, pmovev.f, atomize.f, collide.f, evap.f, lawall.f, chem.f, pmom.f, pcoupl.f, repack.f</td>
</tr>
<tr>
<td>Big iteration</td>
<td>Combustion chemistry</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Emission modeling</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mass and energy contribution due to spray and combustion</td>
<td></td>
</tr>
<tr>
<td>Phase B</td>
<td>Fluid phase calculation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mass, momentum, velocity, temperature, pressure, turbulence properties</td>
<td>ysolve.f, exdif.f, vsolve.f, tsolve.f, psolve.f, pgrad.f, kesolve.f, paccel.f</td>
</tr>
<tr>
<td></td>
<td>(Implicit solver, iterations)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Update droplet velocity</td>
<td></td>
</tr>
<tr>
<td>Phase C</td>
<td>Rezoning grids</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Remapping fluid properties to new grids</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Update cell properties</td>
<td></td>
</tr>
</tbody>
</table>

10.2 Spatial Differencing

Finite volume approach to preserve the local conservative properties is given below:

$$\frac{\partial Q}{\partial t} + \nabla \cdot \vec{F} = S$$  \hspace{1cm} (10.5)
\[ \int \left[ \frac{\partial Q}{\partial t} + \nabla \cdot \vec{F} \right] dV = S \] (10.6)

By using Divergence and Reynolds Transport theorems:

\[ \frac{\partial}{\partial t} \int \vec{Q} dV + \int \vec{F} \cdot d\vec{A} = \int S dV \] (10.7)

10.3 Control Volumes

There are three types of cells used in KIVA3V in general.

1- Regular Cell

2- Momentum Cell

3- Normal-Velocity-Centered-on-Cell-Face Cell

Regular cells are used in calculation of thermodynamic properties such as; \( p, \rho, \rho, T, I, \kappa, \varepsilon \) etc. A typical regular cell was shown in Figure 10.1. The momentum cells are used to calculate the velocity \( \vec{u} \). A typical momentum cell is shown in Figure 10.2. The portion of the momentum cell \((i, j, k)\) is lying within regular cell \((i, j, k)\). The three momentum cell faces lying with the regular cell are shaded. Each momentum cell has 24 such faces in all.

The third type of cells is used to calculate the cell volume changes in phase B for the acoustic sub-cycling and in phase C for the convective fluxing. A typical N-V-C-o-C-F cell is shown in Figure 10.3.

![Figure 10.2. A typical momentum cell](image-url)
The velocity vector $\vec{u}$ is located at the regular cell vertex.

$$\vec{u}_{\theta k} = \vec{u}(x_{\theta k}, y_{\theta k}, z_{\theta k})$$ (10.8)

**Figure 10.3.** A typical N-V-C-o-C-F cell

In Figure 10.3, 2-D schematic of the control volume used for calculating normal velocities on cell faces is shown. Thin lines represent regular cell boundaries while heavy lines delineate the new control volume.

**10.4 Boundary Conditions**

In KIVA3V it is possible to categorize the boundary conditions into three main groups. The first group includes the real boundary conditions (physical boundary conditions) for the combustion chamber globally. The second group covers boundary and initial conditions for the spray droplets and the walls. And the last group includes numerical boundary conditions. However, these main categories also have sub-groups. In Table 10.2 the general classification of boundary conditions are shown.

In following sections these items will be introduced briefly. Again it is possible to find further information about the boundary conditions in KIVA manuals, especially in LA-11560-MS.

**10.4.1 Physical Boundary Conditions**

In general physical boundary conditions can be evaluated in three main categories: Rigid wall, Periodic and Spray injector.
Table 10.2. Boundary conditions in KIVA3V

(1)- Physical Boundary Conditions:

(I) Rigid Wall
   (a) No-slip
   (b) Free-slip
   (c) L-O-W
   (d) Fixed Temperature
   (e) Adiabatic

(II) Periodic

(III) Spray Injector

(2) Boundary/Initial Conditions for the Spray Equation
(For the spray droplets and the walls)

(3) Numerical Boundary Conditions:

(I) Velocity Inflow/Outflow

(II) Pressure Inflow/Outflow

- For rigid wall condition, there are 5 options:

(a) No-slip : gas velocity = wall velocity

\[ \vec{u} = \vec{w}_{wall} \]

(b) Free-slip : (I) normal gas velocity = normal wall velocity

\[ \vec{u} \cdot \vec{n} = \vec{w}_{wall} \cdot \vec{n} \]

(II) The tangential component of \( \vec{\sigma}_n \) = 0

(c) L-O-W : \( \text{lw} = +1 \rightarrow \text{L-O-W} \)
   
   0 \rightarrow \text{Free-slip}
   
   -1 \rightarrow \text{No-slip}
(d) Fixed T  :  (I) For either free-slip or no-slip:

\[ \text{gas temperature} = \text{wall temperature} \]

and \( J_w \) is determined from Eq. (9.14) implicitly.

(II) For L-O-W, \( J_w \) is determined from a modified Reynolds analogy formula

(e) Adiabatic  :  \( J_w = 0 \)

-For periodic, mass averaged case the illustration is like the one in Figure 10.4.

-For fuel spray, the boundary conditions are mainly the assumptions of the spray model. Arbitrary number of fuel injectors can be used. The model is multiple or multi-hole capable. Continuous or pulsed (hollow or solid) injection is possible. Pulsed sprays may be sinusoidal, square wave or user defined via a tabular velocity table. The particle size may be fixed or a distribution of radii at the injectors.

Figure 10.4. Mass averaged case for periodic boundary condition
10.4.2 Boundary Conditions for the Spray Equation

When a spray droplet impinges a rigid wall, KIVA3V sets:

$$\bar{u}_{\text{droplet}} = \bar{u}_{\text{wall}}$$  \hspace{1cm} (10.11)  

The droplet Reynolds no $Re_d = 0$ and there is no heat transfer between the droplet and the wall.

10.4.3 Numerical Boundary Conditions

Six bounding faces of a block should be defined in terms of boundary conditions. The FACEL line of IPREP does this job. There are 10 options that can be used for this identification.

- 1.0: moving
- 2.0: solid
- 3.0: axis
- 4.0: fluid
- 5.0: front periodic
- 6.0: derriere periodic
- 7.0: specified inflow
- 8.0: continuative outflow
- 9.0: pressure inflow
- 10: pressure outflow
CHAPTER 11

STRUCTURE OF COMPUTER CODE AND SIMULATIONS

KIVA3V is a FORTRAN based code. Originally it consists of three independent programs for pre-processing (k3prep), processing (kiva3v) and post-processing (k3post). However, due to computational resources it is not possible to use k3post for post-processing. Instead, GMV (General Mesh Viewer) is used. The flow chart in Figure 11.1 summarizes KIVA3V.

Figure 11.1. Summary of how KIVA3V works

In this study, the grid was generated by both k3prep and ICEM-CFD because especially in complex geometries k3prep is not capable of mesh generation and causes errors in
volume verification. So in this study both meshes prepared by k3prep and meshes prepared by ICEM-CDF were used.

To begin a simulation one needs three input files specially formatted: IPREP, ITAPE5 and CHEM.DAT. IPREP includes the geometric data of the engine combustion chamber. It is a simple text file, but the format (the locations of input values) is very important. Locating the data in a wrong place in the line may cause program not to function. K3prep uses IPREP to generate the mesh structure and creates a data file that all the mesh information is stored in, called OTAPE17. A sample code for IPREP is given in Appendix A and another for ITAPE5 is given in Appendix B.

OTAPE17 is renamed to ITAPE17 and becomes an input file for the main code kiva3v. However, the main code kiva3v needs two other input files: ITAPE5 and CHEM.DAT. ITAPE5 includes the simulation parameters like initial conditions, engine speed etc. It is also a simple text file similar to IPREP. CHEM.DAT includes chemical mechanisms of reactions. All the chemical data is stored in this file. (This file is only read by Valery's Kiva, a modified version of K122298.)

The main code kiva3v produces some OTAPE files and GMV files. For OTAPE files to be post-processed, necessary software couldn’t be obtained. These files include all the data about the simulation in a professional manner and require special software. On the other hand GMV is a freeware, so GMV is used visualize the cases.

Also the main code creates four more files storing; thermodynamic, turbulence, injection and dynamic data in list format. (dat.thermo, dat.turb, dat.inject and dat.dynamic) These files were used to obtain \( P \propto \alpha \) and other characteristic of the simulated engine.

### 11.1 Generation of Bowl Profile Using Analytic Functions

In order to generate an appropriate geometry of the combustion chamber, one needs to know the bowl geometry exactly. In Figure 2.2, the drawing of the piston was given. Here we will define this geometry analytically, dividing the profile into segments.

Dividing the curve into 8 segments:

\[
egin{align*}
[0, 2) & \quad : y=0 & (0, 0) & \rightarrow (0, 2) \\
[2, 19.744) & \quad : 17.744y=-10.245x + 20.49 & (2, 0) & \rightarrow (19.744, -10.245) \\
[19.744, 30.4) & \quad : (x-23.3)^2 + (y+4.097)^2=50.41 & (19.744, -10.245) & \rightarrow (30.4, -4.097) \\
[30.4] & \quad : x=30.4 & (30.4, -4.097) & \rightarrow (30.4, 2)
\end{align*}
\]
Number of sampling points can be increased as much as desired. In Figure 11.2, a schematic view of the NHDD engine piston bowl profile is shown.

![Figure 11.2. Schematic view of NHDD engine piston bowl profile](image)

11.2 Mesh Structure

Using the data obtained from these functions, the bowl profile is generated via I-DEAS and transferred to ICEM-CFD to prepare mesh files. (ITAPE17’s for the main code) In the following pages, three different mesh structures are shown:

Mesh 1: ncells = 21795 nverts = 24320

Mesh 2: ncells = 32146 nverts = 35513

Mesh 3: ncells = 41599 nverts = 45520
**Figure 11.3.** Mesh 1; generated by ICEM-CFD, ncells= 21795 nverts= 24320, in left figure piston is about 42 degrees after BDC and in right figure piston is 2 degrees after TDC.

**Figure 11.4.** Mesh 2; generated by ICEM-CFD, ncells= 32146 nverts= 35513, in left figure piston is about 42 degrees after BDC and in right figure piston is 2 degrees after TDC.
Figure 11.5. Mesh 3; generated by ICEM-CFD, ncells = 41599 nverts = 45520, in left figure piston is about 42 degrees after BDC and in right figure piston is 2 degrees after TDC.

11.3 Experimental Values

At this point, is convenient to give Ford OTOSAN experimental results. In the experiments performed by Ford OTOSAN, a lot of parameters were measured. However, especially in pressure data, some errors may be involved because high pressure transducers can yield errors in low pressure measurements. Since the transducer is selected with respect to the maximum pressure, this situation is quite normal. The pressure at 138 degrees before the TDC is taken 2.28 bars instead of 2.61 bars. By doing so, normal pressure values around the TDC are obtained. In Figure 11.6, Ford OTOSAN experimental pressure diagram is shown. (These values are Set1 values of OTOSAN data.)
Figure 11.6. Reference pressure values (Ford OTOSAN experimental data)

The chart in Figure 11.6 includes pressure data from -138 degrees before the TDC to 80 degrees after the TDC. Our analysis will be in that part of the cycle. Also the other operating conditions had been measured by Ford OTOSAN. These values are given in Table 11.1 and Table 11.2.

Table 11.1 Ford OTOSAN Set 1 experimental data (Part 1)

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<tr>
<th>N_engine</th>
<th>Q_fuel</th>
<th>PHI_inj</th>
<th>P_rail</th>
<th>P_boost</th>
<th>T_boost</th>
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<tr>
<td>rpm</td>
<td>mg-str</td>
<td>°CA</td>
<td>bar</td>
<td>mbar</td>
<td>°C</td>
</tr>
<tr>
<td>1430</td>
<td>128,2</td>
<td>-5,85</td>
<td>1100</td>
<td>1254,5</td>
<td>41,5</td>
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<table>
<thead>
<tr>
<th>P_PFP</th>
<th>Torque</th>
<th>Power</th>
<th>SFC</th>
<th>DT_Inj</th>
<th>T_air</th>
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<td>bar</td>
<td>Nm</td>
<td>KW h</td>
<td>g/kWh</td>
<td>ms</td>
<td>°C</td>
</tr>
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<td>133</td>
<td>1155</td>
<td>173,06</td>
<td>185,75</td>
<td>2214,50</td>
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</tbody>
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<table>
<thead>
<tr>
<th>T_fuel</th>
<th>T_water</th>
<th>T_oil</th>
<th>P_oil</th>
<th>P_com_in</th>
<th>P_com_out</th>
</tr>
</thead>
<tbody>
<tr>
<td>°C</td>
<td>°C</td>
<td>°C</td>
<td>bar</td>
<td>mbar</td>
<td>mbar</td>
</tr>
<tr>
<td>28,8</td>
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<td>102,8</td>
<td>4,0</td>
<td>-17,6</td>
<td>1266,8</td>
</tr>
</tbody>
</table>
Table 11.2 Ford OTOSAN experimental data (Part 2)

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>P_tur_in</td>
<td>P_tur_out</td>
<td>T_com_in</td>
<td>T_com_out</td>
<td>T_tur_in</td>
<td>T_tur_out</td>
</tr>
<tr>
<td>mbar</td>
<td>mbar</td>
<td>ºC</td>
<td>ºC</td>
<td>ºC</td>
<td>ºC</td>
</tr>
<tr>
<td>830,2</td>
<td>25,7</td>
<td>20,8</td>
<td>130,1</td>
<td>635,8</td>
<td>531,4</td>
</tr>
</tbody>
</table>

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<table>
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</tr>
</thead>
<tbody>
<tr>
<td>P_abs_air</td>
<td>F_air</td>
<td>F_air_dry</td>
<td>F_fuel</td>
<td>F_exhaust</td>
<td>smoke</td>
<td>ha</td>
</tr>
<tr>
<td>mbar</td>
<td>kg/h</td>
<td>kg/h</td>
<td>kg/h</td>
<td>kg/h</td>
<td>FSN</td>
<td>g/kg</td>
</tr>
<tr>
<td>1013,3</td>
<td>704,39</td>
<td>697,53</td>
<td>32,47</td>
<td>736,86</td>
<td>0,24</td>
<td>9,74</td>
</tr>
</tbody>
</table>

| O_ppm | HC_ppm | CO2_vol | O2_vol | NOx_gKWh | CO_gKWh | HC_gKWh | air_humidity |
| ppm   | ppm    | Vol%    | Vol%   | g/kWh    | g/kWh   | g/kWh   | %           |
| 93    | 21     | 9,85    | 7,10   | 6,64     | 0,42    | 0,05    | 60,04       |

Now that we know all the information we need, it is the time for adjusting the parameters. Below in Table 11.3, needed parameters for IPREP and ITAPE5 are listed.

Table 11.3. The parameters needed for IPREP and ITAPE5

- bore: 11,2 cm
- stroke: 12,4 cm
- conn. rod.: 22,2 cm
- squish: 0,228 cm
- sim. begin: -138°
- sim. end: 80°
- swirl: 1,4
- comp. ratio: 17,9
- V_bowl: 50,4 cm³
- cyl. wall temp.: 500 K
- head temp.: 500 K
- piston temp.: 500 K
- initial pres.: 2,28 bar
- initial temp.: 314,5 K
- ex. valve open: 59°
- ex. valve close: 27°
- in. valve open: 28°
- in. valve close: 42°

11.4 Cold Flow Simulations: Grid Dependence

The first simulation performed is the type “cold flow”. Since our focus is the air motion in the engine, we first investigate cold flow. The three meshes generated by ICEM-CFD were used as input. The results were checked using Ford OTOSAN experimental data.
According to Ford OTOSAN, 6 degrees before the TDC (just before fuel injection) the measured cylinder pressure is 104.75 bars. The results from Mesh 1 and Mesh 2 are the same (106 bars) and the result from Mesh 3 is 105 bars. The error in Mesh 1 and Mesh 2 is less than 1.2% and in Mesh 3 is less than 0.25%. These errors can be acceptable because some of the data used in the simulations were predicted such as initial temperatures of piston head, cylinder walls etc. The results are given in Figure 11.7.

\[ \text{Cold Flow Pressure} \]

<table>
<thead>
<tr>
<th>pressure [dyne/cm²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.40E+08</td>
</tr>
<tr>
<td>1.20E+08</td>
</tr>
<tr>
<td>1.00E+08</td>
</tr>
<tr>
<td>8.00E+07</td>
</tr>
<tr>
<td>6.00E+07</td>
</tr>
<tr>
<td>4.00E+07</td>
</tr>
<tr>
<td>2.00E+07</td>
</tr>
<tr>
<td>0.00E+00</td>
</tr>
</tbody>
</table>

CA [degrees]

-138 -120 -100 -80 -60 -41 -21 19 38 58 78

Figure 11.7. Cold flow simulation, pressure results

Also it can be possible to see the temperature distributions in these simulations. Since there is no combustion simulated, the temperature curves will be similar to the form of the curve in Figure 11.7.

The temperature distribution in the combustion chamber is shown in Figure 11.8 for the three types of mesh introduced early.
Figure 11.8. Cold flow simulation, temperature results

In Figure 11.9, the turbulent kinetic energy values during the simulation period are shown.

Figure 11.9. Cold flow simulation, turbulent kinetic energy results

As it can be figured out, in this section only the effects of mesh structure are investigated. The input parameters were taken same in three different mesh structures. According to Figure 11.7, Figure 11.8 and Figure 11.9; the three mesh structures give
more or less the same result for cold combustion case as it was expected. This may be due to the lack of chemical reactions and calculations of species in the combustion chamber. All the calculations performed here, are fluid mechanics and thermodynamics calculations.

Taking the above figures and the rest of the figures in this part (Figure 11.7 to Figure 11.13) into account it can be concluded that for a cold flow investigation in such an application may be performed with a mesh similar to Mesh 1. Because increasing the fineness of the mesh (cases Mesh 2 and Mesh 3) does not affect the results seriously. On the other hand using a fine mesh is very time consuming.

In Figure 11.10, the values of the dissipation rate of turbulent kinetic energy ($\varepsilon$) during the simulation period are shown.

![Cold Flow Epsilon](image)

**Figure 11.10.** Cold flow simulation, dissipation rate of turbulent kinetic energy results

Figure 11.11 shows the intensity of turbulence values during the simulation period.
Figure 11.11. Cold flow simulation, intensity of turbulence results

Figure 11.12 shows the length scale of turbulence values during the simulation period.

Figure 11.12. Cold flow simulation, length scale results

The last figure of this cold flow analysis shows turbulent viscosity values during the simulation period in Figure 11.13. As stated before, investigations done by Mesh 1
(ncells= 21795 nverts= 24320) are very similar to those done by Mesh 2 (ncells= 32146 nverts= 35513) and Mesh 3. (ncells= 41599 nverts= 45520).

![Cold Flow Turbulent Viscosity](image)

**Figure 11.13.** Cold flow simulation, turbulent viscosity results

For cold flow conditions, the air motions in the combustion chamber were studied and the results are given in Appendix E. The figures of different meshes are quite similar to each other because of Eulerian phase characteristics. The figures in Appendix E are obtained using 1000 rpm engine speed and 500 K initial engine component (wall) temperature. Other conditions were also simulated and it was seen that, except for the change due to engine speed variations, the results were close to each other. So, as stated above, it was concluded that Mesh 1 is enough for this type of study.

### 11.4.1 Effect of Wall Temperatures

In the second step, a study of effect of wall temperatures such as cylinder head temperature, piston temperature and cylinder wall temperature has been performed. All the simulations in the previous part were performed again setting; tcy1wl, thead and tpistn values to 400, 500 and 600 K set by set. As expected, increase in the temperature of the combustion chamber components caused an increase in the pressure and temperature values. However this effect is almost negligible in cold flow conditions. When combined with the combustion phenomenon, this effect can be much stronger.
Each mesh structure (Mesh 1, Mesh 2, and Mesh 3) was used three times with the varying values of temperature and each situation was evaluated independently. In Figures 11.14, 11.15 and 11.16 pressure variations for different component temperatures are given. (wall temperatures)

**Figure 11.14.** Cold flow simulation, pressure variations for different component temperatures (21795 cells)

**Figure 11.15.** Cold flow simulation, pressure variations for different component temperatures (32146 cells)
Figure 11.16. Cold flow simulation, pressure variations for different component temperatures (41599 cells)

The main reason for the investigation of this effect is that there had been some problems in the simulation data in comparison with the experimental data from Ford OTOSAN. Since the exact geometry of the combustion chamber cannot be created by using k3prep there was an uncertainty in the data. It was suspected that the reason why the experimental data is different from our simulation data could be due to a bad estimation of tcylwl, thead and tpistn values. After using ICEM-CFD and performing these simulations it was concluded that the problem was neither tcylwl, thead and tpistn values nor the mesh structure. As stated early in this chapter, the problem is caused by wrong transducer values in the Ford OTOSAN datasheet. A further step may be investigation of heat loses in terms of engine speed, which will be introduced later.

In Figure 11.17, 11.18 and 11.19, overall temperature variations for different wall temperatures are given.
Figure 11.17. Cold flow simulation, overall temperature variations for different component temperatures (21795 cells)

Figure 11.18. Cold flow simulation, overall temperature variations for different component temperatures (32146 cells)
Figure 11.19. Cold flow simulation, overall temperature variations for different component temperatures (41599 cells)

11.4.2 Effect of Engine Speed

Now that we analyzed the initial temperature effect, we may investigate the heat loses in terms of engine speed. Qualitatively, as the engine speed increases, the heat lose should decrease due to the shorter time for heat transfer. Of course, this is a rough thinking and there are many parameters to be considered additionally.

Three different engine speeds; 1000, 1430 and 1800 rpm were simulated. The engine speeds are chosen such that both they are characteristic speeds for the engine considered and away from each other sufficiently to be able to see the probable difference.

In Figures 11.20, 11.21 and 11.22, the pressure variations are shown for both three different mesh structures and three different engine speeds. Again, from the view point of heat lose in terms of the engine speed; there is not much difference between the cases. The pressure value of Ford OTOSAN at the crank angle -138 degrees (2.61 bar) causes the problem. When it is set to 2.28 bar, the simulation results become compatible to the experimental results.
**Figure 11.20.** Cold flow simulation, pressure variations for different engine speeds (21795 cells)

**Figure 11.21.** Cold flow simulation, pressure variations for different engine speeds (32146 cells)
Figure 11.22. Cold flow simulation, pressure variations for different engine speeds (41599 cells)

It is quite hard to notice from the figures that, in 1800rpm condition the pressure increases more rapidly in comparison to the others. According to the above figures our thesis is right: As the engine speed increases, the heat lose should decrease due to the shorter time for heat transfer.

Actually, phenomena like combustion in internal engines are quite sophisticated and need much more detailed analyses. In an examination of a flame structure, one needs to use grid sizes about Kolmogorov scale in order to see the real situation. This is almost impossible with today’s computational resources. Grid sizes can be locally decreased but this time the transition between grids of different sizes becomes a problem. This is why this study is “air motion” based.

In Figures 11.23, 11.24 and 11.25, the temperature variations are shown for both three different mesh structures and three different engine speeds. The results are more or less the same.
Figure 11.23. Cold flow simulation, temperature variations for different engine speeds (21795 cells)

Figure 11.24. Cold flow simulation, temperature variations for different engine speeds (32146 cells)
Figure 11.25. Cold flow simulation, temperature variations for different engine speeds
(41599 cells)

11.5 Full Simulation Including Combustion

The last step of our study is to simulate the full combustion process occurring in the
Ford OTOSAN NHDD engine. In this stage; both the mesh prepared by k3prep and
ICEM-CFD was used. The mesh which was prepared by k3prep, contains six blocks and
has 63 nbo points for bowl profile generation. The pre-processor k3prep enforces the
cubic or prismatic blocks to curved geometries with the help of these nbo points. This
mesh is shown in Figure 11.26. The number of cells for this mesh structure is 27717 and
the number of vertices is 27880. With these values, it takes place between Mesh 1
(ncells= 21795 nverts= 24320) and Mesh 2 (ncells= 32146 nverts= 35513) in terms of
fineness.
Figure 11.26. Mesh used for combustion case; generated by k3prep, ncells= 27717
nverts= 27880, in left figure piston is about 42 degrees after BDC and in right figure
piston is 2 degrees after TDC.

A set of full combustion simulations was performed with OTOSAN Set 1 values and
ICEM-CFD meshes. (Mesh 1, Mesh 2, Mesh 3) Another set was performed using
OTOSAN Set 1 values and k3prep mesh introduced above. The results are given in
following sections.

11.5.1 Set 1 Values and ICEM-CFD Mesh Results

As usual, our first focus is pressure as an indication parameter for engine power. It is
possible figure out from the pressure diagram (Figure 11.27) that the results are quite
different from experimental case. Also the mesh dependency was noticed. In Lagrangian
phase calculations (like the combustion case); it is necessary to make some adjustments
in simulation parameters with varying meshes. Figure 11.27 was obtained by only
changing the mesh structure. The necessary adjustments are the subject of recent
researches. Once they are defined in a scientific manner, the predictivity of this kind
work will reach a certain level. When the cell size is changed, the calculation parameters
(of course not the physical and experimental ones) should be adjusted in such a way that
this size change is compensated. The most suitable parameters for this job are chemical
mechanism parameters; because, the other parameters are more or less known and
cannot cause this much error. Maybe in some regimes, it can be necessary to change the
chemical model totally. Partially Stirred Reactor model is the most popular model in literature and used as the model.

![Pressure (Grid Dependence)](image)

**Figure 11.27.** Pressure variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3

![Temp. (Grid Dependence)](image)

**Figure 11.28.** Temperature variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3
Figure 11.29. Density variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3

As expected, temperature curves are also different from each other. Because these values are calculated using the same numerical scheme. Thus, the pressure and the temperature results are compatible. The highest pressure according to Figure 11.27 is obtained from Mesh 3 (41599 cells). This means that also the highest temperature should be obtained from Mesh 3. Figure 11.28 verifies this. Figure 11.29 shows the variations of density for the same case.

After analyzing the thermodynamic properties, we may start evaluating turbulence characteristics. Again we have five characteristics: Turbulent kinetic energy, epsilon, intensity, length and turbulent viscosity.

In Figure 11.30, variation of turbulent kinetic energy for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3 is shown. In this case, the highest kinetic energy is obtained using Mesh 1. (21795 cells) Mesh 2 and Mesh 3 are similar in their absolute maximums; Mesh 2 is a little earlier.
Figure 11.30. TKE variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3

Figure 11.31. Epsilon variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3
Figure 11.32. Intensity variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3

Figure 11.33. Length scale variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3
Figure 11.34. Turbulent viscosity variations for full combustion simulations with Mesh 1, Mesh 2 and Mesh 3.

The greatest dissipation is obtained using Mesh 3. It is followed by Mesh 2 and Mesh 1 respectively according to figure 11.31. In Figure 11.32, the highest intensity value is obtained using Mesh 3.

Figure 11.33 shows that length parameter is inversely proportional to the number of cells.

In the last figure of this analysis (Figure 11.34), turbulent viscosity shows a similar character with Mesh 2 and Mesh 3. Mesh 1 is noticeably different from Mesh 2 and Mesh 3.

11.5.2 Set 1 Values and k3prep Mesh Results

In the studies performed by using k3prep mesh, the results are very close to experimental values. (Much better than ICEM-CFD) Furthermore, the character of the pressure curve is more or less same with the experimental curve. Only explanation for this phenomenon can be the difference in the mesh generation. In Figure 11.35, the pressure variation in the combustion chamber is shown in presence of real combustion using k3prep mesh. The characters of the curves are similar to each other but simulation results are a little right-shifted. This is related to fuel and chemical environment characterization.
Figure 11.35. Pressure variation in the combustion chamber using k3prep mesh

In Figure 11.36, the temperature variation in presence of combustion is shown. (k3prep)

Figure 11.36. Temperature variation in the combustion chamber using k3prep mesh

In general, simulation results for the combustion case are compatible with the experimental data.
For combustion case, visualization of the pressure and temperature distribution in the combustion chamber was done. The pressure distributions at various crank angles are given in Appendix C and the temperature distributions at various crank angles are given in Appendix D. These figures are obtained using Mesh 1 with 1430 rpm engine speed.

Also the spray formation and local fuel vapor concentrations were investigated. The figures of spray formation for 1000 rpm are given in Appendix F and the local fuel vapor concentrations figures for 1000 rpm are given in Appendix G.
CHAPTER 12

CONCLUSION

A multi-dimensional modeling of Ford OTOSAN NHDD Engine is presented via the KIVA3V code. Both the physical and chemical modeling calculations are done by this code. An experimental study from Ford OTOSAN is taken as a reference and simulations of the cycle are performed. The experiment engine geometry is generated using a three-dimensional model. For the chemical kinetic modeling, a reduced mechanism of 68 species and 291 reactions is used. In this study the impacts of the engine speed and initial wall temperatures are investigated.

The first part of the study includes the cold flow case. Different mesh structures were tested to obtain the best results and to make the solution independent from the mesh structure. It was seen that the results taken from the simulations do not differ seriously with the increasing cell numbers. This is because of the selection of the mesh numbers and Eulerian phase properties. Mesh 1, Mesh 2 and Mesh 3 (defined before) gave similar results.

Firstly, an investigation of the effect of initial engine component (wall) temperatures was performed. It was seen that for a cold flow analyses, a mesh similar to Mesh 1 is sufficient. This is due to the lack of combustion related calculations such as; instantaneous species concentrations and chemical reactions. Three different initial engine component (wall) temperatures of 400K, 500K and 600K were simulated. As expected, an increase in these values caused the pressure of the combustion chamber to increase. But this effect can be neglected in cold flow conditions.

To understand the engine speed effect, three different engine speeds of 1000rpm, 1430rpm and 1800rpm is simulated. It was seen that the heat lose in terms of engine speed decreases with increasing engine speed. This is due to shorter time for the heat transfer between the in-cylinder environment and the atmosphere.
The second part of this study includes combustion phenomenon. To be able to simulate combustion flame, the grid sizes need to be around Kolmogorov scale. This is almost impossible with today's computational resources. Omitting the analyses of flame, this grid sizes can be increased. This method was preferred in this study.

Combustion study was performed using both ICEM-CFD mesh and k3prep mesh. It was seen that using k3prep mesh gave better results. (More realistic pressure curve form) This is hard to explain why, because meshing capability of ICEM-CFD software is better than k3prep. It uses a more advanced algorithm in comparison to k3prep.

Some problems were detected in the reference data. This is compensated using well known points (high pressure points) as secondary reference. Also there were some problems with the mesh structure. Even if this is the case, the simulation results are compatible with experimental data without a detailed refinement. Of course, in need of refined data, the combustion mechanism should be re-configured.

It is recommended for those who will perform this type study, to use multi-computer facilities. Because, the simulations take very long times in case of fine meshes. (In this study, run times up to a week were recorded.) Again, it is important that the computers should be somehow fast i.e. equipped with high frequency new processors.

This study is also a proof for computational fluid dynamics to decrease the amount of necessary experiments, because it gives an idea about the situation. However; at least with today's technology, this kind of industrial procedure is not possible with experimental support.

In conclusion, the following points can be stated:

About KIVA:

- KIVA3V has an open source code and thus it is suitable for any kind of modification.
- It has deforming mesh capability to simulate valve and piston motions.
- A variety of options for modelling turbulence. (standard k-ε, SGS, RNG k-ε )
- It has a large fuel library.
- It still needs improvement in some aspects. (especially in pre-processing)

About results:

- For a cold flow analysis, Mesh 1 is sufficient enough.
- Initial component (wall) temperature variations do not affect the result in a serious manner.

- Higher engine speeds yield a low heat loss due to shorter transfer time.

- When using several grid structures for an analysis, it is necessary to adjust some parameters to obtain similar results.

- That is why this kind of analysis is called semi-predictive. Without having the experimental values, it is impossible to ensure the right results.

- It can be helpful in reducing the amount of the experimental job. For example, different operating conditions can be measured in detail, and some empirical relations are founded. Then, same group of operating conditions may be simulated in a more predictive manner.
REFERENCES


APPENDIX A

A sample code for IPREP file:

Istanbul Technical University fdg 27000
bore 11.2
stroke 12.4
squish 0.100
thsect 45.0
nblo 6
1 24 15 13 62 1 1 0
5.6 5.6 0.0 0.0 5.6 5.6 0.0 0.0
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
0.0 0.0 0.0 0.0 1.6504 1.6504 1.6504 1.6504
3.0 1.0 5.0 6.0 1.0 4.0
-1.0 0.0 -1.0 -1.0 0.0 -1.0
0.0000 1.1754
0.1300 1.1754
0.2600 1.1408
0.3900 1.0657
0.5200 0.9906
0.6500 0.9156
0.7800 0.8405
0.9100 0.7655
1.0400 0.6904
1.1700 0.6154
1.3000 0.5403
1.4300 0.4653
1.5600 0.3902
1.6900 0.3151
1.8200 0.2401
1.9500 0.1650
2.0800 0.0901
2.2100 0.0335
2.3400 0.0048
2.4700 0.0048
2.6000 0.0209
2.7300 0.0674
2.8600 0.1468
2.9900 0.2769
3.1276 0.4251
3.1023 0.4902
3.1269 0.5902
3.1367 0.6902
3.1228 0.7902
3.1051 0.8902
3.0875 0.9902
3.0699 1.090
3.0522 1.1902
3.0346 1.2902
3.0246 1.3902
3.0471 1.4902

116
3.1142 1.5902
3.2042 1.6504
2.9900 1.6504
2.8600 1.6504
2.7300 1.6504
2.6000 1.6504
2.4700 1.6504
2.3400 1.6504
2.2100 1.6504
2.0800 1.6504
1.9500 1.6504
1.8200 1.6504
1.6900 1.6504
1.5600 1.6504
1.4300 1.6504
1.3000 1.6504
1.1700 1.6504
1.0400 1.6504
0.9100 1.6504
0.7800 1.6504
0.6500 1.6504
0.5200 1.6504
0.3900 1.6504
0.2600 1.6504
0.1300 1.6504
0.0000 1.6504
 2 24 15 3 0 1 1 0
3.2042 3.2042 0.0 0.0 3.2042 3.2042 0.0 0.0
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
1.6504 1.6504 1.6504 1.6504 1.8754 1.8754 1.8754 1.8754
3.0 4.0 5.0 6.0 4.0 4.0
-1.0 -1.0 -1.0 -1.0 -1.0 -1.0
3 5 15 3 0 1 1 0
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
1.6504 1.6504 1.6504 1.6504 1.8754 1.8754 1.8754 1.8754
4.0 1.0 5.0 6.0 1.0 4.0
-1.0 0.0 -1.0 -1.0 0.0 -1.0
4 24 15 26 0 2 1 0
3.2042 3.2042 0.0 0.0 3.2042 3.2042 0.0 0.0
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
1.8754 1.8754 1.8754 1.8754 1.8754 1.8754 1.8754 1.8754
3.0 4.0 5.0 6.0 4.0 2.0
-1.0 -1.0 -1.0 -1.0 -1.0 -1.0
5 5 15 26 0 2 1 0
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
1.8754 1.8754 1.8754 1.8754 1.8754 1.8754 1.8754 1.8754
4.0 4.0 5.0 6.0 4.0 2.0
-1.0 -1.0 -1.0 -1.0 -1.0 -1.0
6 8 15 26 0 2 1 0
5.6 5.6 3.7492 3.7492 5.6 5.6 3.7492 3.7492
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
1.8754 1.8754 1.8754 1.8754 1.8754 1.8754 1.8754 1.8754
4.0 2.0 5.0 6.0 1.0 2.0
-1.0 -1.0 -1.0 -1.0 0.0 -1.0
ncopy 0
tiltflag 0
pentflag 0
wedgeflag 0
translate 0
nlocxy 0
reshape 0
npenny 0
nvguide 0
nvalvport 0
nrunner 0
nsiamese 0
nround 0
npatch 6
  2  1  1  1  2
  3  1  2  1  1  3
  4  5  2  1  1  4
  5  5  3  1  1  5
  5  1  4  1  1  5
  6  1  5  1  1  5
nrelaxb 0
npovtop 0
npovfcone 0
nzcylwall 0
tilt 0
ndish 0
nscallop 0
xoffset 0.0
yoffset 0.0
write17 1.0
plotmesh 1.0
xband 0.0
yband 0.0
zband 0.0
nxplots 0
nyplots 0
0.0
nzplots 0
nvhide 0
APPENDIX B

A sample code for ITAPE5 file:

Istanbul Technical University fdg 27000
irest 2
nohydro 0
lwall 1
lpr 0
irez 2
ncfilm99999
nctap8 1000
nelast99999
ncmon 1
ncaspec 1
-135.0
gmv 1.0
cafilm 5.0
cafin 80.0
angmom 1.0
pgssw 1.0
dti 1.00000e-7
dmxca 0.25
dmax 5.00000e-7
tlimd 1.0
twfilm 9.99e+9
twfin 9.99e+9
fchsp 0.60
bore 11.2
stroke 12.4
squish 0.100
rpm 1430.0
atdc -138.0
datdet 0.0
revrep 2.0
conrod 22.2
swirl 1.4
swiproe 3.11
thsect 45.0
sector 1.0
deaet 0.0
epsy 1.0e-3
epsv 1.0e-3
eps 1.0e-4
eps 1.0e-3
epsk 1.0e-3
epsp 1.0e-3
gx 0.0
gy 0.0
gz 0.0
tcylwl 500.0
thead 500.0
tpiston 500.0
pardon 0.0
a0 0.0
b0 1.0
artvis 0.0
ecrsrv 0.0
adia 0.0
anu0 0.0
visrat -666666667
tcut 9.99e+9
tcute 9.99e+9
cpschem 0.02
omgchem 1.0
turbsw 1.0
sgsl 0.0
trchem 0.0
capa 18.0
pmplct 2.0
lospeed 0.0
airmu1 1.457e-5
airmu2 110.0
airla1 252.0
airla2 200.0
prl 0.74
rpr 1.11
rsc 1.11
xignit 1.0e+4
tlign -1.0
tdign -1.0
calign 9999.9
cadign 10.0
xignl -0.125
xignr +0.125
yignl 1.9388
yignr 2.1888
zignl 9.5275
zignr 9.7775
zignl -0.125
zignr +0.125
yignl -2.1888
yignr -1.9388
zignl 9.5275
zignr 9.7775
kwikeq 0
numnoz 1
numnij 1
numvel 14
t1nij -1.0
td1nij -1.0
cal1nij -5.85
cad1nij 19.0
tspm1 0.1282
tnparc 5000.0
pulse 3.0
injd1 1
kolid 1
tpi 297.05
turb 1.0
breakup 1.0
evapp 1.0
drnoz 0.2
dznoz 14.2
dthnoz 22.5
tiltxy 22.5
tiltxz 75.0
cone 10.0
dcone 10.0
anoz 2.040e-4
smr 1.00e-2 ! 1.00e-2
amp0 0.0
16628.70
20193.90
22000.00
23272.70
24000.00
24500.00
25000.00
25900.00
24500.00
24000.00
24500.00
23272.00
22000.00
20193.90
16628.70
nreg 1
'presi', 2.6109e+6
'tempi', 314.5
'tkei', 0.20
'sci', 1.0
nvalves 0
isoot 0
APPENDIX C

In the figures below, the pressure distribution in the combustion chamber is shown at crank angles; -53, -8, 2, 12 and 52 degrees.
Figure C.1. Pressure distributions in the combustion chamber at various crank angles
APPENDIX D

In the figures below, the temperature distribution in the combustion chamber is shown at crank angles: -53, -8, 2, 12 and 52 degrees.
Figure D.1. Temperature distributions in the combustion chamber at various crank angles
APPENDIX E

The figures in the following pages show the air motions in the combustion chamber at crank angles: -10, -6, -2, 2 and 5 degrees.

The figures are obtained setting:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step</td>
<td>1.000000e-5 sec</td>
</tr>
<tr>
<td>Time step max.</td>
<td>5.000000e-5 sec</td>
</tr>
<tr>
<td>Swirl</td>
<td>1.4</td>
</tr>
<tr>
<td>Cyl. wall temp.</td>
<td>500.0 K</td>
</tr>
<tr>
<td>Cyl. head temp.</td>
<td>500.0 K</td>
</tr>
<tr>
<td>Piston temp.</td>
<td>500.0 K</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>2.28e+6 dyne/cm²</td>
</tr>
<tr>
<td>Initial temp.</td>
<td>314.5 K</td>
</tr>
<tr>
<td>Squish</td>
<td>0.228</td>
</tr>
<tr>
<td>Engine speed</td>
<td>1000 rpm</td>
</tr>
</tbody>
</table>
21795 cells  
(CA = -6°)

32146 cells  
(CA = -6°)

41599 cells  
(CA = -6°)
Figure E.1. Air motions in the combustion chamber at various crank angles
APPENDIX F

The figures in the following pages show the spray formation in the combustion chamber at crank angles; -5, -1, 3, 7, 11 and 13 degrees. The figures are obtained setting:

- Time step: 1.00000e-5 sec
- Time step max.: 5.00000e-5 sec
- Swirl: 1.4
- Cyl. wall temp.: 500.0 K
- Cyl. head temp.: 500.0 K
- Piston temp.: 500.0 K
- Initial pressure: 2.28e+6 dyne/cm²
- Initial temp.: 314.5 K
- Squish: 0.228
- Engine speed: 1000 rpm

Injection Characteristic: Auto adjusted (up shifted or down shifted) by KIVA to ensure injection of right fuel quantity 0.1282 g

Figure F.1. Injection characteristic (arbitrary units)
Figure F.2. Spray formation in the combustion chamber at various crank angles
APPENDIX G

The figures in the following pages show the vapor distribution in the combustion chamber at crank angles; -5, -1, 3, 7, 11 and 13 degrees. The figures are obtained setting:

- Time step: 1.000000e-5 sec
- Time step max: 5.000000e-5 sec
- Swirl: 1.4
- Cyl. wall temp: 500.0 K
- Cyl. head temp: 500.0 K
- Piston temp: 500.0 K
- Initial pressure: 2.28e+6 dyne/cm²
- Initial temp: 314.5 K
- Squish: 0.228
- Engine speed: 1000 rpm

Injection Characteristic: Auto adjusted (up shifted or down shifted) by KIVA to ensure injection of right fuel quantity 0.1282g

Figure G.1. Injection characteristic (arbitrary units)
21795 cells (CA = -1°)

32146 cells (CA = -1°)

41599 cells (CA = -1°)
21795 cells (CA = +30°)

32146 cells (CA = +30°)

41599 cells (CA = +30°)
21795 cells
(CA= +7°)

32146 cells
(CA= +7°)

41599 cells
(CA= +7°)
21795 cells (CA= +11°)

32146 cells (CA= +11°)

41599 cells (CA= +11°)
Figure G.2. Vapor distribution in the combustion chamber at various crank angles
AUTOBIOGRAPHY

Fatih Deniz GENÇ was born in 1979 in Çanakkale. After attending Anatolian High School in Çanakkale, he continued his education in ITU, in Istanbul. In June 2001, he awarded B.Sc. degree in Mechanical Engineering. In 2002, he started attending ITU Science and Technology Institute, Automotive Engineering. He worked for ICDAS in 2003 as continuous casting engineer. He knows English (advanced) and German (intermediate).