Complex Chemistry Modeling
of
Diesel Spray Combustion

P A Niklas Nordin
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Make everything as simple as possible, but not simpler.

- Albert Einstein -
Papers

This thesis is based on the work carried out in the following papers.

Paper I.  N. Nordin and V. Golovitchev,
Numerical Evaluation of n-Heptane Spray Combustion at Diesel-like Conditions,
7th International KIVA Users Meeting at the SAE Congress, Feb 23, 1997, Detroit MI, Book of Abstracts, pp. 1-5

Paper II. V. Golovitchev, N. Nordin and J. Chomiak,
Numerical Evaluation of Dual Oxygenated Fuel Setup for DI Diesel Application,
SP-1276 Advances in SI and Diesel Engine Modeling, SAE Technical Paper Series,
SAE Paper 971596
The 1997 SAE Spring Fuels & Lubricants Meeting, May 5-7, Dearborn MI

Paper III. N. Nordin, V. Golovitchev and J. Chomiak,
Computer Evaluation of DI Diesel Engine Fueled with Neat Dimethyl Ether,
Proceedings of the 22nd CIMAC International Congress on Combustion Engines,
Copenhagen 18-21 May 1998, Vol I

Paper IV. V. Golovitchev, N. Nordin and J. Chomiak,
Neat Dimethyl Ether: Is It Really a Real Diesel Fuel of Promise?,
SAE Paper 982537 presented at the
International Fall Fuels & Lubricants Meeting & Exposition
San Francisco, CA, October 19-22, 1998

Paper V. V. Golovitchev, N. Nordin, J. Chomiak, K. Nishida and K. Wakai,
Evaluation of Ignition Quality of DME at Diesel Engine Conditions,
4th International Conference, ICE99
Internal Combustion Engines: Experiments and Modeling, pp. 299-306
September 12-16, 1999, Capri - Naples

Paper VI. V. Golovitchev, N. Nordin, R. Jarnacki and J. Chomiak,
3-D Diesel Spray Simulations Using a New Detailed Chemistry Turbulent Combustion Model,
Presented 19-22 June 2000, Paris, France at:
CEC/SAE International Spring Fuels & Lubricants Meeting and Exposition
Abstract

This thesis illustrates the application of computational fluid dynamics (CFD) to turbulent reactive two-phase flows in piston engines.

The focus of the thesis lies on numerical simulations of spray combustion phenomena with an emphasis on the modelling of turbulence/chemistry interaction effects using a detailed chemistry approach. The turbulence/chemistry interaction model accounts for the effects of turbulent micro-mixing on the chemical reaction rates. The models have been implemented in the KIVA3-V code [1, 2, 3] and successfully applied to spray combustion analysis in a constant volume and a DI Diesel engine. The limitations and difficulties of representing the spray in a Lagrangian fashion are also addressed.

Three different liquid fuels have been used in the simulations: n-heptane, methanol and dimethyl ether (DME). Detailed and reduced chemical mechanisms have been developed and validated for all these fuels and reasonable agreement between experimental data and numerical simulations has been obtained.
Nomenclature

*When I use a word it means just what
I choose it to mean - neither more nor less.*

- Humpty Dumpty

<table>
<thead>
<tr>
<th>Latin Letters</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c$</td>
<td>Molar concentration</td>
</tr>
<tr>
<td>$C_D$</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat at constant pressure</td>
</tr>
<tr>
<td>$c_{vd}$</td>
<td>Liquid specific heat at constant volume</td>
</tr>
<tr>
<td>$D$</td>
<td>Mass diffusion coefficient</td>
</tr>
<tr>
<td>$D$</td>
<td>Droplet diameter</td>
</tr>
<tr>
<td>$e$</td>
<td>Specific internal energy</td>
</tr>
<tr>
<td>$f_m$</td>
<td>Chemical source term</td>
</tr>
<tr>
<td>$h_m$</td>
<td>Specific enthalpy</td>
</tr>
<tr>
<td>$I$</td>
<td>Identity matrix</td>
</tr>
<tr>
<td>$J$</td>
<td>Heat flux vector</td>
</tr>
<tr>
<td>$k$</td>
<td>Turbulent kinetic energy</td>
</tr>
<tr>
<td>$m_d$</td>
<td>Droplet mass</td>
</tr>
<tr>
<td>$\dot{m}_d$</td>
<td>Droplet evaporation rate</td>
</tr>
<tr>
<td>$m_p$</td>
<td>Parcel mass</td>
</tr>
<tr>
<td>$N_r$</td>
<td>Number of reactions</td>
</tr>
<tr>
<td>$N_s$</td>
<td>Number of species</td>
</tr>
<tr>
<td>$p$</td>
<td>Gas pressure</td>
</tr>
<tr>
<td>$r$</td>
<td>Droplet radius</td>
</tr>
<tr>
<td>$S$</td>
<td>Rate of strain tensor</td>
</tr>
<tr>
<td>$T$</td>
<td>Gas temperature</td>
</tr>
<tr>
<td>$T_d$</td>
<td>Liquid droplet temperature</td>
</tr>
<tr>
<td>$u$</td>
<td>Gas velocity</td>
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<tr>
<td>$u_d$</td>
<td>Droplet velocity</td>
</tr>
<tr>
<td>$u_p$</td>
<td>Parcel velocity</td>
</tr>
<tr>
<td>$V$</td>
<td>Cell volume</td>
</tr>
<tr>
<td>$X_{\text{v,s}}$</td>
<td>Mass fraction fuel vapor at droplet surface</td>
</tr>
<tr>
<td>$X_{\text{v,\infty}}$</td>
<td>Mass fraction fuel vapor far away</td>
</tr>
</tbody>
</table>
Greek Letters

$\Delta t$  Integration step  
$\varepsilon$  Turbulent kinetic energy dissipation rate  $m^2/s^3$
$\mu$  Gaseous dynamic viscosity  $kg/ms$
$\nu$  Gaseous kinematic viscosity  $m^2/s$
$\kappa^*$  Reactive mass fraction  
$\kappa$  Reaction rate multiplier  
$\kappa$  Thermal conductivity  $W/mK$
$\rho$  Gas density  $kg/m^3$
$\rho_l$  Droplet/parcel/liquid density  $kg/m^3$
$\rho_m$  Partial density of the gaseous species  $kg/m^3$
$\rho_s$  Total liquid evaporation rate per unit volume  $kg/m^3s$
$\sigma$  Viscous stress tensor  $N/m^2$
$\tau$  Integration step  $s$
$\tau_u$  Momentum relaxation time  $s$
$\tau_e$  Evaporation relaxation time  $s$
$\tau_h$  Heat transfer relaxation time  $s$
$\tau_m$  Turbulent mixing time  $s$
$\dot{\omega}$  Chemical reaction rate  $mol/m^3s$

Dimensionless Numbers

$Nu$  Nusselt  total / conductive heat transfer ratio
$Oh$  Ohnesorge  viscous / ( inertia * surface tension )$^{(1/2)}$ force ratio
$Pr$  Prandtl  momentum / thermal diffusion ratio
$Re$  Reynolds  inertia / viscous force ratio
$Sc$  Schmidt  momentum / molecular diffusion ratio
$Sh$  Sherwood  mass / molecular diffusion ratio
$T$  Taylor  $Oh\sqrt{We}$
$We$  Weber  inertia / surface tension force ratio
Acknowledgments

Teamwork is essential - it allows you to blame somebody else
- Anonymous

This work was carried out at the Department of Thermo and Fluid Dynamics at Chalmers University of Technology and the Thermofluids Section of Department of Mechanical Engineering at Imperial College of Science Technology and Medicine. I am grateful to many people, but I wish to express my sincere gratitude especially to the people below, who have contributed more than others. If someone feels left out I apologize, it is only because my memory serves me ill.

Chalmers University of Technology

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For her love - Camilla Ljus, it would definitely not be as good without you.

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This document has been typeset using \LaTeX.
1 Introduction

“The time has come”, the Walrus said,
“to talk of many things”
- L. Carroll

1.1 Motivation
The Diesel engine is facing a challenging task. Either reduce emissions or be legislated out of existence. Future environmental legislation will require both soot and NOx emissions to be reduced drastically. It is highly doubtful that the Diesel engine can meet these demands without post/exhaust treatment, since developing and testing a new Diesel engine has been, and still is, done by experiments, which is a time consuming and expensive task. Even though experimental research is reliable it offers little feedback (in terms of what can be improved and how to improve it) as the engine essentially is a black box. What came out and what went in is known, but the important process in-between is not well known. By using computational fluid dynamics (CFD) in conjunction with experiments it is possible to drastically reduce the time and cost of the engine development procedure. Feedback and ideas of how to improve details can also be obtained, since CFD allows the engineer to see what is actually happening. Even though CFD is still not reliable enough to be trusted exclusively, its value cannot be argued. Reliable CFD models are, therefore, the key to better and more predictive computations.

1.2 Turbulent Diesel Spray Combustion
Diesel spray combustion is one of the most difficult problems of applied macroscopic physics as it involves the most difficult problems of turbulence, chemistry and two phase flows. These are problems that are tightly coupled and highly non-linear, with time and length scales that are so small that it’s questionable if they will ever be possible to resolve. The turbulence-chemistry interaction is very strong and it is therefore essential to have a reliable interaction model for this process if accurate predictions of emissions are to be performed. To account for the influence of the turbulent fluctuations on the reaction rate the Partially Stirred Reactor (PaSR) approach has been used. This model is described in detail in Section 3.

Accurate pollutant predictions require a number of species and reactions, in which the number is limited by the computational resources. A realistic approximation typically states that a complex hydrocarbon combustion system contains 1000’s of species with 10000’s of reactions. Using this many species and reactions is not possible today in a CFD application. Still, as always, the more species and reactions that are included, the better the accuracy. It is therefore attractive to be able to include and handle a comprehensive chemical mechanism.
Reducing both soot and NO, is a well investigated problem, known as 'The Diesel dilemma.' It has haunted generations of engineers and will probably continue to do so. Its consequence is that by reducing the soot, NO is increased, and vice versa. However, by reducing the injector orifice and increasing the fuel injection pressure it is possible to reduce them both [17]. Another recent approach is to use oxygenated fuel, in which the oxygen atoms are readily available in the fuel itself. Among these fuels, methanol and dimethyl ether, CH₃OH and (CH₃)₂O, respectively, have been analyzed, and their quality as a possible substitute for hydrocarbon fuels has been evaluated.

1.3 Lagrangian Spray Calculations

The Diesel spray creates a highly turbulent field with very strong gradients. The diameter of the liquid spray is on the order of 0.1 mm and the liquid velocity around 200-400 m/s. The subsequent ignition and combustion involve length scales that are even smaller and resolving this would require an enormous amount of memory and computational time. Hence, using a coarse computational mesh is today a necessity. But, together with models for the sub-grid processes, it is possible to obtain results. Treating the spray in a Lagrangian way is today also a necessity since it does not require the nozzle region to be fully resolved by the computational mesh. In the Lagrangian description, the spray is represented by points, often referred to as parcels or droplets. The more points, the more accurate representation of the spray. These points are then assigned properties which may be as many as desired, some basic ones are location, velocity, diameter, mass, temperature and fuel composition. Since these points are of zero dimension and do not occupy any space in the domain, they only serve one purpose: To act as a marker. The Eulerian equations, for the gas, need to know in which cell the liquid/gas exchange takes place, so that the interaction terms can be distributed in the correct position. These points are then tracked through the domain, in which they move from cell to cell, according to the implemented physics and distribute mass, momentum and energy.

The other approach, where one treats the spray in an Eulerian way, requires the nozzle to be resolved and because of the large difference in scale between the injector orifice and the bore of the cylinder, and limitations in computer power, the computational time using this approach is much longer and often too long for practical purposes. Even though computer speed is doubled every 18-24 months, according to Moore’s law, a practical Eulerian treatment of the spray, with all the physical processes included, will not be realizable for some time. However, with the available computer power it is now possible to have a computational mesh in which the cells are of the same order as the nozzle diameter. This is already a reality when performing Large Eddy Simulations with sprays and it leads to some intricate problems. A simple question like

- In which cell(s) is this parcel/droplet located?

is suddenly a very computationally expensive question to ask, especially since the parcel/droplet may occupy multiple cells. Thus, in order to treat the spray in a truly correct
way and obtain a correct source term distribution of the Lagrangian interaction terms
the “point-representation” has to be replaced by a “sphere-representation”, or rather a
non-zero dimensional representation. Another problem related to this situation, is the
fact that a computational cell may be occupied by only liquid and no gas. Numerically
this leads to singularities, since the gaseous volume tends towards zero, and it has still
not been established whether or not this phenomenon is important enough to include.
While some claim that it can be ignored, it is the authors feeling that ignoring physics
can never be the correct path to follow. This is, however, a question for future research.

1.4 The CFD codes
Two different CFD codes have been used in the work carried out in this thesis. All of
the computations have been carried out using the KIVA3-V code [2] developed at Los
Alamos National Laboratories, mainly by A. Amsden. All of the work carried out on
implementing the Lagrangian description of the spray has been done using the FOAM
(Field Operation And Manipulation) package [36], developed at Imperial College, mainly
by H. Weller. The transition from KIVA to FOAM was based on the limitations in the
fortran77 programming language, which KIVA is written in. Since FOAM is written in
C++, it is a more attractive environment, as the complexity of the CFD code is increased
substantially when a Lagrangian description is added to represent the liquid phase.

1.5 Structure of the Thesis
The basic equations for both the gaseous and liquid phase, together with the sub models
for the spray, are presented in Section 2. This is followed by a detailed description and
discussion of the turbulence/chemistry interaction model in Section 3. In Section 4 the
authors experience from implementing a Lagrangian description of the spray is shared.
The results in Section 5 are findings that have not been included in the papers. The
conclusions are drawn in Section 6, after which future work is discussed in Section 7.
2 Governing Equations

Now is a good time to put your work on a firm theoretical foundation.
- Sam Morgan

This section presents the governing equations for both the Eulerian and Lagrangian representation of the gas and liquid phase. Here, unless stated otherwise, the governing equations have been averaged.

Due to the Eulerian/Lagrangian coupling the Eulerian equations will have extra source terms to account for the phase interaction. The numerical treatment and implementation of these source terms will be discussed in Section 4.

2.1 The Gas (Eulerian) Phase

Performing a calculation involving combustion requires a minimum of 3 components (fuel, oxidizer and products) and the governing equations for a multi-component mixture must therefore be used.

2.1.1 The Continuity Equation

The continuity equation, or rather species transport equation, for one component in a multi component mixture reads

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m u) = \nabla \cdot \left[ \rho \mathcal{D} \nabla \left( \frac{\rho_m}{\rho} \right) \right] + f_m + \dot{\rho}_m \delta_{m1} \quad (1)$$

where $\rho_m$ is the mass density of species $m$, $\rho$ the total gaseous mass density, $u$ the gas velocity, $f_m$ the source/sink term due to chemistry (25) and $\dot{\rho}_m$ the source due to the evaporation of the liquid\(^1\). (By convention the fuel is commonly set to species/component 1.) $\mathcal{D}$ is the mass diffusion coefficient, where we assume Fick’s law of binary diffusion with a single diffusion coefficient as defined in Equation (23). $\mathcal{D}$ includes the turbulent diffusivity replacing the correlations $\rho_m u'$, which are modeled using a Boussinesq hypothesis. Note that all species diffuse equally, which is only true where the diffusion is dominated by turbulent diffusion, as it is here. The Souret and Dufour effects together with thermal radiation have been neglected. By forming the sum, $\rho = \sum \rho_m$, for (1) over all species, the global continuity equation is obtained

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{u} \rho) = \dot{\rho} \quad (2)$$

\(^1\)This thesis only deals with single component fuels. Thus, the Dirac function is limited to just $j = 1$ in the general case with $\delta_{mj}$.
The equation for the liquid evaporation rate, \( \dot{\rho}^* \), is given by the relation

\[
\sum_{V} N_p \dot{m}_d = - \int_{V} \dot{\rho}^* dV = -V \dot{\rho}^*
\]

where the l.h.s sum is the sum over all the spray parcels in the cell volume, \( V \) is the volume of the cell, \( N_p \) the statistical number of droplets in the parcel and \( \dot{m}_d \) is the evaporation rate for a single droplet, given by Equation (42).

2.1.2 The Momentum Equation

The averaged momentum equation for the gas reads

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{\sigma} + \mathbf{F}^* + \rho \mathbf{g} - \frac{2}{3} \nabla (\rho k)
\]

where \((\mathbf{u} \mathbf{u})_{ij} = u_i u_j\), \( p \) is the gas pressure, \( \mathbf{\sigma} \) the viscous stress tensor, defined below, \( \mathbf{F}^* \) the rate of momentum gain/loss per unit volume due to the spray [3, p.16] and \( \mathbf{g} \) the specific body force, which is assumed to be constant.

\[
\mathbf{\sigma} = 2\mu \mathbf{S} + \lambda \nabla \cdot \mathbf{u} \mathbf{I}
\]

where

\[
\mathbf{S} = \frac{1}{2} \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right]
\]

where \( \mu \) and \( \lambda \) are the first and second coefficients of viscosity (including turbulent viscosity), see Equation (22).

2.1.3 The Energy Equation

The internal energy equation reads

\[
\frac{\partial (\rho e)}{\partial t} + \nabla \cdot (\rho \mathbf{u} e) = -\rho \nabla \cdot \mathbf{u} - \nabla \cdot \mathbf{J} + \rho \dot{\varepsilon} + \dot{Q}^e + \dot{Q}^s
\]

where \( e \) is the specific internal energy, exclusive of chemical energy, and \( \mathbf{J} \) is the heat flux vector (8) which is the sum of heat conduction and enthalpy diffusion:

\[
\mathbf{J} = -\kappa \nabla T - \rho \mathbf{D} \sum_m h_m \nabla \left( \frac{\rho_m}{\rho} \right)
\]

where \( T \) is the gas temperature and \( h_m \) is the specific enthalpy of species \( m \). The source terms \( \dot{Q}^s \) and \( \dot{Q}^c \) are due to the chemical heat release, Equation (9), and spray interaction [3, p.19], respectively.

\[
\dot{Q}^s = \sum_{r=1}^{N_r} q_r \dot{\omega}_r
\]
where $\omega_r$ is defined in Equation (26) and $q_r$ is the heat of reaction $r$ at the reference temperature

$$q_r = \sum_{s=1}^{N_s} (\epsilon'_{sr} - \epsilon'_{sr}(h_s)_{r}^{ref}) \tag{10}$$

where $(h_s)_{r}^{ref}$ is the heat of formation of species $s$ at the reference temperature.

### 2.1.4 The Turbulence Equations

Although there are numerous turbulence models available in the literature today, the $k$-$\varepsilon$ model and the RNG version of it, are the only models that have been used throughout the work carried out in this thesis. For sake of completeness they will be presented here as well.

Since the $k$-$\varepsilon$-models originally was developed for incompressible stationary flows, they have been modified to account for the effects of compressibility $(\sigma : \nabla \mathbf{u})$ and spray interaction $(\dot{W}s)$, see [3, p.19].

The turbulent modulation due to the presence of a Diesel spray is a complex and not well known process. In the standard versions of the KIVA codes the spray source in the $k$-equation can only act as a sink, i.e., the turbulent energy is reduced in the presence of a liquid parcel, see [3]. This is, however, in compliance with the assumption that the liquid volume fraction is negligible and the droplets are small in comparison to the turbulent length scales. For a more detailed discussion on this topic see [22].

The $k$-$\varepsilon$-model reads

$$\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} k) = -\frac{2}{3} \rho k \nabla \cdot \mathbf{u} + \sigma : \nabla \mathbf{u} + \nabla \cdot \left[ \left( \frac{\mu}{\Pr_l} \right) \nabla k \right] - \rho \varepsilon + \dot{W}s \tag{11}$$

and

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \varepsilon) = - \left( \frac{2}{3} C_{e1} - C_{e3} \right) \rho \varepsilon \nabla \cdot \mathbf{u} + \nabla \cdot \left[ \left( \frac{\mu}{\Pr_c} \right) \nabla \varepsilon \right]$$

$$+ \frac{\varepsilon}{k} \left( C_{e1} \sigma - C_{e3} \rho \varepsilon + C_s \dot{W}s \right) \tag{12}$$

where $\sigma : \nabla \mathbf{u} = \sigma_{ij} \partial u_i / \partial x_j$ and the different constants are given in Table 1.

The value of $C_s = 1.5$ has been suggested by O’Rourke in [27], based on the postulate of length scale conservation in spray/turbulence interaction. This can easily be shown. Assume constant density and an absence of gradients. Equations (11) and (12) are then reduced to$^2$

$$\frac{\partial k}{\partial t} = \dot{W}s, \quad \frac{\partial \varepsilon}{\partial t} = C_s \frac{\varepsilon}{k} \dot{W}s \tag{13}$$

$^2$If a conclusion, whether the constant $C_s$ should be 1.5, or larger/smaller, one must also neglect $\varepsilon$. Further discussion of this topic can be found in Appendix B
and thus
\[ C_s \frac{\varepsilon}{k} \frac{\partial k}{\partial t} = \frac{\partial \varepsilon}{\partial t}. \] (14)

The turbulent length scale is defined as \( l_t = k^\alpha / \varepsilon \), where \( \alpha = 1.5 \). Differentiation yields,
\[ \frac{\partial l_t}{\partial t} = \frac{\partial}{\partial t} \left( \frac{k^\alpha}{\varepsilon} \right) = \frac{k^\alpha}{\varepsilon^2} \left( \frac{\varepsilon}{k} \frac{\partial k}{\partial t} - \frac{\partial \varepsilon}{\partial t} \right) \] (15)

and for (15) to be zero, Equation (14) gives that \( C_s = \alpha \) for \( l_t \) to be preserved.

It can, however, be argued that the length scale really is conserved, since the dispersed phase, as long as the droplets are small, introduces additional dissipation, without affecting \( \tilde{u} \). Consequently it should lead to a reduction of \( l_t \). Thus looking at Equation (15) again, using (13), yields
\[ \frac{\partial l_t}{\partial t} = \frac{k^\alpha}{\varepsilon^2} \left( \frac{\varepsilon}{k} \frac{\partial k}{\partial t} - \frac{\partial \varepsilon}{\partial t} \right) = \frac{k^{\alpha-1}}{\varepsilon} \tilde{W}^* (\alpha - C_s) < 0 \] (16)

which states that \( C_s \) must be less than \( \alpha = 1.5 \), since \( \tilde{W}^* < 0 \) here, for Equation (16) to be valid. The value of \( \varepsilon \) is constrained to satisfy the inequality
\[ \varepsilon \geq \left( \frac{C_p}{Pr_\varepsilon (C_{e_1} - C_{e_2})} \right)^{\frac{1}{2}} \frac{k^{3/2}}{L_{sgs}} \] (17)

where \( L_{sgs} \) is an input sub grid length scale whose value is typically taken to be \( 4 \delta x \), where \( \delta x \) is a representative computational cell dimension. This prohibits the turbulent length-scale, \( l_t \), to grow beyond \( L_{sgs} \).

In the RNG \( k-\varepsilon \) model, as described in [15], the \( \varepsilon \)-equation is modified to read
\[ \frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{u}) = - \left( \frac{2}{3} C_{e_1} - C_{e_3} + \frac{2}{3} C_p C_n \varepsilon \nabla \cdot \mathbf{u} \right) \rho \varepsilon \nabla \cdot \mathbf{u} \]
\[ + \nabla \cdot \left[ \left( \frac{\mu}{Pr_\varepsilon} \right) \nabla \varepsilon \right] + \frac{\varepsilon}{k^2} \left[ (C_{e_1} - C_{e_2}) \mathbf{\sigma} : \nabla \mathbf{u} - C_{e_3} \rho \varepsilon + C_s \tilde{W}^* \right] \] (18)

where
\[ C_n = \frac{\eta (1 - \eta / \eta_0)}{1 + \beta \eta^3}, \quad \eta = \frac{k}{S_m \varepsilon}, \quad S_m = (2S_{ij}S_{ij})^{1/2}, \] (19)

and
\[ \eta_0 = 4.38, \quad \beta = 0.012 \]

For ideal gases the molecular viscosity, \( \mu_{air} \sim T^m \), where \( T \) is the temperature and \( m=0.5 \), see Equation (22). \( C_{e_3} \) is also dependent on the polytropic exponent, \( n \), in the expression, \( p/\rho^n = \text{const} \), which describes the polytropic relation in a closed thermodynamic system.
Typically, \( n \), ranges from 1.3 to 1.4 and the value 1.4 has been used throughout the computations.

\[
C_{c_3} = \frac{-1 + 2C_{c_1} - 3m(n - 1) + (-1)^\delta \sqrt{6}C_{c_1}C_\eta \eta}{3} \tag{20}
\]

\[
\delta = \begin{cases} 
1, & \nabla \cdot \mathbf{u} \leq 0 \\
0, & \nabla \cdot \mathbf{u} > 0 
\end{cases} \tag{21}
\]

The model constants for the \( k-\varepsilon \)-models are summarized in Table 1.

<table>
<thead>
<tr>
<th>Model</th>
<th>( C_\mu )</th>
<th>( C_{c_1} )</th>
<th>( C_{c_2} )</th>
<th>( C_{c_3} )</th>
<th>( P_{rk} )</th>
<th>( P_{r_\varepsilon} )</th>
<th>( C_s )</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>Equation (20)</td>
<td>0.7194</td>
<td>0.7194</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Table 1: Model constants for the standard and RNG \( k-\varepsilon \) turbulence model.

and the transport coefficients

\[
\nu = \nu_{air} \left[ 1 + \sqrt{\frac{C_\mu k}{\nu_{air} \sqrt{\varepsilon}}} \right]^2, \quad \nu = \frac{\mu}{\rho}, \quad \mu_{air} = \frac{A_1 T^{3/2}}{T + A_2}, \quad \lambda = -\frac{2}{3} \mu \tag{22}
\]

\[
\kappa = \frac{\mu c_p}{P_r}, \quad D = \frac{\nu}{S_c} \tag{23}
\]

where the Prandtl and Schmidt numbers, \( P_r \) and \( S_c \), are input constants and

\[
A_1 = 1.457 \times 10^{-5}, \quad A_2 = 110.0
\]

### 2.1.5 The Chemistry Equations

Any multicomponent mixture involving chemical reactions of the form as in Table 2

1. \( C_7H_{16} + O_2 \rightarrow CH_2O + H_2O \)

: \( \vdots \)

\( N_r \). \( C_7H_{16} + O \rightleftharpoons C_7H_{15} + OH \)

Table 2: Excerpt of a chemical kinetic mechanism

may be written in the form

\[
\sum_{j=1}^{N_r} \partial_j^k c_j \rightleftharpoons \sum_{j=1}^{N_r} \partial_j^\eta c_j, \quad k = 1, N_r \tag{24}
\]
where \( \vartheta \) is the matrix of the stoichiometric coefficients for the forward reactions, \( \vartheta^t \) is the stoichiometric coefficients for the backward reactions and \( c_j \) the molar number for the \( j \)-th species, \( N_r \) is the number of reactions and \( N_s \) the number of species.

The chemical source term in the species transport equation (1) then reads

\[
f_m = M_m \sum_{r=1}^{N_r} (\vartheta^t - \vartheta^r) \dot{\omega}_r
\]

(25)

where

\[
\dot{\omega}_r = k^r_f \prod_{s=1}^{N_s} c_s^{\vartheta^r_s} - k^r_b \prod_{s=1}^{N_s} c_s^{\vartheta^r_s} = k^r_f \Pi_f - k^r_b \Pi_b
\]

(26)

and

\[
k^r = A_r T^{n_r} \exp \left( - \frac{E_a}{RT} \right)
\]

(27)

is the generalized Arrhenius reaction rate for the forward and backward reaction rate coefficients and \( n_r, A_r, \) and \( E_a \) are the corresponding steric factor, collision frequency exponent and activation energy, respectively.

### 2.2 The Liquid (Lagrangian) Phase

This section presents the equation of motion, evaporation and energy for the discrete phase. How to solve them numerically, is discussed in Section 4. The models for atomization, secondary breakup and collisions are also considered.

#### 2.2.1 The Equation of Motion

Although the momentum equation (Newton’s II law) for a discrete particle is very simple

\[
m_d \frac{du_d}{dt} = F
\]

(28)

where \( m_d, u_d \) and \( F \) are the droplet mass, droplet velocity and the force acting on the droplet, respectively, it presents, as will be shown, some intricate problems. From the pioneering work of Basset (1888), Boussinesq (1903) and Oseen (1927) the most general form of \( F \) is often referred to as the BBO equation and although it is still a subject of controversy, see [13], this is of minor importance in systems where the density ratio between the discrete and continuous phase is of the order \( 10^2 \) or higher. Under these conditions the added mass, Basset, Magnus (rotating droplets are not considered), Saffman, pressure and buoyancy force are often neglected and the BBO equation is reduced to just the drag and gravitational force (Although the gravitational force in Diesel sprays can also be neglected, it is included due to its simplicity). The acting force on the droplet is thus,

\[
F = -\frac{\pi D^2}{8} \rho C_D |u_d - u| (u_d - u) + m_d g
\]

(29)

\[
\]
where \( C_D \) is the drag coefficient. There are numerous proposals for the expression of the drag coefficient \( C_D \) [37, 32, 8, 22].

In this work the relation below has been used, ignoring all effects, such as evaporation rate, deformation and proximity (high liquid volume fraction) effects.

\[
C_D = \begin{cases} 
\frac{24}{Re_d} \left( 1 + \frac{1}{6} Re_d^{2/3} \right) & \text{Re} < 1000 \\
0.424 & \text{Re} > 1000 
\end{cases}
\]  

(30)

where

\[
Re_d = \frac{\rho |u_d - u| D}{\mu}
\]  

(31)

When solving the equation of motion in practice, Equations (28) and (29) are combined and written in the form

\[
\frac{du_d}{dt} = -\frac{u_d - u}{\tau_u} + g
\]  

(32)

where \( \tau_u \) is the momentum relaxation time defined below

\[
\tau_u = \frac{8 m_d}{\pi \rho C_D D^2 |u_d - u|} = \frac{4 \rho D}{3 \rho C_D |u_d - u|}
\]  

(33)

2.2.2 The Droplet Energy Equation

The liquid droplet receives its energy from the gas, which is used to increase the liquid temperature and overcome the latent heat of evaporation in order to evaporate the fuel. Unless the gas is saturated with fuel vapor, evaporation is always present, i.e., \( \dot{m}_d < 0 \), the evaporation process will receive its energy from the droplet. Thus, if the transferred heat, from the gas, is insufficient, the droplet temperature will decrease. The equation for the heat transfer to the liquid droplet is given by

\[
m_d \frac{dh_d}{dt} = \dot{m}_d h_v(T_d) + \pi D\kappa Nu(T - T_d) f
\]  

(34)

where

\[
f = \frac{z}{e^z - 1}, \quad z = -\frac{c_v \dot{m}_d}{\pi D\kappa Nu}
\]  

(35)

\( f \) is a factor [35] which corrects the rate of heat exchange due to the presence of mass transfer. In the review by Gösmán [11], various correlations for the Nusselt number are discussed in more detail. The correlation used here is

\[
Nu = 2.0 + 0.6 Re^{1/2} Pr^{1/3}
\]  

(36)

where the Prandtl number is defined as

\[
Pr = \frac{\mu c_p}{\kappa}
\]  

(37)
and all properties are evaluated using the film temperature, i.e., the 1/3-rule
\[ T_f = \frac{2T_d + T}{3}. \]  

Solving Equation (34) in practice is performed by introducing a characteristic heat transfer relaxation time, \( \tau_h \), defined as
\[ \tau_h = \frac{m_d c_l d}{\pi D \kappa N u}. \]

where \( c_l d \) is the specific heat for the liquid. Rearranging Equation (34), where
\[ h_d = c_l d (T_d - T_{ref}) \]

and using Equation (42), for the mass transfer, yields
\[ \frac{dT_d}{dt} = \frac{T - T_d}{\tau_h f} - \frac{1}{c_l d \tau_e} \]

where \( \tau_e \) is defined later in Equation (45).

### 2.2.3 The Droplet Mass Equation

In Diesel engines, the temperature and pressure are very high and the critical properties for hydrocarbons are very low, for instance the critical temperature and pressure for n-Heptane are 540.2 K and 2.74 MPa, thus, evaporation in classical terms does not really occur. These effects have not been addressed yet and are a subject for future research. They will therefore be ignored here.

The condensation process is not present in Diesel engines, thus, the only transfer of mass is from the liquid phase to the gas phase. Evaporation from a spherical liquid droplet has experimentally been established to follow the \( D^2 \)-law, i.e.,
\[ \frac{dD^2}{dt} = C_{evap} \]

see, for instance, [16]. However, the evaporation rate is more commonly expressed in terms of mass, or diameter, and the rate of evaporation for a single droplet is given by the expression
\[ \frac{d\dot{m}_d}{dt} = \dot{m}_d = -\pi DD \rho_v S h \ln \frac{p}{p_v} = -\pi DD \rho_v S h \ln \left( 1 + \frac{X_{v,s} - X_{v,\infty}}{1 - X_{v,s}} \right) \]

where \( \rho_v \) is the density of the fuel vapor close to the surface. This is estimated using the ideal gas law
\[ \rho_v = \frac{p}{R_v T_m} \]
where \( p \) is the gas pressure and assumed to be equal to the fuel vapor pressure close to the surface. The evaporation rate is increased by the relative velocity, which is accounted for by the Ranz-Marshall correlation\(^3\) \( Sh \), where \( Sh \) is the Sherwood number and here defined as

\[
Sh = 2.0 + 0.6 Re^{1/2} Sc^{1/3}
\]

In practice Equation (42) is solved by using an evaporation relaxation time, \( \tau_e \), as defined below:

\[
\tau_e = \frac{md}{\pi D\bar{S}h \rho \ln(1 + B)}
\]

where

\[
B = \frac{X_{v,s} - X_{v,\infty}}{1 - X_{v,s}}
\]

The evaporation rate is then given by the expressions

\[
\frac{dm_d}{dt} = -\frac{md}{\tau_e}, \quad \frac{dD}{dt} = -\frac{D}{3\tau_e}
\]

Since, the mass or diameter is always reduced, the equation above should be solved implicitly as it prevents the diameter, or mass, from becoming negative if too large time steps are used.

Although the pressure in a Diesel engine is typically above the critical conditions for the fuel, the following observation is important. If the liquid starts to boil, the vapor pressure rises above the ambient pressure, which yields \( B \to \infty \), and the evaporation relaxation time tends to zero, which in turn leads to the evaporation rate \( \dot{m}_d \to \infty \). In fact Equation (42) is no longer valid. Unless the liquid is close to the critical point, this infinite evaporation rate is not physical. The evaporation rate at boiling point therefore has to be coupled with the energy equation (34), since the evaporation rate is then governed by how fast heat can be supplied to the liquid.

Under boiling conditions the evaporation rate equation is deduced from (34), where the l.h.s. is equal to zero, since the temperature is constant under boiling conditions. The boiling mass transfer rate is then given by

\[
\frac{dm_d}{dt} = -\frac{\pi D\kappa Nu}{c_{p,v}} \ln \left( \frac{c_{p,v}}{h_v} (T - T_d) + 1 \right)
\]

Or using a characteristic boiling relaxation time

\[
\frac{dD}{dt} = -\frac{D}{\tau_{boil}}
\]

where

\[
\tau_{boil} = \frac{D^2 \rho_d c_{p,v}}{2\kappa Nu \ln \left( \frac{c_{p,v}}{h_v} (T - T_d) + 1 \right)}
\]

\(^3\)Originally proposed by Frössling (1938) [10].
Since Equation (42) becomes singular close to the boiling point, the mass transfer should be switched from (42) to (48) when \( \tau_{\text{bail}} > \tau_e \) and the saturation pressure is close enough to the surrounding pressure, where close enough is a matter of numerical robustness.

### 2.2.4 The Atomization Model

Since the purpose of the Lagrangian approach is to remove the necessity for resolving the nozzle, the initial conditions for the spray parcels must be specified. This can be done by using either an atomization model or by specifying the initial size and spray angle as constants, which can be seen as a very simple atomization model.

As both approaches need to be tuned for optimal performance, the latter approach has been used in the current work, since it is both simpler, faster and more straight-forward. Using an atomization model is, however, physically more correct, but any advantage of using an atomization model is clouded by the uncertainties in current breakup models.

### 2.2.5 The Breakup Model

When the liquid parcels have been injected they start to deform and break up. If the Weber number is high enough that is. The purpose of the breakup model is to reduce the characteristic size of the liquid parcels, due to aerodynamic forces, and, if the model includes it, to introduce new parcels, which are being stripped off the larger sized (parent) parcels. Today, there exist a number of breakup models and although the TAB model is the one that has been used the most (which is standard in the KIVA code), the Kelvin-Helmholtz Rayleigh-Taylor (KHRT) breakup model by Reitz, see [31, 34, 33] will be presented here, for reference, as it has been implemented in the KIVA3-V [2] code as well as the FOAM package [36]. The details of implementation can be found in Section 4.

The KHRT breakup model has two modes for breakup. The KH mode works as follows. New, child, parcels with the size

\[
r_c = B_0 \Lambda
\]

are stripped from the parent parcel and the radius of the parent parcel is reduced according to the rate expression

\[
\frac{dr}{dt} = -\frac{r - r_c}{\tau_{kh}}, \quad \tau_{kh} = \frac{3.788 B_1 D}{\Omega \Lambda}
\]

where \( B_0 = 0.61, B_1 = 40 \) are model constants and

\[
\Omega = \frac{0.34 + 0.38 W e^{1.5}}{(1 + Oh)(1 + T^{0.8})} \sqrt{\frac{\sigma}{\rho_d e^3}}
\]

\[
\Lambda = 9.02(1 + 0.45 \sqrt{Oh})(1 + 0.4 T^{0.7})
\]

\[
(1 + 0.865 W e^{1.67})^{0.6}
\]
where $\Lambda$ is the wavelength of the fastest growing wave $\Omega$, see Figure 1.

The Weber number for the gas is defined as

$$We = \frac{\rho|u_{rel}|r}{\sigma},$$

the Ohnesorge number is defined as $Oh = \sqrt{We\over \rho \varepsilon}$, and the Taylor number as $T = Oh \sqrt{We}$. The liquid Weber number $We_l$ is defined similar to $We$, but with the gas density replaced by the liquid density. The liquid Reynolds number is defined as

$$Re_l = \frac{\rho_l |u_{rel}|r}{\mu_l}.$$

The RT mode of breakup works in a slightly different way. The wavelength $\Lambda_t = \pi/K$, where

$$K = \sqrt{\frac{|g_t(\rho_t - \rho)|}{3\sigma}}, \quad g_t = (g + \frac{du_t}{dt}) \frac{u_t}{|u_t|}$$

is compared to the droplet size and if $\Lambda_t < r$, it is assumed that RT waves have started to grow on the surface of the droplets. (The droplet acceleration is obtained using Equation (32)). The life time of the growing RT waves is then tracked from then on, and when the life time exceeds the characteristic RT time $\tau_t = 1/\Omega_t$, where

$$\Omega_t = \sqrt{\frac{2}{\sqrt{2} \sigma}} \frac{|g_t(\rho_t - \rho)|^{3/2}}{\rho_t + \rho}$$

catastrophic breakup occurs, which immediately creates much smaller droplets. The RT breakup splits the parcel so that the new statistical number is increased by a factor of $r/\Lambda_t$ and the new droplet size is corrected to ensure conservation of mass.
2.2.6 The Collision Model

Among the spray sub-models, the \textit{weakest} model is the collision model. This is due to the built-in grid dependency, which will be explained below. First, collisions between parcels are only significant when the liquid volume fraction is high. Although all Diesel sprays are dense at the beginning, this is, however, a question of mesh resolution, since a computational mesh with small cells will yield a higher liquid volume fraction than a mesh with larger cells. The collision model by O’Rourke [26] states that:

\begin{quote}
Collision between two parcels occurs when they occupy the same computational cell and the probability for collision is higher than a threshold value based on the collision frequency,
\end{quote}

where the collision frequency is defined as

\[ v = \frac{\pi}{4V} N_{d,\text{small}} (D_{\text{small}} + D_{\text{large}})^2 |U_{d,\text{small}} - U_{d,\text{large}}| E_{12} \]

where $E_{12}$ is the collision efficiency\(^4\) [26]. Reducing the cell size will have two effects, increasing the chance for collision, according to Equation (58). But, it will also reduce the domain in which the parcels can meet. And since two parcels not in the same cell have zero probability of colliding, the probability increase in Equation (58), by reducing $V$, is of no importance. In the extreme, if the cell size is of the same order as the droplet size, only one droplet will occupy the cell and no collisions will occur.

Another weakness of this formulation is that there is an equal chance for collision regardless of whether the parcels are moving towards or away from each other, see Figure 2, and the chance for collision is much higher if the place of collision is inside a cell than

\begin{figure}[h]
  \centering
  \includegraphics[width=0.5\textwidth]{collision_example.png}
  \caption{Two different collision possibilities, in which the top pair of parcels have equal chance of colliding as the bottom pair.}
\end{figure}

if it is between two cells, where the latter is difficult to control in a complex geometry. These effects are investigated and discussed in more detail in Section 5.

Although the collision models developed by Berlemont [5] are more accurate, they are computationally very demanding.

Therefore, the following mesh independent formulation is hereby suggested

\(^4\text{In the KIVA codes } E_{12} = 1.0.\)
Collision between two parcels occurs if their trajectories intersect and the intersection point is reached at the same time, and within the integration step.

These conditions are, however, also quite computationally demanding if they are applied to all pairs of parcels. Therefore, to sort out impossible collisions, two prerequisites have to be met. First, from Figure 3 it can be deduced that in order for two parcels to collide they have to travel towards each other, or \( U_{12} > 0 \), where

\[
U_{12} = (U_1 - U_2) \cdot \frac{x_2 - x_1}{|x_2 - x_1|}.
\]

The second condition is that the parcels’ relative displacement must be larger than the distance between them, or \( U_{12} \Delta t > |x_2 - x_1| - (r_1 + r_2) \).

If these two requirements are met, the parcels have a chance of colliding and the postulate above can be expressed in mathematical terms. If, \( \alpha_0 \in [0, \Delta t] \) and \( \beta_0 \in [0, \Delta t] \), where \( \alpha_0 \) and \( \beta_0 \) is the solution to the system

\[
p_1 = x_1 + \alpha U_1, \quad p_2 = x_2 + \beta U_2, \quad \frac{\partial |p_2 - p_1|}{\partial \alpha, \beta} (\alpha_0, \beta_0) = 0.
\]

collision will occur if a random number, \( \xi \in [0, 1] \), is less than the collision probability \( P \), where

\[
P = \left( \frac{r_1 + r_2}{\max(r_1 + r_2, \Delta_{12})} \right) C_1 e^{-C_2 |\alpha_0 - \beta_0|/\Delta t}.
\]

where \( \Delta_{12} = |p_2(\beta_0) - p_1(\alpha_0)| \) is the minimum distance between the two trajectories and \( C_1 \) and \( C_2 \) are model constants. Where \( C_1 \) is the spatial probability decay outside the swept cylinders by the droplets and \( C_2 \) is the temporal probability decay. \( C_1 \) allows for trajectories that are 'close' to also have a chance of colliding. Since both \( \alpha_0 \) and \( \beta_0 \) contain the information of when the collision occurs in time, the term \( e^{-C_2 |\alpha_0 - \beta_0|/\Delta t} \) takes into account that the parcels must be at the same place at the same time.

This new condition for collision has been implemented in the KIVA code and the outcome of the collision is treated in the same way as the original model.
3 The Turbulence/Chemistry Interaction Model

We all agree that your theory is crazy,
but is it crazy enough?
- Niels Bohr

This section deals with how the chemical source terms in the species transport equation (1) have been modeled. The modeling approach uses a special technique, in which a reference species is introduced to compute both the reaction rate and the characteristic chemical time. As this procedure is closely connected with the modeling, it is explained in detail.

3.1 Introduction

It is not possible, with current computer technology, to resolve the flame structure for practical purposes. Because of the thinness and complex structure of the flame, the computational cell size has to be several orders of magnitude larger than required to resolve the flame structure.

And since it is only possible to resolve variables, e.g., species concentrations, on a scale which is of the same order as the cell size, the conditions in the combustion zone are thus, in principle, unknown. And since the source term, $f_m$, in the species transport equation (1) is a function of the combustion zone parameters, it is dependent on variables, not on a grid level, but on a sub-grid level. Hence, using only grid level information 'straight on' is, in most cases, not appropriate as the combustion region structure unresolved. Because of this, correlating the sub-grid conditions with grid level conditions is a necessity, since the grid level conditions are the only information available.

The remainder of this section deals with one approach to how to treat this problem.

3.2 Background

With the introduction of the Eddy Break-Up model (EBU) by Magnusen and Hjertager [24] in 1976, it became possible to treat turbulent diffusion combustion in a successful manner. Since then, the EBU model has become widespread and widely used in many CFD codes. The success of the model can mainly be attributed to two things, the simplicity of the model, plus, at the time, lack of other diffusion flame models. Although it was first and simple, it was not too simple. On the contrary. In a recent study by Gran [14], in which different alternatives for accounting for finite rate chemistry in turbulent combustion are investigated, it is concluded that the EBU concept is the most attractive approach for practical purposes. Since the introduction of the EBU model, other models

\[ \text{\footnotesize{5Although this study was not directly related with spray combustion.}} \]
have been derived, based on other principles, such as the flamelet concept [29], the probability density function (PDF) approach [30] or the Lagrangian approach [6]. There have also been extensions to the EBU concept. However, all of these approaches, except for the Lagrangian, have difficulties handling complex chemistry. The standard EBU only uses one global reaction. Although it is possible to extend it for complex chemistry, it is not clear how to do this. For instance, one way, different from the one used here, can be found in [7].

The flamelet concept is based on the assumption that the chemical time scale is much faster than the turbulence time scale. The flame is, hence, treated using a laminar approach, where the turbulence and chemistry have been decoupled. This is not appropriate for Diesel spray combustion as this concept cannot treat the important slow chemistry conditions, since this assumption is not valid. And for predicting the, for emissions, important flame lift-off [9], this is crucial. Although, the PDF, theoretically, is the most correct approach, the number and complexity of the various (unknown) correlations between species and temperature, make the system untreatable. Using a Lagrangian approach, the probabilistic Eulerian Lagrangian (PEUL) model can treat complex chemistry, although slow chemistry is treated separately using a reduced mechanism. In addition, fulfilling the balance equations locally is a problem in this approach. Thus, it leaves some room for improvement.

The Partially Stirred Reactor (PaSR) concept by Karlsson [17] is an extension of the EBU approach. The derivation is, however, somewhat ad hoc and based on several postulates. It has, however, proven to work very well for turbulent Diesel spray combustion and provides the first complex chemistry treatment of the problem.

This work is a continuation of the work carried out by Karlsson [17].

### 3.3 The Reference Species Technique

Solving a chemical system in a fully coupled fashion, when the number of reactions is of the order of about 100, is far too expensive. Hence, to treat a detailed mechanism, another approach has been developed in which the reaction set is solved sequentially, i.e., the reactions are accounted for one after another and the species are updated after each reaction and fed into the next reaction. Although the correctness of this is yet to be proven, it is based on the same reasoning as the widely used time splitting technique, which is used for instance in the KIVA codes, and thus, it appears to be acceptable. An alternative procedure is yet to be developed. Still, due to the stiffness of the system a special technique, using a reference species for each reaction, has been applied. This approach is appropriate when the integration step is larger than the smallest chemical time scale, since the same algorithm can be applied to all reactions without checking whether they are slow or fast (equilibrium).

Normally, by using this approach, the species in danger of being driven to negative concentration restricts the integration step.
3  THE TURBULENCE/CHEMISTRY INTERACTION MODEL

The reference species technique is used in the KIVA codes, [1, 2, 3], but is explained nowhere. It will therefore be explained here.

Consider the following elementary reaction

\[ \vartheta_1 c_1 + \vartheta_2 c_2 \xrightleftharpoons{k_f,k_b} \vartheta_3 c_3 + \vartheta_4 c_4 \]  \hspace{1cm} \text{(62)}

where \( \vartheta_i \) and \( c_i \) are the reaction stoichiometric coefficients and molar concentrations, respectively. For simplicity, it is assumed that all \( \vartheta_i = 1 \), since it is more specific for detailed chemistry, where the maximum value of \( \vartheta_i \) is two for the radical recombination reactions.

The rate equation for the above reaction is

\[ \frac{dc_1}{dt} = \frac{dc_2}{dt} = -\dot{\omega}, \quad \frac{dc_3}{dt} = \frac{dc_4}{dt} = \dot{\omega} \]  \hspace{1cm} \text{(63)}

where \( \dot{\omega} \) is defined similar to (26), but without the subscript.

When solving Equation (63), it is commonly accepted that one use an implicit scheme, since the reaction rate \( \dot{\omega} \) is dependent on both temperature and concentration and can differ in value by several orders of magnitude when the reactions proceed. The problem is illustrated by discretizing (63) for the forward reaction and assuming \( \dot{\omega} > 0 \)

\[ \frac{c_1^{n+1} - c_1^n}{\tau} = -\dot{\omega}^x \quad \Rightarrow \quad c_1^{n+1} = c_1^n - \tau \dot{\omega}^x \]  \hspace{1cm} \text{(64)}

where \( \dot{\omega}^x \) is either evaluated at \( x = n \), \( x = n + 1 \) or a combination of both.

If \( \dot{\omega}^x \) is evaluated at \( x = n \), it is clear from (64) that if the time step, \( \tau \), is sufficiently large, there is a danger of \( c_1^{n+1} \) becoming negative. Obviously, this is incorrect, since the concentrations should tend towards the equilibrium solution \( \dot{\omega} = 0 \), which for \( i = 1 \) yields

\[ c_i^{eq} = \left( \frac{k_bc_3c_4}{k_fc_2} \right)^{c_q} \]  \hspace{1cm} \text{(65)}

To overcome this deficiency, \( \dot{\omega}^x \) is evaluated at \( x = n+1 \) semi-implicitly in the following way. Differentiating \( \dot{\omega} \) with respect to time yields (\( k_f \) and \( k_b \) are held constant)

\[ \frac{d\dot{\omega}}{dt} = k_f \left( \frac{dc_1}{dt} c_2 + c_1 \frac{dc_2}{dt} \right) - k_b \left( \frac{dc_3}{dt} c_4 + c_3 \frac{dc_4}{dt} \right) \]  \hspace{1cm} \text{(66)}

which together with (63) yields

\[ \frac{d\dot{\omega}}{dt} = - (k_f(c_2 + c_1) + k_b(c_4 + c_3)) \dot{\omega} = -\alpha \dot{\omega} \]  \hspace{1cm} \text{(67)}

where

\[ \alpha = k_f(c_2 + c_1) + k_b(c_4 + c_3) \]  \hspace{1cm} \text{(68)}
Discretizing Equation (67) with a semi-implicit scheme yields
\[
\frac{\dot{\omega}^{n+1} - \dot{\omega}^n}{\tau} = -\alpha^n \dot{\omega}^{n+1} \quad \Rightarrow \quad \dot{\omega}^{n+1} = \frac{\dot{\omega}^n}{1 + \alpha^n \tau}
\] (69)

To update the species using \(\dot{\omega}^{n+1}\), with the above form of \(\dot{\omega}\), would not be appropriate either since the expression
\[
c_i^{n+1} = c_i^n - \tau \frac{\dot{\omega}^n}{1 + \alpha^n \tau} \xrightarrow{\tau \to \infty} c_i^n - \dot{\omega}^n = c_i^n - \left[ \frac{k_f c_1 c_2 - k_b c_3 c_4}{k_f (c_1 + c_2) + k_b (c_3 + c_4)} \right]^{n}
\] (70)
does not tend toward the equilibrium concentration \(c_i^e\), see Equation (65). In order to overcome this deficiency, the reference species concept is introduced. The reference species is defined as 'the species most in danger of being driven negative', thus, it is the species which is being consumed by the reaction and has the lowest concentration. For the sake of argument let’s assume the reference species to be \(c_r = c_1\), i.e., species one. The partner to species one is, thus, \(c_2\). Note, thus, that \(c_2 > c_1\) and by assuming that \(k_f c_2\) is larger than the other terms in (68) we have
\[
\alpha^n \approx \left( k_f c_2 \right)^n
\] (71)

With the above expression for \(\alpha^n\), \(\dot{\omega}^{n+1}\) can now be evaluated. For the reference species this yields
\[
c_i^{n+1} = c_i^n - \tau \frac{\dot{\omega}^n}{1 + \alpha^n \tau} \xrightarrow{\tau \to \infty} c_i^n - \dot{\omega}^n = c_i^n - \left( \frac{k_f c_1 c_2 - k_b c_3 c_4}{k_f c_2} \right)^n = \left( \frac{k_b c_3 c_4}{k_f c_2} \right)^n
\] (72)

This way, the equilibrium condition for each reaction is automatically ensured and there is no need to treat equilibrium reactions separately from the slow, kinetically controlled reactions\(^6\).

### 3.4 The Partially Stirred Reactor Concept

In the Partially Stirred Reactor (PaSR) approach, a computational cell is split into two different zones, one zone, in which all reactions occur, and another, in which no reactions occur. Thus, the composition changes due to mass exchange with the reacting zone. Furthermore, the reacting zone is treated as a perfectly stirred reactor (PSR), in which the composition is homogeneous (every species is assumed to be perfectly mixed with the other ones). This allows us to disregard any fluctuations when calculating the chemical source terms.

\(^6\)This statement is not really true, since \(c_i^e\) requires the equilibrium values of all the species. However, obtaining the true equilibrium value requires an iterative procedure which is computationally demanding and therefore avoided.
Because the computational cell is divided into two zones, the question now arise of how to split the cell into the reacting and non-reacting part. How large is the mass fraction of the mixture taking part in the combustion, and what governs the composition of it?

As it turns out, the key issue in the PaSR approach lies in answering these questions, as they describe the connection between the sub-grid information and the grid level information.

The reactive mass fraction will be defined below as the calculation is advanced one time step, from $c_0$ to $c_1$, see Figure 4.

![Figure 4: Conceptual picture of a PaSR](image)

First, the model distinguishes between three molar concentrations:

- $c_0$ is the averaged concentration in the feed of the cell and may be considered as the initial averaged concentration in the cell.
- $c$ is the unknown concentration in the reaction zone on a sub-grid level in the unknown reactive fraction of the cell material.
- $c_1$ is the sought for, time averaged reactor-exit concentration. This is also the averaged concentration in the cell.

Having established this, the reactor exit concentration can be obtained, from mass conservation considerations, looking at Figure 4, as

$$c_1 = \kappa^* c + (1 - \kappa^*) c_0$$  \hspace{1cm} (73)

where $\kappa^*$ is the mass fraction of the mixture that reacts. Investigating Equation (73) further, it is obvious that $c_1$ can be obtained using a linear interpolation between $c_0$ and $c$. Thus, plotting $c_0$, $c$ and $c_1$ in the diagram of Figure 5, the following observations can be made.

The whole process can be divided into two sub-steps, proceeding in parallel. In Figure 5, they are marked as $I$ and $II$:
I The initial concentration in the reaction zone changes from $c_0$ to $c$ as it reacts,

II The reactive mixture, $c_1$, is mixed with the unreactive mixture, $c_0$, by turbulence, resulting in the averaged concentration $c_1$

Since $c_1$ is the initial value for the next time step, the time between $c_0$ and $c_1$ must be the integration step, $\tau$. And since the turbulence mixes $c$ with $c_0$, the time difference between $c$ and $c_1$ must be the characteristic time for turbulence, $\tau_{mix}$. The total reaction time for path I in Figure 5, can, thus, be considered as being increased by the mixing time, from $\tau$ to $\tau + \tau_{mix}$.

From Figure 5 the following relations can be obtained, assuming that the slope of the curve is equal to the reaction rate in the reaction zone, $c$.

$$\frac{c_1 - c_0}{\tau} = \frac{c - c_1}{\tau_{mix}} = f_m(c) \quad (74)$$

The last assumption,

$$\frac{c - c_1}{\tau_{mix}} = f_m(c) \quad (75)$$

is also in agreement with the main assumption of the stationary flamelet approach in [20, p.630]. Thus,

$$\frac{c_1 - c_0}{\tau} = \frac{c - c_1}{\tau_{mix}} \quad (76)$$

which can be rearranged as

$$c_1 = \kappa^* c + (1 - \kappa^*) c_0, \quad \kappa^* = \frac{\tau}{\tau + \tau_{mix}} \quad (77)$$
3 THE TURBULENCE/CHEMISTRY INTERACTION MODEL

which clearly states that if the integration step is larger than the turbulent mixing time, \( i.e., \kappa^* \approx 1 \), then most of what comes out of the reactor will be from the reaction zone. Having established the reactive fraction, \( \kappa^* \), it remains to eliminate the unknown parameter \( c \) in order to obtain \( c_1 \).

Let us recapitulate the chemical source term in the species transport equation:

\[
    f_m(c) = \sum_{r=1}^{N_r} f_m^r = M_m \sum_{r=1}^{N_r} \left( \frac{\varphi'_{mr} - \varphi'_{mr}}{\varphi'_{mr} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}} - k_b^* \prod_{s=1}^{N_s} c_s^{q_{sr}}} \right) \\
    = M_m \sum_{r=1}^{N_r} \left( \frac{\varphi'_{mr} - \varphi'_{mr} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}}}{\varphi'_{mr} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}}} \right)^{\xi_1} \\
    - M_m \sum_{r=1}^{N_r} \left( \frac{\varphi'_{mr} - \varphi'_{mr} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}}}{\varphi'_{mr} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}} + \varphi'_{mr} k_r^* \prod_{s=1}^{N_s} c_s^{q_{sr}}} \right)^{\xi_2} \\
    = \sum_{r=1}^{N_r} (\xi_1 - \xi_2) = \xi_1 - \xi_2
\]

where \( \xi_1 \) and \( \xi_2 \) are both positive. Above, the reaction rate \( f_m(c) \), is evaluated at the reaction zone conditions \( c \). However, since \( c \) is sub-grid information, it must be replaced by something known on a grid level.

Using Taylor expansion yields

\[
    f_m(c) = f_m(c_1) + \frac{\partial f_m}{\partial c} (c - c_1) + \frac{1}{2} \frac{\partial^2 f_m}{\partial c^2} (c - c_1)^2
\]

where the diagonal elements in \( \frac{\partial f_m}{\partial c} \) are zero and the off-diagonal elements are neglected. It should be noted that the Taylor expansion does not contain any derivatives of a higher order than two. Further, it is assumed that the dominating term in the Jacobian is with respect to the reference species, \( i.e., \partial f_m/\partial c_r \). The chemical time can then be defined from the Jacobian element

\[
    \frac{1}{\tau_c} = \frac{\partial f_m}{\partial c_r}
\]

(Obtaining the chemical time involves the same assumptions as when obtaining (71), which is discussed in Section 3.3). Equation (79) now reads

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

By substituting the expression for \( c \) in (81) with (77), we obtain

\[
    \frac{c_1 - c_0}{\tau} = f_m(c) = f_m(c_1) - \frac{1}{\tau_c} \left[ \left( \frac{c_1}{\kappa^*} - \frac{1}{\kappa^* c_0} \right) - c_1 \right]
\]
which leads to

$$\frac{c_1 - c_0}{\tau} = f_m(c_1) - \frac{1}{\tau_c \kappa^*} \left( c_1 - \kappa^* c_1 - (1 - \kappa^*) c_0 \right) = f_m(c_1) - \frac{1 - \kappa^*}{\tau_c \kappa^*} \left( c_1 - c_0 \right) \quad (83)$$

The terms containing $c_1 - c_0$ can, now, be grouped together as

$$\left( \frac{1}{\tau} + \frac{1 - \kappa^*}{\tau_c \kappa^*} \right) (c_1 - c_0) = f_m(c_1) \quad (84)$$

and after manipulating the lhs, it takes the form

$$\left( \frac{1}{\tau} + \frac{\tau_{mix}}{\tau_c \tau} \right) (c_1 - c_0) = \frac{c_1 - c_0}{\tau} \frac{\tau_c + \tau_{mix}}{\tau_c} \frac{1}{\kappa} = f_m(c_1) \quad (85)$$

which finally yields

$$\frac{c_1 - c_0}{\tau} = \kappa f_m(c_1) \quad (86)$$

where

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}} \quad (87)$$

and the final result can be summarized as:

$$f_m(c) = \kappa f_m(c_1) \quad (88)$$

This is the correlation for the chemical source term on a sub-grid level, based on the resolved information. Note that, $f_m(c_1)$ is treated implicitly, by using information from the next time step, as described in detail in Section 3.3.

The exchange process between the fresh, unreacting mixture and the burned gases is accounted for by the characteristic time $\tau_{mix}$.

There is a wide range of scales in turbulent flows, from the largest eddies down to the molecular level, and to account for all these different scales using only one characteristic value is of course a great simplification. The question is what to base the representation $\tau_{mix}$ on. In a study by Kjeldman [19] three different options have been investigated. They were related to the Kolmogorov time scale,

$$\tau_k \sim \left( \nu/\varepsilon \right)^{1/2},$$

the Taylor time scale,

$$\tau_t \sim k/\varepsilon,$$

and a geometrical mean of the Kolmogorov and Taylor time scales,

$$\tau_{kc} \sim \sqrt{\tau_k \tau_t},$$

which was proposed by Karlsson and Chomiak [18]. Kjeldman reported that the Karlsson and Chomiak approach was better than using only the Kolmogorov time, but the best
results were obtained using the Taylor scale. This result is in agreement with the findings here, where \( \tau_{mix} \) has been obtained from the \( k-\varepsilon \) equation,

\[
\tau_{mix} = C_{mix} \frac{k}{\varepsilon},
\]

and the model constant \( C_{mix} \) was set to 0.005. This constant can, however, vary between 0.001-0.3, depending on the flow. It should be noted that using \( \tau_{mix} \sim k/\varepsilon \) might not always yield the best results, depending on the flow situation, as well as the chemical mechanism. Moreover, the small value of \( C_{mix} \) might be an indication that the Karlsson and Chomiak approach will yield better results using a larger constant in front of \( \sqrt{\tau_{k}} \).

### 3.5 The PaSR Model: Observations and Implications

Treating the reactive fraction in a Lagrangian fashion, the governing equation for the reacting species on a sub-grid scale is

\[
\frac{dc}{dt} = D_{sgs} \nabla^2 c + f(c)
\]

where \( D_{sgs} \) is the sub-grid diffusion. Solving (90) presents some fundamental problems. First, the problem is not well posed, since calculating \( c(t_{n+1}) \) requires \( c(t_n) \), which is unknown. Second, the spatial resolution is too coarse to resolve the discretized operator \( \nabla \).

Since the \( \nabla \) operator is unresolved, the operator \( D_{sgs} \nabla^2 \) is modeled by the turbulent characteristic time as

\[
D_{sgs} \nabla^2 \approx -\frac{1}{\tau_{mix}}
\]

where \( \tau_{mix} \) is obtained from the turbulence model. Note that \( c \) must be replaced by \( c - c_1 \) in order to satisfy the equilibrium constraint \( c \to c_1 \) as \( dc/dt \to 0, f(c) \to 0 \). Equation (90) now reads

\[
\frac{dc}{dt} = -\frac{c - c_1}{\tau_{mix}} + f(c),
\]

which is the same equation as used in the probabilistic Eulerian Lagrangian (PEUL) model \([6]\); if \( \tau_{mix} = \tau_{IEM} \), where \( \tau_{IEM} \) is defined as the characteristic time for Interaction Exchange with the Mean.

However, using relation (74) we obtain

\[
\frac{dc}{dt} = -f(c) + f(c) = 0
\]

implying that \( c \) is in equilibrium/steady-state.

This implies that the reactions in the reactive zone proceed at a rate determined by how strong the mixing, or interaction with the mean, is.
Further, let us consider the reaction rate for reaction \( i \)

\[
f^i_m(c) = \xi^i_1 - \xi^i_2 \tag{94}
\]

and recall the definition of the reference species, \( c_r \), which is used to calculate the reaction rate. Linearizing Equation (94) around \( c_r \), by using the information at the current time step, we find that the linear form of (94) is given by (since \( c_r \) is only present in \( \xi^i_2 \))

\[
f^i_m(c) = (\xi^i_1)^0 - (\xi^i_2)^0 \frac{c_r}{c^0_r} \tag{95}
\]

Differentiating (95) yields,

\[
\frac{df^i_m(c)}{dt} = -\frac{(\xi^i_2)^0}{c^0_r} \frac{dc_r}{dt} = -\frac{(\xi^i_2)^0}{c^0_r} f^i_m(c), \tag{96}
\]

since \( (\xi^i_1)^0 \) and \( (\xi^i_2)^0 \) are held constant. To obtain the reaction rate at the next time step, a semi-implicit scheme is applied to (96), (superscript zero is the value at this time step and superscript one denotes the value at the next time step)

\[
\frac{df^i_m(c)}{dt} = f^1 - f^0 = -\frac{(\xi^i_2)^0}{c^0_r} f^1 \tag{97}
\]

which yields,

\[
f^1 = \frac{f^0}{c^0_r + (\xi^i_2)^0 \tau} c^0_r = -\frac{1}{\tau_c} c^0_r, \quad \tau_c = -\frac{c^0_r + (\xi^i_2)^0 \tau}{f^0} \tag{98}
\]

Equation (98) yields an expression for both the reaction rate at the next time step and the chemical time. By inserting (98) in (88) we find

\[
f^i_m(c) = \kappa f^i_m(c^1) = \frac{\tau_c}{\tau_c + \tau_{mix}} f^i_m(c^1) \tag{99}
\]

With the above expression for the reaction rate (99) two limiting extremes can be identified, the homogeneous rate, \( \tau_{mix} \to 0 \), and, the mixing controlled rate, where the term \( f^0 \tau_{mix} \) is dominant.

Investigating the first case, \( \tau_{mix} \to 0 \), yields

\[
f^i_m(c) = \frac{f^0 c^0_r}{c^0_r - f^0 \tau_{mix} + (\xi^i_2)^0 \tau} \to \frac{f^0}{1 + (\xi^i_2)^0 \tau/c^0_r} \tag{100}
\]
where the reaction rate is reduced to a quasi-laminar approach, where $c = c^1$, according to Equation (77), in the reaction rate terms.

Investigating the second case, where $f^0_{m\text{mix}}$ dominates, yields

$$f^i_m(c) = \frac{f^0_{c_0} \cdot c_0}{c_r - f^0_{c_0} \cdot \left( \frac{c_0}{1 + s} \right)} \rightarrow -\frac{c_r}{\tau_{\text{mix}}} \tag{101}$$

which is equivalent to the eddy break-up rate, in particular the Magnussen and Hjertager [24] reaction rate. To illustrate this, let us start with the expression for the reaction rate given in [24]

$$f(c) = -A \frac{c^3}{k} \min \left( c_f, \frac{c_o}{s} \cdot \frac{B_c p}{1 + s} \right) = -A \frac{1}{\tau_{\text{mix}}} \min \left( c_f, \frac{c_o}{s} \cdot \frac{B_c p}{1 + s} \right) \tag{102}$$

where $A$ and $B$ are model constants and $c_f$, $c_o$ and $c_p$ are the fuel-, oxidizer- and product concentration, respectively. It should be noted that the Magnussen model is valid only for one global reaction, in the form,

$$c_f + sc_o \rightarrow (1 + s)c_p \tag{103}$$

If a more detailed mechanism is used with, for instance, two and/or more than one reaction, it is not clear how to use the Magnussen model. Moreover, the uncertainties in determining the model constants increase dramatically. The product term, $B_c p / (1 + s)$ is not important in our analysis because it is introduced to describe the temperature level corresponding to the moment when mixture ignition is achieved.

Supposing, for simplicity $s = 1$, in the reaction of the form (103), the quasi-laminar reaction rate is given by the expression

$$|f(c)| = k_f c_f c_o \tag{104}$$

which, essentially reads

$$|f(c)|_{\text{PaSR}} \sim c_f c_o = c_f (1 - c_f) \tag{105}$$

which reduces to the Magnussen and Hjertager reaction rate

$$|f(c)|_{\text{Magnussen}} \sim \min(c_f, 1 - c_f) \tag{106}$$

The plot of the different expressions for the rates, $|f(c)|$, can be seen in Figure 6. Thus, to describe the Magnussen limiting species, the minimum operator is introduced and from this, it becomes clear that the Magnussen limiting species and the reference species are equivalent, as the minimum operator can be seen as approximating the function $c(1 - c)$.

Another interesting observation is that the PaSR reaction rate (99) can be deduced in a completely different way.

The total electrical resistance, $R$, of two parallel connected resistances $R_1$ and $R_2$ is obtained in the following way

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2} \tag{107}$$
Figure 6: The reaction rates as a function of fuel concentration. The two PaSR graphs differ by a constant two.

and by viewing the two limiting reaction rates, (100) and (101) as parallel processes, the overall reaction rate can be written as

\[
\frac{1}{f_m^1(c)} = \frac{1}{f(\tau_{mix} \to 0)} + \frac{1}{f(\tau_{mix} \to \infty)} = \frac{1 + (\xi_2^0 \tau / c_r^0)}{\tau_{mix} / c_r^0} = \frac{c_r^0 + (\xi_2^0 \tau - f_0 \tau_{mix})}{f_0 c_r^0}
\]

(108)

which obviously is equivalent to (99).

In light of this, an analogy between electrical circuits and combustion can be drawn. As the resistance of two parallel connected resistances is determined by their harmonic average\(^7\), likewise the overall reaction rate in the PaSR model is determined by the harmonic average of the quasi-homogeneous rate and the turbulent mixing controlled rate. It is important to note that both rates must be defined using the same limiting, or reference, species.

Even though the reactor is split into two parts, there is only one common temperature for both zones. It has not been established whether or not this simplification is important. The production of NO\(_x\) is sensitive to the temperature and may require the conditions in the reaction zone to be restored and this may require keeping track of two different temperatures. This is a question for future research and has not been investigated here.

\(^7\)The harmonic average only differs by a factor of two since it is defined as \(\frac{2}{\frac{1}{R_1} + \frac{1}{R_2}}\)
4 Implementing a Lagrangian Representation of the Spray

This one is tricky - it involves imaginary numbers, like eleven.
- Bill Watterson (Calvin and Hobbes)

4.1 Introduction

This section deals with how to implement a Lagrangian representation of the spray in an Eulerian framework. At first glance, this might seem trivial, but as will be shown below, there are some intricate details which can lead to erroneous behavior if care is not taken.

It is the author's experience that the way the spray models have been implemented is of importance since this can, and must, influence the behavior of the spray sub-models. Hence, comparing spray sub-models for different codes can be misleading, since a model's behavior, good or bad, might depend on the implementation and not on the model itself.

By revealing these details it is the author's wish that by doing so it will help someone and any mistakes made by the author will be discovered.

The implementation below describes how the models have been implemented in FOAM [36]. This is something that might belong in a manual, but as this is a universal problem for all CFD codes, this thesis might be the proper place. Moreover, this knowledge, or information, has not been found anywhere.

4.2 Tracking

Tracking the parcels is the most fundamental operation. This includes the 'in-which-cell-am-I' functionality. Of course, the parcels must have a position, but they must also belong to a cell. This is fundamental if the parcels are to interact with the surrounding Eulerian field. Currently, there are two main approaches for tracking a parcel, they will here be referred to, for lack of a better word, the Lose-Find (LF) algorithm and the Face-To-Face (F2F) algorithm. The LF algorithm moves the parcel along its path, \( \mathbf{u}_d \Delta t \), disregarding the mesh, and then finds out which cell it belongs to by performing a search. This approach is very easy to implement and suitable for explicit codes in which the integration step must be small and therefore the parcel does not move much. The search algorithm thus starts by looking for the parcel in the same cell (which is where it most often is). If the parcel does not belong to the same cell, but has moved into a new cell, the algorithm searches the neighboring cells, until the parcel is either found or the search is expanded further to cover the entire mesh. However, searching the entire domain is a time-consuming task and should be avoided; it is most probably an indication that there is a problem in the tracking, or search, algorithm.

For an implicit code, in which the integration step is much larger, this procedure is inappropriate and there is no guarantee, since there is no check, that the parcel passes
every cell along its path. See Figure 7, in which a parcel moves from position \( I \) to \( II \) during one time step, thereby missing several cells in-between.

![Figure 7](image)

Figure 7: Possible scenario using the LF tracking when the time step is too large.

This situation is unacceptable for both accuracy and stability reasons, as it will create a source field which is very 'spiky' and has a high intensity, since the LF algorithm distributes the source from the parcel to only one cell during the full time step. This limits the maximum time step and the advantages of using an implicit code are thereby diminished.

The F2F tracking algorithm only requires one search, which is performed when the parcel is first introduced into the domain. From then on there is no need to look for it again (if the tracking algorithm is robust enough). Consider Figure 8, in which the parcel

![Figure 8](image)

Figure 8: Parcel in a cell.

is inside a cell and its position and velocity are \( \mathbf{x} \) and \( \mathbf{u}_p \), respectively. A cell is defined by its faces and the cell faces are defined by their outward pointing face normals, \( \hat{n}_i \), and some arbitrary point on the face, most commonly the face center, \( \mathbf{c}_i \). A parcel does not leave its cell during the integration step if \( \lambda_i > 1 \) for all \( i \), where

\[
\lambda_i = \frac{(\mathbf{c}_i - \mathbf{x}) \cdot \hat{n}_i}{(\mathbf{u}_p \Delta t) \cdot \hat{n}_i}. \tag{109}
\]

If the parcel does not change cell, all the Lagrangian source terms in the Eulerian equations can be calculated and the parcel moved to the end of its trajectory.
However, if some $\lambda_i < 1$, the parcel hits face $i$ and $\lambda = \min(\lambda_i) > 0$ is the face it hits first. If the parcel hits a face, the parcel is then moved for $\lambda \Delta t$ time to its new position on face $i$, which is $x_{\text{new}} = x_{\text{old}} + \lambda u_i \Delta t$. The source terms are calculated for cell $i$ and the parcel now belongs to the neighboring cell of face $i$. This procedure is then repeated until the parcel has moved the whole integration step $\Delta t$.

This ensures the parcel going through every cell it passes without any error in the source term calculation as it changes cells and there are no time step restrictions due to its velocity.

Using the F2F tracking technique has, however, some quite intricate loop-holes that may result in the parcels being lost, if care is not taken. These loop-holes and how to avoid them are discussed in Appendix A.

As for the 'in-which-cell-am-I' functionality, the easiest way to check whether or not a parcel belongs to a cell is by checking that $\beta_i \leq 0$ for every face, where

$$\beta_i = (x - c_i) \cdot \hat{n}_i$$

(110)

$x$ is the position of the parcel, $c_i$ a reference point on face $i$ and $\hat{n}_i$ the face normal. This is a fool-proof method when the cell is a tet, but on a hex mesh, this method will fail if the situation looks as in Figure 9. However, using the F2F tracking algorithm on a hex mesh, the tet decomposition has already been performed and thus the tet’s are already available.

4.3 The Equation of Motion

Discretizing and integrating the equation of motion for a parcel presents some problems that can be categorized under the following categories:

- Turbulent dispersion (Unresolved random fluctuations in the Eulerian phase).
- Lagrangian / Eulerian description discrepancy.
• Lagrangian / Eulerian coupling.

The meaning of each one of these will be covered in detail below.

All of the three problems mentioned above are present not only in the momentum equation, but in the mass and energy equations as well.

4.3.1 Turbulent Dispersion

Because the Eulerian momentum equations have been averaged, in some way, the instantaneous velocity \( \mathbf{u} \), acting on the parcel, is thus unknown. Writing Equation (32) in terms of the known averaged and unknown fluctuating velocity then reads

\[
\frac{d\mathbf{u}_d}{dt} = -\frac{\mathbf{u}_d - (\bar{\mathbf{u}} + \mathbf{u}')}{\tau_u} + \mathbf{g}
\]

(111)

where \( \mathbf{u}' \) is the velocity fluctuation, which has to be modeled, see for instance [12, 28] (\( \mathbf{u}' \) is also included in the evaluation of \( \tau_u \) and \( C_D \)). In order to obtain the velocity of the parcel at the next time level, Equation (111) has to be integrated, and since the analytical expression of the r.h.s of (111) is unknown, it is assumed to be constant during the integration step. Hence, integrating (111) yields:

\[
\mathbf{u}_d(t_0 + \Delta t) - \mathbf{u}_d(t_0) = -\left( \mathbf{u}_d(t_0 + \Delta t) - (\bar{\mathbf{u}}(t_0) + \mathbf{u}') \right) \frac{\Delta t}{\tau_u} + \mathbf{g} \Delta t
\]

(112)

where the parcel velocity on the r.h.s has been evaluated implicitly and the gaseous velocity explicitly. Thus, the velocity for the next time step is obtained from

\[
\mathbf{u}_d(t_0 + \Delta t) = \frac{\mathbf{u}_d(t_0) \tau_u + \Delta t (\bar{\mathbf{u}}(t_0) + \mathbf{g} \tau_u)}{\Delta t + \tau_u} + \frac{\Delta t}{\Delta t + \tau_u} \mathbf{u}'
\]

(113)

The dispersion effect will also be present when calculating the parcel position,

\[
\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d, \quad \Rightarrow \quad \mathbf{x}_d(t_0 + \Delta t) - \mathbf{x}_d(t_0) = \int_{t_0}^{t_0 + \Delta t} \mathbf{u}_d(\tau) d\tau
\]

(114)

which is evaluated explicitly, and the random fluctuation accounting for the turbulence, \( \mathbf{x}' \) is added

\[
\mathbf{x}_d(t_0 + \Delta t) = \mathbf{x}_d(t_0) + \Delta t \mathbf{u}_d(t_0) + \mathbf{x}'
\]

(115)

The purpose of including \( \mathbf{x}' \) and \( \mathbf{u}' \) is to account for the influence of the random turbulent fluctuations on the parcel. The turbulent dispersion is important when the relative velocity is relatively low, like in particles transported by air, see for instance [23]. In diesel spray applications, it is, however, of minor importance, since the relative velocity is very high and the liquid evaporates quickly.

The implementation of turbulent dispersion will not be described here. It is modeled using the 'random walk procedure' as described in [28, 4]
4.3.2 Lagrangian-Eulerian Description Discrepancy

Because the parcel moves continuously through the computational mesh and the gaseous velocity is stored in fixed positions, either cell centers or vertices, how to evaluate the gaseous velocity, \( \mathbf{u} \) in Equation (113), at the parcel position is an open question. The different strategies are either to use the velocity at the position closest to the parcel, or to interpolate the velocity, using a set of the closest positions. In Figure 10, taken from [4], the 2-D spray patterns from four different CFD codes are shown. From left to right, they are SPICE, KIVA, CHAMPION and FLUENT. They represent the same case, at the same time, and although the turbulent dispersion makes the sprays look more 'random' and different breakup models have been used, one important and obvious, observation can be made. They all are very different. The most significant reason for the difference in

![Figure 10: Spray patterns for different CFD codes.](image)

the spray pattern is due to the difference in how the evaluation of the relative velocity is performed. The SPICE and CHAMPION code use interpolation, while the others; KIVA and FLUENT, use the value at the closest position. The parcels at the tip of the spray are traveling in an adverse pressure gradient, hence the radial velocity component, at the tip, is in the outward direction. The effect this has on the parcels is most visible in the non-interpolating codes, KIVA and FLUENT, where the parcels close to the axis of symmetry tend to go outwards, thus creating a hollow-like shape. For the codes using interpolation the tip of the spray is sharper. This behavior depends on the discontinuity in the gaseous velocity field, as seen by the parcel. Thus, if this behavior is to be avoided, the type of interpolation used is important, since not all methods of interpolation are continuous. It also matters if the velocities are stored in a staggered arrangement or not.
The most common and easiest method of interpolation is inverse distance weighting, where the velocity, \( \mathbf{n} \), is evaluated by using the closest vertices, or faces, as

\[
\mathbf{n}(\mathbf{x}) = \frac{1}{\sum \alpha_i} \sum_i (\alpha_i \mathbf{n}_i), \quad \alpha_i = \frac{1}{\max(\delta, |\mathbf{x} - \mathbf{n}_i|)}.
\]

(116)

where \( \mathbf{x} \) is the parcel position and \( \mathbf{n}_i \) the position at which the velocity \( \mathbf{n}_i \) is stored. \( \delta \) is some small number to prevent division by zero. As the parcel moves from one cell to another it changes the set from which the velocity is interpolated and for the method above, this switch makes \( \mathbf{n} \) appear to be non-continuous. Therefore, another method will be presented below, in which the parcel experiences a continuous flow field.

This, however, assumes that the parcel is in a tetrahedron. In Figure 11, the distance from vertex \( i \), where the gaseous velocity, \( \mathbf{u}_i \), is stored, to base \( i \) is \( \alpha_i + \beta_i \) and the distance from base \( i \) to the parcel is \( \alpha_i \). The interpolated velocity at the parcel position, \( \mathbf{x} \), is then

\[
\mathbf{u}(\mathbf{x}) = \sum_{i=1}^{4} \frac{\alpha_i}{\alpha_i + \beta_i} \mathbf{u}_i.
\]

(117)

Calculating all the \( \alpha_i \) and \( \beta_i \) is, however, quite expensive.

Using an interpolated velocity also requires some consideration when calculating the momentum contribution to the gas. If the parcel only interacts with the cell it is in, problems can easily arise. Consider the situation depicted in Figure 12, in which the parcel is in cell 2. The velocity of the parcel is \( \mathbf{U}_d \) and \( \mathbf{U}_2 < \mathbf{U}_d < \mathbf{U}_1 \).

The interpolated Eulerian velocity at the parcel position can, thus, be larger than the velocity of the parcel. This means that the parcel experiences an acceleration and will increase its velocity. Thus, it will gain momentum, which it must take from the Eulerian phase. And, since the parcel only interacts with the cell it is in, this will reduce the momentum in that cell and, hence, lower the Eulerian velocity.

But, how can a parcel gain momentum in a cell which has a lower velocity than the parcel itself? This problem has not been addressed, since it is not as serious for the
momentum as it is for the energy, which will be addressed in Section 4.4. In fact, it appears to reduce the grid dependency, which will be shown in Section 5. It is also a question of interpretation. Is the the velocity in the cell a representative average or just the value at the position it is stored?

4.3.3 Lagrangian-Eulerian Coupling

The last item, regarding the equation of motion, is how to handle the Lagrangian-Eulerian coupling. One of the purposes with the FOAM implementation is portability and modularity. The spray package should function like an add-on module and it should be easy and fast to add to an already existing code, with a minimum of modifications. The Lagrangian and Eulerian calculations have therefore been fully decoupled. Advancing the calculation one time step is performed in the following manner:

The Eulerian solution is frozen at time level $n$ and the parcels are advanced one by one, to time level $n+1$. All the source terms in the mass, momentum and energy equation are thus evaluated using the information from time level $n$. When the Lagrangian phase is done, the Eulerian calculation is performed using the Lagrangian source terms from time level $n + 1$.

Performing a calculation in a fully coupled manner would not only be very expensive, but most likely also unstable, at least for the momentum. This can easily be realized. Imagine a parcel traveling along a path, thus modifying the gas field. It is not likely that it will travel along the same path through the same cells in every iteration if the gaseous velocity field changes. Thus, if a parcel is close to a face, and it passes a different cell every iteration, convergence will never be obtained. And since Murphy’s Law often applies, coupled momentum calculations should be avoided. This problem is also linked with the parcel only interacting with the cell it is currently in. Another consequence of the decoupling should also be mentioned. Imagine a constant volume vessel, filled with zero velocity air. The first parcels injected into the vessel will experience zero gas velocity,

---

8Edward A. Murphy, Jr. - *If there are two or more ways to do something, and one of those ways can result in a catastrophe, then someone will do it* (1949). Murphy’s Law is, however, more commonly known as - *Anything that can go wrong, will*, which is Finagle’s Law of Dynamic Negatives
the relative velocity will therefore be higher than it should and the liquid penetration will most likely be under-predicted. Liquid penetration therefore not only depends on breakup, or the evaporation model, but also on the integration step.

4.4 The Liquid Mass and Heat Transfer

The decoupling of the Lagrangian and Eulerian calculation is most important for the energy equation. Integration step restrictions in implicit CFD codes are mainly due to the energy/evaporation and too large time steps may result in negative gas temperatures. This is due to the fact that every parcel passing a cell experiences the same temperature. Thus, if many parcels pass through the same cell, the energy required to evaporate the parcels may result, when the total energy drainage is summed up, in that there is more energy taken out of the cell than is actually available, hence, the negative temperature, which most certainly will crash the calculation. One way to overcome this deficiency is to pass a copy of the enthalpy and species field to the Lagrangian phase. When the parcel evaporates these copies are modified and subsequent parcels experience a more correct environment. So, when the 100:th parcel passes through a cell, the parcel will experience a colder environment and the temperature is less likely to be driven to a negative value.

As in the previous section, the question now arises - How to evaluate the temperature at the parcel position. As mentioned earlier, the gaseous temperature at the parcel position is not obtained by interpolation. This is due to the following reason.

Imagine Figure 12 again, but now with the temperature instead of velocity [25]. The droplet is in cell 2 and $T_2 < T_d < T_1$.

Interpolating the gaseous temperature may thus result in the gaseous temperature being higher than the droplet temperature. Hence, heat is transferred from the cell, with a lower temperature than the droplet, to the droplet and the 2:nd law of thermodynamics has been violated.

And the conclusion is that interpolation is not always better.

When solving the mass and energy equation numerically, a semi-implicit method is preferable, especially for the evaporation, as this prevents the mass, or diameter, from being driven to negative values. Hence the new diameter of the droplet is obtained as

$$\frac{D^{n+1} - D^n}{\Delta t} = -\frac{D^{n+1}}{3\tau_c^n} \quad \Rightarrow \quad D^{n+1} = \frac{D^n}{1 + \Delta t/(3\tau_c^n)}$$ (118)

As the mass of the parcel becomes lower than some small value it is removed from the computations and the mass, momentum and energy added to the gas for consistency. The new parcel temperature is also obtained semi-implicitly from (40) as:

$$\frac{T_d^{n+1} - T_d^n}{\Delta t} = (T^n - T_d^{n+1}) \left( \frac{f}{\tau_h} \right)^n - \left( \frac{h_v}{c_l d_i \dot{\tau}_c} \right)^n$$ (119)
which yields

\[ T_{d}^{n+1} = \left[ 1 + \frac{f}{\tau_{h}} \Delta t \right]^{-1} \left[ T_{d} + \Delta t \left( \frac{f}{\tau_{h}} T - \frac{h_{v}}{c_{l,d} \tau_{r}} \right) \right]^{n} \tag{120} \]

### 4.5 The Breakup Model

The purpose of the secondary breakup model is to reduce the characteristic size of the parcels due to aerodynamic forces. Among the spray sub-models, it is the secondary breakup model that has attracted the most attention. Modifying the breakup model is relatively straightforward, since the mass, heat and momentum transfer depend on the size of the droplets. It is, thus, by controlling the size of the parcels possible to influence both evaporation rate history and liquid penetration, with only one model.

The rate expression used to calculate the size of the parent parcel in Equation (52) is discretized using an implicit method:

\[ \frac{r_{n+1}^{n+1} - r_{n}^{n}}{\Delta t} = \frac{r_{n+1}^{n+1} - r_{c}}{\tau_{kh}} \quad \Rightarrow \quad r_{n+1}^{n+1} = \left[ 1 + \frac{\Delta t}{\tau_{kh}} \right]^{-1} \left( r_{n}^{n} + \frac{\Delta t}{\tau_{kh}} r_{c} \right) \tag{121} \]

The size of the child parcel, \( r_{c} \), stripped from the parent parcel, is used to calculate how much mass that has been stripped from the parent parcel. But, since adding a parcel every time step would lead to a dependence of time step and an abundance of small droplets, a limit of how much mass must be stripped before a new parcel is introduced into the calculation, is used. This is typically 5-10% of the parent parcel mass.

If a new parcel is introduced, the child parcel inherits the statistical number of droplets from the parent parcel and its radius is set to \( r_{c} \). The new parent radius is deduced, as normal, from the rate equation and the number of droplets in the parent parcel is set so that the liquid mass is conserved.

The RT mode of the KHRT breakup model does not introduce any new parcels. When RT breakup occurs, the parcels new statistical number of droplets is set to

\[ N_{p,new} = \max(1, \frac{r}{A_{l}}) N_{p,old} \tag{122} \]

and the new radius is set to conserve mass.

### 4.6 The Lagrangian Solution Procedure

Because of the decoupling of the liquid and gas phase, the liquid phase is treated first. This is done in the following way:

1. Existing parcels are moved up to the current time, while at the same exchanging heat, mass and momentum. During this phase the source terms for the phase interaction are calculated.
2. The mass and number of parcels to be injected during the current time step are calculated and the new parcels are injected, either sequentially or all at the same time, and moved up to the current time.

3. Clean up the spray. Parcels with very small mass are removed from the calculation.

4. The various sub-models are applied sequentially: breakup, collision and turbulent dispersion.

The parcels have now been moved from time level \( n \) to time level \( n + 1 \).
5 Results and Discussion

"Oh bother", said Pooh
- A.A. Milne

The results summarized in this section are findings that have not been included in the papers. The reader is, therefore, referred to the papers for results regarding experimental comparisons and engine applications.

In this section, the various parametric studies behind the above mentioned results are presented, since these studies often have to be left out of the papers due to volume restrictions in the material presented for publication.

All the studies below have been done in a constant volume, since this allows for more control over the simulation.

By including many species and reactions in the simulations, the computational time is naturally increased. However, the increase is not dramatic. Typical run times are in the order of one hour to one day for a 2D case and one to two weeks for a 3D case, depending, of course, on how long the simulation time is.

The computers used to perform the simulations were either LINUX based PCs or an SGI Origin2000.

5.1 Mesh Dependence Analysis

The liquid penetration is sensitive to the cell size, especially in the radial direction. As can be seen in Figure 13, by reducing the cell size in the radial direction, the liquid penetration is increased and in general, using a finer mesh will increase the liquid penetration. The breakup model used for obtaining the results in Figure 13 was the TAB model. The TAB model is known to produce very small droplets close to the injector. To investigate the
reasons behind the sensitivity to cell size, two different 2-D axi-symmetric grids were used with cell sizes $\Delta r = 1.0$ mm and $\Delta r = 0.5$ mm, while the cell size along the axis of symmetry was 1.0 mm. The breakup model was turned off and two different sizes of the initial droplet size were used on each grid. They were 1.0 $\mu$m and 0.01 $\mu$m. The injector velocity was set to a constant 223 m/s. Since the drag, heat and mass transfer depend on the relative velocity, investigating the relative velocity close to the injector was performed by averaging the relative velocity for all droplets closer than 3.0 cm from the injector.

![No interpolation]

**Figure 14:** Averaged relative velocity for the parcels within 3.0 cm from the injector and the corresponding leading droplet position, with no interpolation

![Interpolation]

**Figure 15:** Averaged relative velocity for the parcels within 3.0 cm from the injector with interpolation

In Figure 14, the difference in relative velocity for the 1.0 $\mu$m droplets is very small,
while the difference for the 0.01 μm droplets is very large. The momentum exchange is much larger for the smaller droplets. Hence, if the cells are small enough to capture the velocity gradient close to the injector, this will result in a gaseous jet with a velocity close to the liquid parcels and, thus, a low relative velocity. When the grid is too coarse, the numerical diffusion, together with the fact that the momentum increase yields a lower increase in velocity, results in a much higher relative velocity.

In Figure 14, no interpolation was used to calculate the relative velocity and to investigate the effect of using interpolation, the same cases are shown in Figures 15.

As can be seen, by comparing Figure 15 with 14, when using interpolation, the difference in both relative velocity and liquid penetration is reduced. This will, thus, reduce grid sensitivity since the phase exchange depends on, especially, the relative velocity.

5.2 Turbulent Parameters Analysis

The influence of the turbulence parameters on vapor penetration was investigated in Figure 16. The two parameters varied were the turbulent energy, $k$, and the turbulent length scale $l_t$. As can be seen, the largest influence on the penetration is obtained by varying the turbulent length scale, where the general trend is that increasing the turbulent length scale reduces the vapor penetration. This can be explained by the change in turbulent viscosity $\nu_t$.

$$
\nu_t = C_\mu \frac{l_t^2}{\varepsilon} = C_\mu k^{1/2} l_t
$$

Hence, the turbulent viscosity is linearly dependent on the length scale, while the variation in $k$ is only to the power of $1/2$. Thus, increasing the initial turbulent length scale will increase the gaseous effective viscosity, which reduces the penetration length. Increasing
the turbulent energy should, thus, also decrease the penetration length, but the total effect is unclear as the longest penetration, for a given \( h \), is for the medium value of \( k \).

The reduction in penetration is due to the diffusion of the fuel vapor.

5.3 Collision Modeling

As pointed out in Section 2.2.6, the standard collision model in the KIVA code is very grid dependent. To show this, two impinging jets are set up in a constant volume as in Figure 17. To minimize the influence of the gas, the breakup model was turned off and the size of the droplets were set to the size of the nozzle, with a diameter of 0.1 mm. This allows the droplets to move relatively undisturbed the gaseous field, preventing them from following any eventual gas motion. The turbulent dispersion was also turned off. To investigate the influence of the size of the grid cells and where the collision occurs in the mesh, four different grids were used, where the number of grid cells in the horizontal direction was varied between 10, 11, 20 and 21. Since the expected place of collision is in the center of the domain, the collisions will occur on a grid line, for an even number of horizontal cells, and in the center of a cell, for an odd number of horizontal cells. In Figure 17, the top row is the 20-cell case and the bottom row is the 21-cell case. No collision model was used (for reference) in the left, in the center the original collision model is used and to the right the mesh independent collision formulation is used. Looking at Figures 17(b) and 17(e), in which the original collision model has been used, it is clear that the chance for collision is practically reduced to zero when the parcels meet at a grid line. By doubling the cell size, the probability for collision is reduced by half. However, by doubling the size of the cell, a larger number of parcels occupies the same cell and the effect can be seen by comparing Figure 17(e) with 18(e). Many more parcels collide in the larger sized cells case 18(e), than in 17(e), where the cells are half the size. This feature is very unattractive, since the standard procedure to check for a grid-independent solution will not work in this case. In fact, by reducing the cell size in absurdum, parcels will move independently of the others and never collide, since the cells are too small to hold more than one droplet.

Investigating the results from the mesh independent formulation, it is obvious that the results are truly mesh independent. Although this method is more expensive, it is still attractive as it offers a solution to an otherwise unsolvable problem. In the simulations below the constant, \( C_2 = 0 \), in Equation (61), which means that all parcels crossing each others path, within the time step, will collide. This overpredicts the collision frequency and was used here only for demonstration purposes.

5.4 Micro Mixing Time

To investigate the influence of different micro mixing times, \( \tau_{mix} \). Constant injection with a liquid temperature of 300K into a gas with 50bar, 800K was set up. The 'cold' liquid was chosen to make the flame liftoff longer, hence enhancing any difference in \( \tau_{mix} \). The
5 RESULTS AND DISCUSSION

Figure 17: Comparison of collision models for two different grids, with 'smaller' cells

figures in Figure 19 are arranged in increasing order, where the shortest expression for $\tau_{mix}$ is at the top and the longest at the bottom. It is immediately clear that by increasing the mixing time, the flame lift off is increased, which is in compliance with Equations (87) and (88).
Figure 18: Comparison of collision models for two different grids, with 'larger' cells
5 RESULTS AND DISCUSSION

Figure 19: The temperature field for continuous spray injection using different mixing times.

(a) $\tau_{mix} = 0$

(b) $\tau_{mix} = 0.2 \sqrt{\tau_k \tau_l}$

(c) $\tau_{mix} = 0.02 \tau_l$

(d) $\tau_{mix} = 0.2 \tau_l$
6 Conclusions

*I do not feel obliged to believe that the same God who has endowed us with sense, reason, and intellect has intended us to forgo their use.*

- Galileo Galilei

This thesis presents the application of CFD to spray combustion analysis. Improved sub-models for turbulence/chemistry interaction using a detailed chemistry approach is presented. The computer model was applied to a constant volume apparatus with n-heptane and DME as a fuel and reasonable agreement with experimental data was achieved, although spray simulations are sensitive to the cell size.

When comparing numerical spray combustion simulations with experimental data, it is important to know the initial conditions of the turbulence characteristics and to use a correct injection rate schedule of the liquid fuel, since the simulation is especially sensitive to these parameters. However, it is not certain that the best result would be obtained if the experimental results of these parameters were obtained and used in the simulation, as this might depend on the choice of turbulence model, as well. In this thesis the $k$-$\varepsilon$, either standard or RNG, has been used throughout and no special investigation of this statements has been performed. However, the $k$-$\varepsilon$ model is 'tuned' only for stationary situations, while spray combustion is a highly transient phenomenon.

Constant volume calculations are attractive, since they offer the possibility to study the influence of each parameter. In an engine calculation, in which the cell size and turbulent parameters are more difficult to control, it is even more important that experimental results are available to validate the calculations. Still, when the problem setup has been tuned, good agreement can be obtained.

In contrast to single-phase flows where it is almost always possible to obtain mesh independent results, which are dependent only on the models, Lagrangian spray calculations do not obey this 'law,' because the smaller the cell size does not always yield a better result. If a complete solution to this problem could be discovered, it would be a major breakthrough in the modeling.
7  Future Work

*I like work; it fascinates me. I can sit and look at it for hours*

- Jerome K. Jerome

In order to accurately predict the emissions in spray combustion, a minimum requirement is, at least, that the initial fuel vapor distribution is correct. Since this is supplied by the spray models, it is important to have as accurate and reliable behavior of the spray as possible. Future work will focus on improving the Lagrangian treatment of the spray in regions with a high liquid volume fraction.

It is still an open question whether or not this effect is important enough to include. A bug-free implementation of the above mentioned phenomena in a CFD code built on fortran77 is an extremely tedious and time consuming task. However, by using object-oriented programming techniques it is hoped that a proper investigation of this can be turned into a reality. Improving the PaSR model is also, as always, a question for future research.
8 Summary of Papers

Numerical Evaluation of n-Heptane Spray Combustion at Diesel-like Conditions

This paper focuses on 2D axi-symmetric spray combustion simulations in a constant volume with n-heptane as a fuel. A detailed chemical mechanism was implemented in the KIVA code with the purpose of verifying the chemistry model and finding an optimal grid size for the behavior of the spray. For this purpose, local measurements, using Raman spectroscopy, of mixture concentration was used together with ignition delay and liquid spray penetration measurements, obtained at Aachen [21].

Numerical Evaluation of Dual Oxygenated Fuel Setup for DI Diesel Application

Using methanol as a diesel fuel is promising due to the reduction of particulate and NOx emissions. However, the poor ignition quality of methanol necessitates the use of an ignition improver. In this study, Dimethy Ether (DME) was selected, since gaseous DME can be manufactured from methanol on board the vehicle through a catalytic system, and the ignition quality of DME is excellent. When adding DME to the intake-air, care should be taken as to how much DME is to be added. Adding the wrong amount can prove to have the opposite effect of that which is intended. To study this, a chemical mechanism was developed and implemented in the KIVA code and the optimal addition amount of DME was numerically evaluated.

Computer Evaluation of DI Diesel Engine Fueled with Neat Dimethyl Ether

Dimethyl ether has, due to Haldor Topsoe A/S (see below), received an increasing amount of interest as a potential diesel fuel. However, there is a lack of fundamental data in the kinetics of DME oxidation at high pressures and temperatures. This paper focuses on developing a detailed chemical mechanism of methanol+DME/Air oxidation and comparing the ignition delay times obtained in shock tube experiments. The chemical mechanism was implemented into the KIVA code and applied to a constant volume application and a 2D axi-symmetric Volvo DI Diesel engine with methanol as a fuel and DME in a purely gaseous state.

Neat Dimethyl Ether: Is It Really Real Diesel Fuel of Promise?

This paper is a continuation of the work carried out in the paper described above, Computer Evaluation of DI Diesel Engine Fueled with Neat Dimethyl Ether.
Haldor Topsøe A/S stated in 1995 that dimethyl ether has the potential of being a real diesel fuel in the future. It has low particulate emissions and excellent ignition qualities and it does not require any special treatment of the fuel injection equipment, since it is non-corrosive to metals.

This paper is a numerical evaluation of how valid that statement was. For this purpose a detailed chemical mechanism was developed and implemented in the KIVA code. The chemical mechanism was compared with experimental data for ignition delay times with good agreement. The lack of spray combustion experiments with DME as a fuel prevented any such comparisons and the model was tuned with n-heptane as a fuel.

**Evaluation of Ignition Quality of DME at Diesel Engine Conditions**

Previously lacking constant volume experimental data for DME, this paper is a continuation of the paper above and presents a comparison with the experiments performed at the University of Hiroshima. Good agreement is obtained and the simulations confirm the high ignition quality of DME.

**3-D Diesel Spray Simulations Using a New Detailed Chemistry Turbulent Combustion Model**

This is a presentation of the latest models for turbulence/chemistry interaction together with a new chemical mechanism, to which a soot model has been added and the physical properties of the n-heptane have been replaced with the properties of a real Diesel #2 grade fuel. The Volvo engines AH10A245 and D12C were simulated using a 3D sector mesh, and the simulations were compared with experimental data for the pressure trace. Fair agreement was obtained.
A Robust Face-To-Face Tracking

To track parcels through any mesh in a reliable and robust way is only possible when the cells are tetrahedral. This rather strong conclusion will be shown below. Since many CFD codes use hexahedral cells this requires the hex-cells to be split into tets. An operation quite costly if performed every time it is required. Thus, the optimal way is to perform this decomposition in the beginning, or every time the mesh has changed, and then store this information.

Because of the face to face addressing, a parcel is not allowed to travel through a vertex which in a discrete world, where the representation of a real number is finite, has a 100% chance of happening. Looking at Figure 20, this means that a parcel going from cell 1 to cell 4 is not allowed to travel along path II, going directly from cell 1 to cell 4. Path I, however, is perfectly valid. This is due to the fact that a face is only shared by two cells, and when a parcel hits a face it must go into the the other cell sharing this face. Thus, if the parcel travels along path II, it can either go into cell 2 or cell 3, but not cell 4. Hence, the vertices, and edges as well, are holes, through which the parcels can escape, and this is one way to lose them.

![Diagram](attachment:diagram.png)

Figure 20: Two theoretically possible ways for a parcel to go from cell 1 to cell 4

The other way to lose parcels is face-warpage, which happens when a face is described by more than three points. Thus, for a hexahedral cell, in which a face has four points, it is possible for one point, or more, to not lie on the face plane. Because a face is described by a face normal and a face point only, a situation like in Figure 21, where face α is warped, may occur. Cells 1 and 2 only share two vertices. The other two vertices for face α may thus be arranged so that one of them is higher, and the other lower, than the 2 shared vertices. Resulting in a situation depicted in Figure 21.

A parcel going from cell 1 hits face i. Because only cells 1 and 2 share face i, the parcel is now believed to travel into cell 2. Hence, the parcel moves to cell 2 and has now been 'lost'. This will not be discovered unless a check is performed every time the parcel changes cells, which slows down the calculations and makes the whole point of the F2F algorithm useless.
Figure 21: Tracking a parcel on a warped mesh.

To remedy face warpage it is necessary to decompose the cells into tetrahedrals using the vertices. This ensures that the parcel enters the correct cell as it crosses a face, and a situation like Figure 21 becomes impossible.

B  The turbulence/spray interaction constant \( C_s \)

The value of \( C_s = 1.5 \) (in front of the spray/turbulence interaction term in the \( \varepsilon \)-equation) is chosen on basis that this conserves the turbulent length scale, \( l_t \). It is, however, shown below that \( C_s = 1.5 \) is the worst possible choice.

By assuming no gradients and constant density, and without neglecting \( \varepsilon \), in the \( k-\varepsilon \) equations, they are reduced to

\[
\frac{\partial \rho k}{\partial t} = -\rho \varepsilon + \hat{W}^*, \quad \frac{\partial \rho \varepsilon}{\partial t} = \frac{\varepsilon}{k} \left( -C_{\varepsilon_2} \rho \varepsilon + C_s \hat{W}^* \right) \tag{124}
\]

After some manipulation, the equation for the turbulent length scale can be written as

\[
\frac{\varepsilon}{k^{\alpha-1}} \frac{\partial \rho l_t}{\partial t} = (\alpha - C_s) \hat{W}^* + \left( C_{\varepsilon_2} - \alpha \right) \rho \varepsilon \tag{125}
\]

where the turbulent length scale is \( l_t = k^\alpha/\varepsilon \) and \( \alpha = 1.5 \).

It is not possible to draw any definite conclusion about the value on \( C_s \), and its influence on the length scale since the magnitude of \( \varepsilon \) is unknown.

The conclusion that \( C_s = 1.5 \) conserves the length scale is therefore erroneous.

In fact, by setting \( C_s = \alpha = 1.5 \) Equation (125) is reduced to

\[
\frac{\varepsilon}{k^{\alpha-1}} \frac{\partial \rho l_t}{\partial t} = (C_{\varepsilon_2} - \alpha) \rho \varepsilon > 0. \tag{126}
\]

Thus, if \( C_s = 1.5 \), the only conclusion that can be drawn, is that the turbulent length scale increases, when it should decrease.
Comment

It is generally agreed that it is not possible to reconstruct a CFD code using the documentation only, meaning that there are undocumented features and tricks, never mentioned in text, that make the code work.

It is the authors experience that this also applies to model descriptions, and this is not discovered until one tries to implement the model. It is therefore the author’s wish that all details of the models described herein and how they have been implemented are made perfectly clear, and for those using the KIVA3-V code all models are therefore available at the KIVA JumpStation, http://www.tfd.chalmers.se/~nordin/KJS/, for anyone to download.
References


REFERENCES


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