Doctoral Thesis

Modelling of combustion and nitric oxide formation for medium-speed DI diesel engines
a comparative evaluation of zero- and three-dimensional approaches

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Modelling of Combustion and Nitric Oxide Formation for Medium-Speed DI Diesel Engines: A Comparative Evaluation of Zero- and Three-Dimensional Approaches

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2001
Abstract

The present study explores the potential of both zero- and three-dimensional methods for the simulation of combustion and nitric oxide formation in medium-speed diesel engines.

For a broad range of operating conditions as well as geometrical configurations we validate the results of simulations with both types of model against experimental data, mainly in terms of rate of heat release histories and nitric oxide emissions. The variations investigated include modifications of initial conditions in terms of charge air composition and thermodynamic state as well as variations of the injection boundary conditions associated with the use of different injection systems and the variation of injection system parameters. Additionally, the effects of engine size and injector geometry are considered.

The results of the validations are analysed with respect to the performance of both the complete models as well as the respective sub-models for the key processes, in particular ignition, combustion and nitric oxide formation. In both types of model, similar approaches are employed: Ignition is simulated by solving the evolution equation of a progress variable on the basis of the chemical time scale for ignition, which, in the three-dimensional model, is determined from an approximation of detailed ignition chemistry. Combustion is regarded as governed by the chemical time scales during the premixed combustion phase and by the turbulent time scales mainly during the mixing-controlled combustion phase; where the turbulent time scales are determined from variants or derivatives of the $k – \varepsilon$ turbulence model. The transition between the two combustion modes is modelled on the basis of phenomenological considerations. Finally, for the simulation of nitric oxide formation, detailed models of the post-flame chemistry are employed.

The ignition model yields excellent results, both in terms of the ignition delay predictions under engine conditions and of the simultaneous predictions of the ignition location in a constant-pressure spray combustion chamber for a variety of operating temperatures.
and pressures in the case of the three-dimensional variant.

The qualitative predictions of heat release rate patterns are in good agreement with the experimental data, the limitations in terms of quantitative agreement are attributed to deficiencies of the turbulence models employed.

The present study shows, by various means, that the quality of the emission predictions can be substantially increased by applying more detailed mechanisms, which take into account additional reaction paths involving intermediates such as $HO_2$, $NH$, $HNO$, $NO_2$, and $N_2O$ on top of the commonly employed extended Zeldovich mechanism. However, the performance of the nitric oxide formation model is, to leading order, affected by the quality of the combustion predictions. Additionally, the rate of mixing of the hot combustion products and the surrounding fresh air is of decisive importance for $NO$ formation through determining the residence time at high temperature and adequate oxygen availability. In the zero-dimensional model, this effect was utilized in order to tune the model to match experimental emission data.

This well-tuned model proved particularly efficient for the fast, even quantitative, investigation of effects associated with variations in initial conditions as well as (moderate) injection boundary condition modifications. By nature, it is incapable of dealing with more complex situations involving geometry-related phenomena.

In those cases, the three-dimensional model clearly reveals its superiority. Though it is not capable of predicting $NO$ emissions quantitatively, it yields the correct trends, not only for the variations in initial conditions and injection boundary conditions, but also for the geometry variations. In particular, for situations involving effects of interactions of multiple sprays, as we demonstrate for the case of a variation in injector orifice number and size.

Moreover, it allows the isolated study of such effects under strongly idealized conditions in order to obtain the necessary insight into the basic mechanisms and the relevance of local effects.
Zusammenfassung

Gegenstand der vorliegenden Arbeit ist die Untersuchung des Potenzials von sowohl null- als auch dreidimensionalen Modellen für die Simulation der Verbrennung und Stickoxidbildung in mittelschnelllaufenden Dieselmotoren.


Die Resultate dieser Untersuchungen werden hinsichtlich der Leistungsfähigkeit sowohl der beiden Gesamtmodelle als auch der Untermodelle für wichtige Teilprozesse bewertet, insbesondere der Modellansätze für die Beschreibung von Zündung, Verbrennung und Stickoxidbildung. In beiden Arten von Modellen werden ähnliche Ansätze verwendet: Die Zündung wird mittels einer Fortschrittsvariablen auf der Basis einer charakteristischen Zeit für die Zündung beschrieben, welche in der dreidimensionalen Simulation über eine auf den Resultaten detaillierter Reaktionsmechanismen für die Zündung basierende Näherung bestimmt wird. Für die Verbrennung wird angenommen, dass die Umsatzraten während der einzelnen Phasen durch die jeweils relevanten charakteristischen Zeiten bestimmt werden: Derjenigen für die Chemie während der vorgemischten und derjenigen der Turbulenz während der mischungskontrollierten Phase, wobei letztere aus Varianten oder Derivaten des $k-\varepsilon$ Modells bestimmt werden. Der Übergang zwischen den Phasen wird auf der Basis phänomenologischer Betrachtungen modelliert. In der Simulation der Stickoxidbildung schliesslich
kommen detaillierte Reaktionsmodelle für die Gasphasen-Chemie in den Hochtemperaturregionen ausserhalb der Flamme zum Einsatz.


Unter Anwendung verschiedener Verfahren konnte gezeigt werden, dass der Einsatz detaillierter Reaktionsmechanismen die Qualität der Stickoxid-Emissionsprognosen deutlich steigert. Dabei wird der üblicherweise verwendete erweiterte Zeldovich Mechanismus durch zusätzliche Reaktionspfade unter Berücksichtigung der Zwischenprodukte $HO_2$, $NH$, $HNO$, $NO_2$ und $N_2O$ erweitert. In erster Linie wird die Qualität der Emissions-Vorhersagen allerdings durch die Genauigkeit der Verbrennungsmodelle bestimmt. Zusätzlich hat die Geschwindigkeit der Vermischung der heissen Verbrennungsprodukte mit der umgebenden Frischluft einen entscheidenden Einfluss auf die Stickoxidbildung, insofern als sie die Verweilzeit bei hohen Temperaturen und ausreichender Sauerstoff-Verfügbarkeit bestimmt. Im Fall des nulldimensionalen Modells wurde dieser Zusammenhang benutzt, um das Modell auf quantitative Übereinstimmung mit gemessenen Emissionswerten abzustimmen.

Dieses sehr gut abgestimmte Modell hat sich als in hohem Grad geeignet erwiesen, um schnell und zudem quantitativ korrekt Aussagen über den Einfluss von veränderten Anfangsbedingungen sowie von nicht allzu ausgeprägten Modifikationen der einspritzzeitigen Randbedingungen zu machen. Hingegen ist es aufgrund des Verzichts auf die detaillierte Betrachtung räumlicher Effekte nicht in der Lage, für komplexere Fälle, bei denen Einflüsse der Brennraum-
oder Strahlgeometrie eine Rolle spielen, realistische Ergebnisse zu liefern.

In diesen Fällen zeigt sich die Überlegenheit des dreidimensionalen Modells. Auch wenn damit keine quantitativ korrekten Vorhersagen der NO Emissionen möglich sind, so stimmen die berechneten Trends mit dem im Experiment beobachteten Motorverhalten doch gut überein. Dies nicht nur für Veränderungen der Anfangsbedingungen und Einspritz-Randbedingungen, sondern auch für die geometriebedingten Einflüsse. Dies gilt insbesondere für Fälle, bei denen Wechselwirkungen zwischen einzelnen Strahlen von entscheidender Bedeutung sind, wie am Beispiel des Einflusses von Düsenlochdurchmesser und -anzahl gezeigt wird.

Außerdem können mit Hilfe von dreidimensionalen Simulationen solche Einflüsse auch isoliert unter idealisierten Bedingungen betrachtet werden, um ein besseres Verständnis der grundlegenden Zusammenhänge sowie der Auswirkung lokaler Effekte auf das Gesamtverhalten zu erzielen.
Sommaire

Ce mémoire est consacré à l'exploration du potentiel des méthodes de simulation zéro et tridimensionnelles de la combustion et de la formation des oxydes nitriques dans les moteurs diesels à vitesse moyenne.

Dans une large plage de conditions d'exploitation, les résultats des simulations obtenus avec ces deux méthodes sont comparés aux mesures correspondantes, surtout à l'égard du déroulement de la combustion et des émissions d'oxydes nitriques. Les variantes étudiées comprennent des modifications des conditions initiales, comme des variations de condition thermodynamique et de composition de la charge aussi bien que des variations des conditions limites associées à l'injection du carburant, spécialement l'application de différents systèmes d'injection et la variation de paramètres de ces systèmes. En plus sont pris en considération des effets de la largeur du moteur et de la géométrie de l'injecteur.

Les résultats sont analysés par rapport au rendement non seulement des méthodes intégrales mais aussi des modèles des procédés principaux : Mise en feu, combustion et formation des polluants. Dans les deux modèles, des approches similaires sont utilisées : La mise en feu est décrite à l'aide d'une variable d'avancement sur la base du temps caractéristique qui dans la simulation tridimensionnelle repose sur une approximation des résultats des mécanismes détaillés des réactions chimiques gouvernant la mise en feu. La combustion est basée sur la considération des temps caractéristiques associés aux différentes phases : Ceux de la chimie à la phase de pré-mélange et ceux de la turbulence à la phase contrôlée par la diffusion turbulente. Le temps caractéristique de la turbulence est déterminé en appliquant des variantes ou des dérivés du modèle $k – \varepsilon$. La transition entre les deux phases de combustion est modélisée sur une base phénoménologique. Finalement, en simulant la formation des oxydes nitriques nous appliquons des mécanismes détaillés des réactions se produisant dans les régions à haute température.
Le modèle de la mise en feu produit des résultats excellents, non seulement quant à la prédiction des retards d'allumages en conditions d'exploitation du moteur, mais aussi pour la prédiction correcte simultanée du lieu d'allumage en reproduisant les expériences effectuées dans une bombe à combustion à injection diesel pour une large plage de variation des conditions d'opération en températures et pressions, dans le cas de la simulation tridimensionnelle. Qualitativement, les prédictions de l'écoulement de la combustion sont en bon accord avec les expériences, les différences quantitatives sont apparemment largement dues aux défauts des modèles de turbulence.

Par de multiples procédés, nous avons démontré que la qualité des prédictions de la formation des polluants peut être augmentée de manière significative par l'emploi des mécanismes plus détaillés que le Zeldovich étendu, qui est normalement appliqué. Les détails additionnels sont associés à la considération de chemins de réaction supplémentaires, tenant compte des espèces chimiques intermédiaires, en particulier $HO_2$, $NH$, $HNO$, $NO_2$ et $N_2O$. Il est vrai que la chimie de la formation des oxydes nitrés n'a pas le plus grand effet sur la prédiction des émissions. La qualité du modèle de la combustion est en tout cas primordial. En plus, la rapidité du mélange entre les produits de la combustion sortant de la flamme et les résidus de la charge environnante influence la prédiction de la formation des oxydes nitrés en déterminant le temps de résidence à conditions favorables (les températures hautes en combinaison avec des concentrations d'oxygène suffisamment élevées). Dans le cas de la méthode zéro dimensionnelle, cet effet a été utilisé pour mettre les résultats numériques en accord quantitatif avec les mesures.

Cette méthode bien adaptée a démontré son potentiel pour une évaluation rapide et efficace des effets associés à la variation des conditions initiales et, dans une moindre mesure, aux modifications des conditions limites dues à l'injection. Par contre, de par sa nature, elle n'est pas capable de fournir des prédictions réalistes dans des situations plus complexes reliées à des interactions de multiples jets ou entre jets individuels et parois.
Dans ce genre de situation, la supériorité de la méthode tridimensionnelle est évidente. Même si elle ne peut produire des résultats quantitatifs corrects, les tendances obtenues sont toujours conformes aux expériences, pas seulement dans le cas de modifications des conditions initiales ou des conditions limites, mais aussi lorsque est modifiée la géométrie. Ceci est démontré de façon remarquable dans le cas de variation du nombre et du diamètre des orifices de l'injecteur.

En outre, cette méthode permet d'étudier de manière isolée l'effet de l'interaction entre jets dans des conditions grandement idéalisées afin d'obtenir un plus haut degré de compréhension des mécanismes de base et des effets locaux gouvernant le comportement global.
Acknowledgments

The present thesis was prepared during my work at the Laboratory of Internal Combustion Engines and Combustion Technology at the Swiss Federal Institute of Technology (ETH) in Zurich and it was completed while employed at Wärtsilä Switzerland Ltd.

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<td>$a$</td>
<td>oxygen-fuel mass ratio</td>
</tr>
<tr>
<td>$b$</td>
<td>temperature exponent in the Arrhenius relation</td>
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<tr>
<td>$c$</td>
<td>molar concentration</td>
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<tr>
<td>$c_d$</td>
<td>aerodynamic drag coefficient</td>
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<tr>
<td>$c_{dr}$</td>
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</tr>
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<td>$c_p$</td>
<td>specific heat at constant pressure</td>
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<td>$d$</td>
<td>diameter</td>
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<td>$e$</td>
<td>third body efficiency</td>
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<td>$f$</td>
<td>droplet distribution function</td>
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<td>$w$</td>
<td>velocity</td>
</tr>
<tr>
<td>$x$</td>
<td>position</td>
</tr>
<tr>
<td>$y$</td>
<td>droplet deformation</td>
</tr>
<tr>
<td>$A$</td>
<td>pre-exponential factor in the Arrhenius relation</td>
</tr>
<tr>
<td>$B$</td>
<td>transfer number</td>
</tr>
</tbody>
</table>
constant
$C_{ig}$ ignition progress variable
$D$ diffusion coefficient
$E$ energy
$F$ force
$G$ surface area
$H$ enthalpy
$I$ internal energy
$I$ unit dyadic
$J$ total number of zones
$K$ equilibrium constant
$L$ latent heat of vaporization
$P$ probability density function
$Q$ heat
$R$ cylinder radius
$S$ source term
$S_{ij}$ strain rate
$T$ temperature
$U$ mean strain rate
$V$ volume
$W$ work
$X$ spray penetration
$Y$ species mass fraction
$Z$ mixture fraction
$\alpha$ spray angle
$\beta$ pressure exponent
$\gamma$ combustion progress variable
$\delta$ Kronecker symbol
$\epsilon$ turbulent kinetic energy dissipation rate
$\eta$ ratio of turbulent to mean-strain time scale
$\zeta$ factor or function
$\theta$ gas phase properties vector of quantities driving the diffusion process in the conservation equation of $\phi$
$\kappa$ collision probability
$\lambda$ thermal conductivity
$\mu$ dynamic viscosity
$\mu_0$ bulk viscosity
ν  stoichiometric coefficient
ξ  representative quantity
ρ  density
σ  surface tension
ς  chemical symbol
τ  time scale
υ  droplet number
φ  gas phase properties vector
χ  scalar dissipation rate
ψ  droplet properties vector
ω  specific reaction rate
Γ  transport coefficient
Ξ  dissipation rate of change due to strain rate effects
ϒ  overall third body efficiency
Φ  fuel/air equivalence ratio
Ψ  function
Ω  frequency of oscillation
\(m\)  molar mass
ℜ  universal gas constant

**Variations of a symbol \(o\)**

<table>
<thead>
<tr>
<th>Variant</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(o)</td>
<td>absolute value</td>
</tr>
<tr>
<td>(o_T)</td>
<td>vector of components in the individual directions</td>
</tr>
<tr>
<td>(o^T)</td>
<td>transpose of (o)</td>
</tr>
<tr>
<td>(o')</td>
<td>fluctuation about the ensemble average</td>
</tr>
<tr>
<td>(o'')</td>
<td>fluctuation about the mass-weighted average</td>
</tr>
<tr>
<td>(\bar{o})</td>
<td>mass-weighted average</td>
</tr>
<tr>
<td>(\tilde{o})</td>
<td>ensemble average</td>
</tr>
<tr>
<td>(\hat{o})</td>
<td>mean value in the vicinity of a droplet, see (27)</td>
</tr>
<tr>
<td>(\dot{o})</td>
<td>transfer rate</td>
</tr>
</tbody>
</table>
### Subscripts, superscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>absolute zero</td>
</tr>
<tr>
<td>a</td>
<td>aerodynamic</td>
</tr>
<tr>
<td>b</td>
<td>backward</td>
</tr>
<tr>
<td>bu</td>
<td>breakup</td>
</tr>
<tr>
<td>c</td>
<td>concentration</td>
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<td>conv</td>
<td>convection</td>
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<tr>
<td>comb</td>
<td>combustion</td>
</tr>
<tr>
<td>cyl</td>
<td>cylinder</td>
</tr>
<tr>
<td>dr</td>
<td>droplet</td>
</tr>
<tr>
<td>diff</td>
<td>related to diffusion/mixing-controlled combustion</td>
</tr>
<tr>
<td>ebo</td>
<td>enforced burnout</td>
</tr>
<tr>
<td>eff</td>
<td>effective (combining laminar and turbulent)</td>
</tr>
<tr>
<td>end</td>
<td>end</td>
</tr>
<tr>
<td>eq</td>
<td>equilibrium</td>
</tr>
<tr>
<td>evap</td>
<td>due to evaporation</td>
</tr>
<tr>
<td>f</td>
<td>forward</td>
</tr>
<tr>
<td>g</td>
<td>gas</td>
</tr>
<tr>
<td>i</td>
<td>species index</td>
</tr>
<tr>
<td>if</td>
<td>droplet species index</td>
</tr>
<tr>
<td>ig</td>
<td>ignition</td>
</tr>
<tr>
<td>ini</td>
<td>initial</td>
</tr>
<tr>
<td>inj</td>
<td>injection</td>
</tr>
<tr>
<td>j</td>
<td>zone index</td>
</tr>
<tr>
<td>l</td>
<td>particle index</td>
</tr>
<tr>
<td>lam</td>
<td>laminar</td>
</tr>
<tr>
<td>m</td>
<td>system boundary index</td>
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<tr>
<td>max</td>
<td>maximum</td>
</tr>
<tr>
<td>mix</td>
<td>mixing</td>
</tr>
<tr>
<td>n</td>
<td>normalized</td>
</tr>
<tr>
<td>o</td>
<td>injector orifice</td>
</tr>
<tr>
<td>p</td>
<td>spray particle</td>
</tr>
<tr>
<td>prem</td>
<td>related to premixed combustion</td>
</tr>
<tr>
<td>prep</td>
<td>prepared</td>
</tr>
<tr>
<td>prod</td>
<td>products</td>
</tr>
</tbody>
</table>

xx Nomenclature
prog progress
r reaction index
rad due to radiation
reac due to reaction
ref reference
rest rest
s steady state
st stoichiometric
turb turbulent
tr, trans transition
A activation
D dissipation
FG fresh gas
I total number of species
J total number of zones
L total number of particles
M total number of system boundaries
P production
R total number of reactions
S spray
V volume
W wall
ι representative species for ignition
⊥ component perpendicular to main direction

Non-dimensional numbers

Symbol Description
Da Damköhler number
Ka Karlovitz number
Le Lewis number
Nu Nusselt number
Pr Prandtl number
Re Reynolds number
Sc Schmidt number
Sh Sherwood number
We Weber number
### Abbreviations used in the text

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMO</td>
<td>International Maritime Organisation</td>
</tr>
<tr>
<td>WHO</td>
<td>World Health Organisation</td>
</tr>
<tr>
<td>DI</td>
<td>direct injection</td>
</tr>
<tr>
<td>PLN</td>
<td>Pump-Line-Nozzle (injection system)</td>
</tr>
<tr>
<td>CR</td>
<td>Common-Rail (injection system)</td>
</tr>
<tr>
<td>EGR</td>
<td>exhaust gas recirculation</td>
</tr>
<tr>
<td>VTG</td>
<td>variable turbine geometry (turbocharger)</td>
</tr>
<tr>
<td>TDC</td>
<td>top dead centre</td>
</tr>
<tr>
<td>BDC</td>
<td>bottom dead centre</td>
</tr>
<tr>
<td>CA</td>
<td>crank angle</td>
</tr>
<tr>
<td>IVO</td>
<td>inlet valve opening</td>
</tr>
<tr>
<td>IVC</td>
<td>inlet valve closing</td>
</tr>
<tr>
<td>SOI</td>
<td>start of injection</td>
</tr>
<tr>
<td>EVO</td>
<td>exhaust valve opening</td>
</tr>
<tr>
<td>bsfc</td>
<td>brake specific fuel consumption</td>
</tr>
<tr>
<td>PDF</td>
<td>probability density function</td>
</tr>
<tr>
<td>ODE</td>
<td>ordinary differential equation</td>
</tr>
<tr>
<td>TAB</td>
<td>Taylor analogy breakup (model)</td>
</tr>
<tr>
<td>ETAB</td>
<td>enhanced Taylor analogy breakup (model)</td>
</tr>
<tr>
<td>EDC</td>
<td>eddy dissipation concept (model)</td>
</tr>
<tr>
<td>EBU</td>
<td>eddy breakup (model)</td>
</tr>
<tr>
<td>ALE</td>
<td>arbitrary Lagrangian-Eulerian (method)</td>
</tr>
<tr>
<td>DDM</td>
<td>discrete droplet model</td>
</tr>
<tr>
<td>RNG</td>
<td>renormalization group (technique)</td>
</tr>
<tr>
<td>0-D</td>
<td>zero-dimensional (model)</td>
</tr>
<tr>
<td>3-D</td>
<td>three-dimensional model</td>
</tr>
<tr>
<td>MRC</td>
<td>maximum rate constraint</td>
</tr>
<tr>
<td>ROI</td>
<td>rate of injection</td>
</tr>
<tr>
<td>ROHR</td>
<td>rate of heat release</td>
</tr>
<tr>
<td>ROFC</td>
<td>rate of fuel consumption</td>
</tr>
<tr>
<td>CPU</td>
<td>central processing unit</td>
</tr>
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</table>
1 Introduction

Direct injected diesel engines are representing the most efficient converters of chemical energy into mechanical work among the thermodynamic single cycle machines. The additional exploitation of the remaining thermal energy of the exhaust gas and heat recovery from the cooling systems allows even higher total energy utilization ratios.

When considering the medium-size to large engine segment, the engine’s ability to operate on almost every grade of fuel including heavy and high-ash fuels or even crude oil represents an additional advantage: It makes them ideal candidates for the application in installations requiring high availability, i.e. high numbers of operating hours at almost permanently high power, as found in the transportation industry, in particular in marine applications, and power generation, both in pure power and co-generation plants. In all those installations, the fuel costs represent a major fraction of the total operating costs. Hence, the applicability of low-quality fuels, which are considerably cheaper as a consequence of the fewer refinement steps involved in their processing, is a prerequisite for competitiveness of engines designed for the application in these markets. Marine engines additionally have to cope with the fact that the fuel quality can vary considerably between bunkering regions.

Apart from the continuous operating mode in power stations, as required e.g. for the power supply of smaller or isolated units such as islands and production sites, diesel engines also interesting options for installations designed for more intermittent operation. Their short start-up time identifies them as ideal option for use as emergency gensets and, in combination with the power output available, as a valuable alternative for covering peak load requirements, in particular when considering the medium-speed (typically between 400 and 1000 rpm) range.

For many years, the development of medium-speed engines mainly focused on the further increase of power output, efficiency and reliability as well as the reduction of investment costs. Emission limits
were unknown to the marine engines, and most power plants faced rather large restrictions due to their location in developing countries with no strict emission legislation. The same applied to the emergency gensets operated in regulated regions: They were subject to considerably less severe restrictions than power stations for continuous use. Note that the strict limits imposed on the latter by legislation in the developed countries usually required the application of exhaust gas aftertreatment, which practically eliminated the need for optimization of those engines for emissions.

In recent years, however, the situation gradually changed in both the marine and the power segment:

In 1998, the International Maritime Organization (IMO) published the first internationally valid emission legislation [1] that came into force in the beginning of 2000. It limits the nitric oxide emission of marine diesel engines according to the curve shown in Figure 1:

![Figure 1: NO₂ emission limit for marine diesel engines according to the IMO MARPOL regulations, Annex VI [1].]
Depending on the rated speed of the engine, the maximum allowable level is defined. Compliance of the engine requires an emission level determined in a prescribed test cycle and corrected for variations in ambient conditions from a given reference below this limit. The test cycle to be applied and the weighting factors for the individual operating conditions are depending on the type of application (main propulsion or auxiliary engine, propeller law or constant or variable speed). The regulations apply to all ships entering service after January 1st, 2000 and all engines subject to major modifications or replacement after that date.

Note that the curve in Figure 1 was defined after a thorough analysis of the emission levels of engines in operation: Based on the statistical evaluation of the data obtained, a correlation between engine speed and emission level was determined. Then, the allowable emission as a function of engine speed was prescribed in order to achieve an overall improvement against the level given by this correlation, which was in the order 20%. Additionally, a cut-off value of 17 g/kWh was defined, applicable in the low-speed range.

The introduction of this regulation marks only one step in a process that gained considerable momentum in the meantime: Apart from the next level of the IMO regulation, envisaged for some time after 2005, various local authorities are considering [2] or already introduced [3] additional or more stringent limits for gaseous or particulate emissions. Some authorities are preparing for [4] or already started offering ([5], [6], [7]) financial incentives to further reduce the emissions from ships in particular regions and harbours. In addition, various classification societies ([8], [9]) as well as local authorities [10] presented voluntary emission control programs that can also be expected to have an effect on the industry.

On the power generation side, similar considerations apply: On the one hand, the already existing regulations in developed countries are partly being tightened up further ([11], [12]), thus bringing installations based on conventionally optimized engines with exhaust gas aftertreatment to the limits. Partly, even emergency gensets are no longer exempted from these regulations [11]. On the other hand, the
World Bank introduced general emission limits complementing its Guideline for Diesel Engine Plant Specification and Bid Evaluation [13]. This was done in order to enforce the World Health Organization (WHO) standards on ambient air quality [14] for projects worldwide receiving World Bank funding. The limits prescribed in their Pollution Prevention and Abatement Handbook [15] were recently even further lowered by individual countries [16].

All those procedures shifted the focus of engine development: The additional consideration of emission constraints makes the entire optimization process much more difficult, in particular as some of the former optimization goals exhibit a trade-off behaviour with respect to emissions. In many cases, the re-tuning of the engine for compliance with emissions standards can only be achieved at the expense of efficiency.

An effective control of the effects of variations of individual operating and design parameters on engine efficiency and reliability as well as emissions requires a more fundamental insight into the governing in-cylinder phenomena, including the mechanisms of pollutant formation. However, the complex interactions of the individual phenomena, including fuel preparation and mixing, combustion and the actual generation of emissions are not too well understood. Therefore, more advanced simulation methods need to be developed that allow both a fast and efficient pre-selection of concepts and the in-depth analysis of the in-cylinder processes.

Note that the new challenges associated with the introduction or tightening of emission limits also considerably promoted the investigation of new or alternative concepts and the introduction of innovative technologies, which additionally increased the need for predictive tools: As a consequence of the replacement of various mechanically or hydraulically actuated systems by electronically controlled ones (e.g. Common-Rail injection and Variable Valve Timing) many of the former limitations in terms of flexibility practically vanished. Additionally, several auxiliary systems were also further developed towards more flexible operation (e.g. Variable Turbine Geometry turbochargers). Due to this increasing flexibility,
the adjustment of an engine has turned into a multiple-parameter optimization problem that requires new techniques already for the experimental investigation in order to keep the number of variants to be tested within reasonable limits [17]. In this context, predictive simulations are believed to help in identifying the most promising concepts and thus limiting the range of the individual parameters already prior to the experiments. Again, the in-depth analysis of the effect of variations of the individual parameters on the in-cylinder processes can yield the additional insight required for an efficient optimization.

For many years, simulations were only employed in the thermodynamic layout of medium-speed engines, based on purely zero-dimensional models employing empiric approaches for heat release modelling and partly even involving some rough estimates of emission levels. These empiric approaches are, however, to a large extent based on the experience from the older engines and, therefore, not applicable any more to the new generations of highly flexible engines, as no experience is available on the sensitivity to the various additional parameters.

In order to model the effect of these additional parameters on combustion and emission formation, two approaches can be used:

On the one hand, the zero-dimensional models may be extended in order to predict the heat release rate as a consequence of the injection, mixture formation and combustion processes, which involves dimensional considerations with respect to spray propagation. The additional discretization of the cylinder content into multiple zones allows a more realistic description of the temperature and composition inhomogeneity inside the combustion chamber, which must be considered a prerequisite for more accurate nitric oxide emission predictions.

On the other hand, three-dimensional models enable the determination of both combustion and nitric oxide formation on the basis of the spatial distribution of the individual species. However, in view of the large dimensions involved and the high Reynolds numbers, the flow field cannot be fully resolved and the sub-grid scale pro-
cesses have to be modelled appropriately. Moreover, as the computational resources presently available dictate the use of rather coarse grids.

In terms of the applicability of these two approaches in an industrial context, one of the main differences between these two approaches is the response time of an individual simulation: For a multi-zone model, these correspond to several minutes, whereas three-dimensional simulations typically take at least several hours, possibly days. Therefore, the achievable accuracy of either model has to balance the computational effort required.

To our best knowledge, to date no attempt has been made to compare the performance of both types of model in terms of predictions of heat release and nitric oxide emission formation. Therefore, the present study is believed to complement the present understanding of the advantages and deficiencies associated with either approach.

The goal of the present investigation is twofold: On the one hand, we explore the potential of both types of simulation tools for predicting combustion and nitric oxide emission formation in medium-size diesel engines, as the basis for a comparative evaluation. On the other hand, we aim at gaining additional insight into the fundamental processes governing pollutant formation in those engines. In that context, the effect of the detail of the chemical scheme employed in the simulation of nitric oxide emission formation is of particular interest.

For that purpose, both zero- and three-dimensional models are considered, largely based on physical modelling: In order to be able to investigate effects associated with variations in the injection boundary conditions, both approaches include detailed models of the key sub-processes associated with spray propagation and mixture formation. Combustion is modelled via characteristic time scale models, taking into account effects of chemistry and turbulent mixing. The emission formation models, finally, enable the consideration of detailed mechanisms of nitric oxide formation.
2 Modelling Fundamentals

The modelling of turbulent, reactive, multi-phase flow systems as encountered in the combustion process of diesel engines is based on the fundamental laws of thermodynamics. Further, it makes use of the general concepts of fluidmechanics for the description of gas phase phenomena on the basis of a continuum approach. Additionally, it involves statistical methods, in particular for modelling of the behaviour of dispersed liquid and/or solid phases.

In this chapter, a brief summary of the general correlations will be given, whereas the following chapters will focus on the specific applications in the two modelling approaches.

2.1 Classical Thermodynamics

The thermodynamic state of an open chemical system (open with respect to size and composition) is defined by a finite number of independent thermodynamic variables. The pressure $p$, the volume $V$ and the mole numbers of the participating species $n_i$, $i = 1, ..., I$ constitute a common and convenient choice of this basic set of independent variables. From these quantities, all other properties can be determined as dependent variables. The temperature $T$ is related to the independent quantities through an equation of state, which for an ideal gas reads

$$pV = \sum_{i} n_i R T$$  \hspace{1cm} (1)

The state of a system is subject to changes due to transfer processes, both internal and across the system boundaries. These changes can be described by means of conservation equations for the masses of the individual species, the total mass in the system and the internal energy. The mass of an individual species $m_i$, determined through the species mole number $n_i$ and its molar weight $m_i$, is altered by chemical reactions and the exchange of mass across the $M$ system boundaries.
The conservation equation for the total mass in the system, \( m \), results from summation over all species mass conservation equations. Since \( m \) is conserved in chemical reactions, it is only subject to changes due to the exchange of mass across the system boundaries.

\[
\frac{dm}{dt} = \sum_I \sum_M \dot{m}_{i,m}
\]  \hspace{1cm} (3)

The internal energy of the system \( I \) and its enthalpy \( H \) are related to the independent properties through the caloric equation of state

\[
H = \sum_I m_i \left( h^0_i + \int_0^T c_{p,i}dT \right)
\]  \hspace{1cm} (4)

and the thermodynamic identity

\[
I = H - pV.
\]  \hspace{1cm} (5)

Changes of the internal (plus kinetic) energy must, according to the first law of thermodynamics, balance the rates of work done by body forces and surface stresses, of heat transfer as well as of enthalpy transfer (through mass transport) across the system boundaries and of the heat released (or absorbed) in chemical reactions.

\[
\frac{d}{dt} \left( I + m \frac{w^2}{2} \right) = -p \frac{dV}{dt} + \dot{W} + \dot{Q}
\]

\[
+ \sum_I \sum_M \dot{m}_{i,m} \left( h_{i,m} + \frac{w_{m}^2}{2} \right) + \dot{Q}_{reac}
\]  \hspace{1cm} (6)
2.2 Fluidodynamics

The governing equations of fluid dynamics are essentially applications of the general principles of mass, momentum and energy conservation to fluid flow systems. The resulting conservation equations for a reacting, multi-component gas mixture can be derived either from continuum fluid mechanics or kinetic theory (see e.g. Williams [18]).

2.2.1 Conservation Equations

The general structure of all the conservation equations is identical: The rate of change of the individual quantity plus its convective transport must balance the sum of a diffusion and a production term (referred to as source term below). They can hence be expressed in a compact form as follows:

\[
\frac{\partial (\rho \phi)}{\partial t} + (\nabla \cdot \mathbf{u}) \rho \phi = \nabla \cdot (\rho \Gamma_\phi \nabla \theta(\phi)) + S_\phi
\]  

(7)

In (7), \( \phi \) denotes the vector of gas phase properties, \( \phi = (1, Y_i, \mathbf{u}, i) \), and the individual components thus represent the continuity equation and the conservation equations for species mass density, momentum and specific internal energy, respectively.

Table 1 summarizes the transport coefficients \( \Gamma_\phi \), the properties \( \theta(\phi) \) driving the diffusion process and the source terms \( S_\phi \) associated with the different components of the gas phase properties vector \( \phi \) in (7).

The general formulation of equation (7) already implies the common assumptions of a Newtonian fluid and of the validity of Fick’s law of diffusion. Soret and Dufour effects are neglected and a single diffusion coefficient as well as a Lewis number of unity are assumed.

The Lewis number \( Le \) relates the energy transport via conduction to the one associated with mass diffusion as

\[
Le = \frac{\lambda}{\rho D c_p}.
\]  

(8)
Table 1: Transport coefficients, driving gradient quantities and source terms for the individual components of $\varphi$.

<table>
<thead>
<tr>
<th>$\varphi$</th>
<th>$\Theta(\varphi)$</th>
<th>$\Gamma_\varphi$</th>
<th>$S_{\varphi}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>-</td>
<td>0</td>
</tr>
<tr>
<td>$Y_i$</td>
<td>$Y_i$</td>
<td>$D$</td>
<td>$\frac{dc_i}{m_i dt }_{\text{reac}}$</td>
</tr>
<tr>
<td>$u$</td>
<td>$u$</td>
<td>$\frac{\mu}{\rho}$</td>
<td>$- \nabla p + \nabla \cdot \left( \mu \left( \nabla u \right)^T \frac{2}{3} \nabla \cdot u I + \mu_0 \nabla \cdot u I \right) + \rho g$</td>
</tr>
<tr>
<td>$i$</td>
<td>$T$</td>
<td>$\lambda$</td>
<td>$- p \nabla \cdot u + \nabla \cdot \left( \rho D \sum h_i \nabla Y_i \right) + \frac{\dot{Q}<em>{\text{reac}}}{V} + \frac{\dot{Q}</em>{\text{rad}}}{V}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$+ \left( \mu \left( \nabla u + (\nabla u)^T \frac{2}{3} \nabla \cdot u I \right) - \mu_0 \nabla \cdot u I \right) : \nabla u$</td>
</tr>
</tbody>
</table>

For convenience, the transport coefficients for species and heat diffusion are usually related to the molecular viscosity through the definition of the dimensionless Schmidt and Prandtl numbers, $Sc$ and $Pr$, respectively.

$$Sc = \frac{\mu}{\rho D} \quad (9)$$

$$Pr = \frac{\mu c_p}{\lambda} \quad (10)$$

From equations (8), (9), (10) it is apparent that the Lewis number $Le$ can also be expressed as $Sc/Pr$.

This set of equations is valid only for single phase flow systems, which are either laminar or can be fully resolved. However, engine flows are highly turbulent and the spatial and temporal discretization required for a full resolution of the flow field is far from tractable in view of computing resources available now and in the visible future.
Therefore, the conservation equations have to be simplified in order to account for the discretization errors associated with the coarse grids and large timesteps that have to be used in practice. Those errors are specifically due to the inadequate reproduction of the governing length and time scales associated with turbulent motion. This simplification also involves the introduction of appropriate models for processes in the sub-grid scale.

### 2.3 Turbulence

Viewed on a larger scale, turbulent flows are mainly characterized by their randomness. As a result of the practical constraints with respect to spatial resolution, their description must, therefore, rely on statistical rather than deterministic approaches. For this purpose, following the concept of Reynolds [19], all quantities are decomposed into mean values and fluctuations from the mean value. In this context, the term “mean” refers to either the time or the ensemble average, depending on the nature of the problem. Thus, for the fluid property $\varphi$, we obtain

$$\varphi(x, t) = \bar{\varphi}(x, t) + \varphi'(x, t) \tag{11}$$

Inserting (11) into the basic equations (7) and averaging them to obtain the modified conservation equations for the mean quantities gives rise to a significant number of additional terms related to the correlation of individual fluctuations. Especially the correlations involving the density fluctuation make the resulting equations hard to handle. To facilitate this task, Favre [20] introduced the concept of mass averaging, which was originally developed for the analysis of high speed turbulent boundary layers ([21], [22]) but is now widely accepted as a convenient means to handle all turbulent flows with significant density variations (c.f. [23]). All quantities except the pressure and the density are decomposed according to

$$\varphi(x, t) = \bar{\varphi}(x, t) + \varphi''(x, t), \tag{12}$$

where the tilde denotes the mass averaged quantity $\bar{\rho}\varphi/\bar{\rho}$ and the double prime the fluctuation from this value, which implicitly in-
cludes density variations and the associated coupling effects. Re-
peaing the procedure of inserting the decomposition rule into the
conservation equations and averagi ng results in a substantially sim-
ppler expression:

$$\frac{\partial (\rho \tilde{\phi})}{\partial t} + (\nabla \cdot \tilde{u})(\rho \tilde{\phi}) = \nabla \cdot (\rho \Gamma_\theta \nabla \theta) - \rho u'' \phi'' + S_\phi \quad (13)$$

Note that the equation of state (1) is also subject to a modification
involving the correlation of temperature and mass fraction fluctu-
a tions. However, if the variation of the mixture molecular weight is
sufficiently small, it reduces again to a correlation between mean
pressure, density and temperature.

The additional quantities in the diffusion terms in equation (13)
are referred to as Reynolds stresses (for the velocity components)
and fluxes (for the species mass fractions and specific internal en-
ergy), which require modelling for closure of the system of equa-
tions. Different techniques were established to tackle this problem,
including moment methods of various orders and the widely used
$k - \varepsilon$ models.

Classical moment methods are based on a correlation of the Rey-
nolds stresses and fluxes with the gradients of the mean values

$$- \rho u'' = \mu_{turb}(\nabla \tilde{u} + (\nabla \tilde{u})^T) - \frac{2}{3}(\rho \dot{k} + \mu_{turb} \nabla \cdot \tilde{u})I \quad (14)$$

$$- \rho u'' \phi'' = \rho \Gamma_{\phi,turb} \nabla (\tilde{\theta}(\phi)),$$  \hspace{1cm} (\phi = Y_i, i)  \quad (15)

with a turbulent viscosity $\mu_{turb}$ and corresponding turbulent trans-
port coefficients $\Gamma_{\phi,turb}$ for species and heat diffusion. The turbu-
ulent transport coefficients are related to the turbulent viscosity via
turbulent Schmidt and Prandtl numbers defined in analogy to their
laminar counterparts (compare (9), (10)). This procedure implicitly
assumes that the different transport processes are associated with
identical length scales. The quantity $\dot{k}$ appearing in ((13), (14)) is the
turbulent kinetic energy, which will be defined below. Note that the
bulk viscosity $\mu_0$ is usually neglected in the modelling of turbulent
flows, since it is very small compared to typical values of the turbulent viscosity, which in first moment methods is determined e.g. in terms of a mixing length model ([24], [25], [26]).

Second moment methods are based on the derivation of conservation equations for the Reynolds stresses and fluxes, thereby introducing triple correlations as new unknown terms in these equations. This shifts the closure problem to the next level in the hierarchy of equations, which is argued to improve accuracy; however, it also increases the computational expense considerably. Though, in the recent few years, great effort has been put in the further development of these methods, they are still in the stage of being considered a next generation modelling concept [27].

The $k - \varepsilon$ model represents sort of an intermediate between first and second moment methods: It employs the gradient transport models of the former ((14), (15)), but models the transport coefficient $\mu_{turb}$ as a function of the turbulent kinetic energy $k$, defined by

$$k = \frac{1}{2}(u'' \cdot u'')$$  \hspace{1cm} (16)

and its dissipation rate $\varepsilon$, for which an additional transport equation is formulated. This is expected to improve the performance in terms of sensitivity to changes in turbulence intensities and scales over first moment methods. The transport equation for $k$ can be derived from the momentum conservation equation, basically by summing over the conservation equations for the mass-averaged diagonal terms in the Reynolds stress tensor (for details, see e.g. [23]).

$$\frac{\partial (\bar{\rho} k)}{\partial t} + (\nabla \cdot \bar{u})(\bar{\rho} k) = \nabla \cdot (\bar{\rho} \Gamma_k \nabla k) - \frac{2}{3} \bar{\rho} k \nabla \cdot \bar{u} - \bar{\rho} \varepsilon$$ \hspace{1cm} (17)

$$+ \left( \mu_{eff} \left( \nabla \bar{u} + (\nabla \bar{u})^T \frac{2}{3} \nabla \cdot \bar{u} \mathbf{I} \right) - \mu_0 \nabla \cdot \bar{u} \mathbf{I} \right) : \nabla \bar{u}$$

For convenience, the transport coefficient $\Gamma_k$ is again related to the viscosity by defining a Prandtl number equivalent for the transport of turbulent kinetic energy. The source term consists of a pro-
duction and a dissipation term. Production of turbulent kinetic energy is due to interaction with the mean flow and is represented by an expression analogous to the viscous forces source term in the energy conservation equation formulated for laminar flow (compare Table 1). In fact, in modelling of turbulent flows, the respective term is replaced by a term relating to the viscous dissipation of turbulent kinetic energy.

\[
\left(\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \frac{2}{3} \nabla \cdot \mathbf{u} \mathbf{I}\right) - \mu_0 \nabla \cdot \mathbf{u} \mathbf{I}\right) \nabla \mathbf{u} \rightarrow \bar{\rho} \bar{\varepsilon}
\]  

(18)

The generation of turbulent kinetic energy \(k\) is reflected in an additional source term \(F_{turb}\) relating to \(k\) in the momentum conservation equation. This term results after inserting (14) and combining the laminar and turbulent viscosities into an effective value,

\[
\mu_{\text{eff}} = \mu + C_\mu \frac{k^2}{\bar{\varepsilon}},
\]

(19)

already employed in (17), to

\[
F_{turb} = -\nabla \left(\frac{2}{3} \bar{\rho} \bar{k}\right)
\]

(20)

This modelling approach reflects the general picture of the spectral character of turbulence, where energy is extracted from the mean flow by the large eddies, then eventually transferred to ever smaller eddies until it is finally dissipated into heat at the low end of the spectrum by the smallest flow structures.

The transport equation for the dissipation rate \(\varepsilon\) is usually derived from physical but less rigorous arguments and structured very similar to (17):

\[
\frac{\partial (\bar{\rho} \bar{\varepsilon})}{\partial t} + (\nabla \cdot \mathbf{u}) (\bar{\rho} \bar{\varepsilon}) = \nabla \cdot (\bar{\rho} \Gamma_{\varepsilon} \nabla \bar{\varepsilon}) - \frac{2}{3} C_{\varepsilon_3} \bar{\varepsilon} \nabla \cdot \mathbf{u} \\
- C_{\varepsilon_2} \bar{\varepsilon} + C_{\varepsilon_1} \frac{\bar{\varepsilon}}{k}\left(\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \frac{2}{3} \nabla \cdot \mathbf{u} \mathbf{I}\right) - \mu_0 \nabla \cdot \mathbf{u} \mathbf{I}\right) \nabla \mathbf{u}
\]  

(21)
In fact, one of the main reasons for the popularity of the $k-\varepsilon$ model is related to the simplicity of its implementation and application: As the structure of the new transport equations is identical to that of the classical equations for the gas phase properties, the solution procedure for those variables can easily be adopted for the new ones as well. However, even if the $k-\varepsilon$ model is regarded as the standard turbulence model today, we have to keep in mind that some of its basic assumptions restrict its performance. Specifically, the assumptions of isotropy and turbulent gradient flux in a form similar to classical diffusion in laminar flow are not valid in many practical turbulent combustion systems. Also, the $k-\varepsilon$ model is known to yield poor predictions of axisymmetric and strongly swirling flows ([28], [29]).

For zero-dimensional models, where effective transport properties are again needed to determine the rates of processes related to turbulent transport, an additional strong assumption has to be introduced: Since the flow field is not resolved spatially, turbulence has to be considered as homogeneous. If some information about the mean flow is available, the energy exchange between the mean flow and the turbulence can again be modelled. Since this transfer is governed by the dynamics of the large scale eddies and the energy extracted from the mean flow is subsequently dissipated on the small scales [30], turbulence evolution can basically be described on the basis of a consideration of the dynamics of those large scale eddies alone. These can be characterized by two characteristic quantities, the integral length scale $l_I$ and a (rotational) velocity representative of the turbulence intensity $u'$. For a variable density flow, simple evolution equations for these two quantities can be formulated [31].

\[
l_I(t) = l_I(t_{ini}) \left( \frac{\rho(t_{ini})}{\rho(t)} \right)^{\frac{1}{3}} \tag{22}
\]

\[
\frac{du'}{dt} = \frac{1}{3} \frac{u'd\rho}{\rho dt} + C_P \frac{u'^2}{l_I} - C_D \frac{u^2}{l_I} \tag{23}
\]
The integral length scales have to be initialized according to typical dimensions of the turbulence generating process, for instance the valve lift for intake flow generated turbulence or the injector orifice diameter for turbulence caused by injection.

### 2.4 Spray

The mathematical description of a liquid phase dispersed in a gaseous environment is based on the spray equation formulation - a statistical approach, first introduced by Williams [32]. It considers a droplet distribution function \( f(\psi, t)\, d\psi \), which denotes the number density of droplets in a particular state interval \( d\psi \) around the state \( \psi \) at time \( t \).

The dimension of the state vector \( \psi \) depends on the nature of the problem, it includes at least the position \( x \), the velocity \( v \) and a quantity representative of the droplet size, typically the radius \( r \) of a volume-equivalent sphere. For conditions, where heat and mass transfer processes between the droplets and the gas phase occur, the droplet temperature \( T_{dr} \) has to be included - in case of a multi-component liquid, the mass fractions of the individual components have to be considered as well. If the droplet Weber number,

\[
We = \frac{\rho_{dr}(v - u)^2 r}{\sigma},
\]  

(24)

approaches the critical value of 6, parameters representing the distortion of the droplet, like the nondimensionalized deviation from sphericity \( y \) should be included. \( We \) relates the disturbing (aerodynamic) and restoring (surface tension) forces acting on the droplet surface. For Weber numbers higher than 6, the disturbing forces are dominant and the droplets are unstable. Hence, breakup processes have to be considered, which in a number of models involves the consideration of the deformation velocity of the droplet \( y \) as additional droplet state variable.

The evolution of the droplet distribution function has to take into account all processes, which alter individual droplet state variables.
These processes can relate to interactions of the individual droplet both with the gas phase and with other droplets. The evolution is described by the spray equation:

\[
\frac{\partial f}{\partial t} + \frac{\partial}{\partial \psi} f \dot{\psi} = \dot{f},
\]

where the second term on the left hand side represents the sum of all contributions due to changes of the individual state variables and the source term \( \dot{f} \) is usually composed of collision and breakup induced changes of the distribution function.

### 2.4.1 Aerodynamic Effects

Droplet position and velocity are changing due to aerodynamic drag and gravitational forces, though the latter are of minor relevance for high-pressure-driven injection systems as found in engines. In zero-dimensional models, the momentum transfer can be modelled simply by means of empiric correlations for spray penetration. In fluiddynamic models however, the interaction between the liquid and the gas phase has to be considered in some more detail.

The acceleration of a droplet is defined by

\[
\dot{v} = \frac{3}{8} \frac{\rho_g}{\rho_{dr}} \frac{|\mathbf{u} - \mathbf{v}|}{r} (\mathbf{u} - \mathbf{v}) c_d ( + g ),
\]

where the drag coefficient \( c_d \) is computed from standard correlations as a function of the droplet Reynolds number \( Re_{dr} \). In this context, the droplets are commonly treated as rigid spheres. The effective gas velocity \( \mathbf{u} \) includes a turbulent component \( \mathbf{u}' \) representative of the local turbulence level, thus modelling the effect of turbulent dispersion [33]. For the computation of gas phase properties, it is common practice to apply a ‘two-thirds rule’ in the estimation of average temperature and composition in the vicinity of droplets, e.g.

\[
\hat{T} = \frac{T + 2T_{dr}}{3}.
\]
In the gas phase, the momentum transfer to or from the droplets is reflected in additional source terms \( F_{S,a} \) and \( Q_{S,a} \) in the momentum and energy conservation equations. These terms are obtained by integrating over all momentum and energy rates of change of all droplets in the respective volume \( \Delta x \) about \( x \) at time \( t \), which result from aerodynamic effects. Analogously, source terms for the turbulent kinetic energy and its dissipation rate are determined (\( \dot{W}_{S,a} \) and \( C_S(\varepsilon / k)\dot{W}_{S,a} \)), by assuming that turbulent kinetic energy is depleted by the work required for the turbulent dispersion of the droplets [33].

\[
F_{S,a} = - \int_{\Delta x} f \rho \frac{4\pi r^3}{3} \dot{v} d\psi
\]

\[
Q_{S,a} = - \int_{\Delta x} f \rho \frac{4\pi r^3}{3} \cdot \dot{v} \cdot (v - u) d\psi
\]

\[
\dot{W}_{S,a} = - \int_{\Delta x} f \rho \frac{4\pi r^3}{3} \dot{v} \cdot u' d\psi
\]

Note that it is commonly assumed that the droplet volume density with respect to the gas volume is negligible. Consequently, no full coupling is required. The spray is then regarded as an ensemble of volume-less point-sources. This assumption has some implications on the spatial resolution applicable, since it is only valid if typical grid dimensions are large compared to the size of individual droplets (see also discussion in Appendix C.3).

2.4.2 Evaporation

Evaporation and/or condensation phenomena in sprays are usually dealt with by considering the spray as an ensemble of individual non-interfering droplets. Phase transition processes at the surface of such individual droplets can be described by applying energy and mass conservation to the liquid and the gas phase, respectively, and bal-
ancing them at an interface. In this procedure, a quasi-steady assumption is usually applied to the interface.

The solution presented here and employed throughout the present work is based on the steady-state analysis of the evaporation of a droplet in a quiescent environment, extended to convective conditions, as documented e.g. in [34]. It involves a considerable number of additional assumptions: Spherical symmetry, quasi-steady flow, constant pressure and gas properties, single-component droplets of constant density with negligible solubility of the gas phase components, negligible radiation and impact of chemical reactions, and the validity of a binary diffusion law with Lewis number unity. Even under these strongly idealized conditions, this results in coupled evolution equations for droplet temperature and radius, which have to be solved simultaneously.

\[
\frac{dr}{dt} = -\frac{(\rho D)_g \dot{T}}{2pr_d r} B Sh \tag{31}
\]

\[
\frac{dT_d r}{dt} = \frac{3}{\rho_d r c_d r} \left( \dot{Q}_d r - \rho_d r c_d r \frac{d r}{d t} L(T_d r) \right), \tag{32}
\]

where the rate at which heat is transferred to or from the droplet per unit surface area is given by a Ranz-Marshall type correlation:

\[
\dot{Q}_d r = \frac{\lambda_g (\dot{T})(T - T_d r)}{2r} Nu \tag{33}
\]

The Nusselt and Sherwood numbers, \( (Nu, Sh) \) in ((31), (33)), are related to the Reynolds number \( Re \) and the Prandtl, respectively Schmidt numbers, \( (Pr, Sc) \), through identical functional relationships.

\[
Nu \text{ or } Sh = \left( 2 + C(Re)^{\frac{1}{5}} (Pr \text{ or } Sc)^{\frac{1}{3}} \right)^{\frac{1}{2}} \ln(1 + B) \tag{34}
\]

2.4 Spray
In (31) and (34), $B$ denotes the transfer number, which is assumed to be the same for heat and mass transfer.

The effect of phase transition has to be accounted for by introducing additional source terms in the gas phase conservation equations: $\dot{\rho}_S$ in the continuity equation, $\dot{\rho}_S\delta_{if}$ in the species mass fraction conservation equation, $F_{S,\text{evap}}$ in the momentum equation and $Q_{S,\text{evap}}$ in the energy equation. These terms are again obtained from integration over all mass and heat transfer contributions of all droplets in the respective volume $\Delta x$ about $x$ at time $t$ to

$$\dot{\rho}_S = -\int \rho \frac{d}{dt} 4\pi r^2 dr \frac{d\psi}{\Delta x}$$ \hspace{1cm} (35)$$

$$F_{S,\text{evap}} = -\int \rho \frac{d}{dt} 4\pi r^2 dr v d\psi$$ \hspace{1cm} (36)$$

$$Q_{S,\text{evap}} = -\int \rho \frac{d}{dt} \left(4\pi r^2 dr (I_{dr}(T_{dr}) + \frac{1}{2}(v - u)^2) + \frac{4\pi r^3}{3} c_{dr} dT_{dr} \right) d\psi$$ \hspace{1cm} (37)$$

2.4.3 Collision and Breakup, Droplet-Wall Interactions

Processes related to the interaction of individual droplets as well as the interaction of droplets with the system boundaries are additionally affecting the droplet distribution function $f(\psi, t)d\psi$. In contrast to the processes listed above, which result in rather continuous modifications of individual components of the state vector $\psi$, these processes act in a discontinuous manner on the distribution function.

Collisions between droplets are particularly important in the dense spray region close to the injector. Depending on the collision intensity, related mainly to the relative velocity and the collision angle as well as minimum distance during impact, however also a function of
liquid properties, the outcome of collisions can take on various forms ([35], [36]): For lower collision intensities, the droplets may not coalesce, but simply exchange part of their momentum, resulting in a deflection from their original direction of flight. With higher collision intensity, the droplets coalesce, forming a single, stable droplet, whereas for further increased collision intensities the resulting droplet is not stable any more and increasing degrees of shattering are observed.

The modelling of collisions in spray systems is commonly based on the work of O’Rourke [35]: It considers the probability of collision of a larger ‘collector’ droplet with smaller droplets located in the same volume increment $\Delta x$. This probability is assumed to follow a Poisson distribution with mean value

$$\kappa = \frac{\upsilon_2}{\Delta x} \pi(r_1 + r_2)^2|\upsilon_1 - \upsilon_2|dt,$$

(38)

where the subscripts 1, 2 denote the properties of the ‘collector’ and smaller droplets, respectively. In case of collision, the outcome is then determined by considering the probabilities of the individual options.

The present understanding of droplet breakup processes is largely based on Reitz and Bracco’s [37] study of the mechanisms of disintegration of a stationary, round liquid jet, which led to the introduction of a classification of breakup processes with respect to the relative liquid-gas velocity. Generally, the breakup of droplets is one possible result of instabilities occurring at the liquid-gas interface. Two types of disturbances are distinguished: Kelvin-Helmholtz or Rayleigh-Taylor instabilities.

Kelvin-Helmholtz instabilities arise from viscous forces acting on the liquid-gas interface as a consequence of the relative tangential motion. They are characterized by small wavelengths and consequently lead to the stripping of droplets with diameters roughly equal to this wavelength off the liquid surface. Rayleigh-Taylor instabilities are the result of the acceleration of a droplet acting perpendicular-
lar to the interface in combination with the droplets inertia acting against the acceleration.

Depending on the droplet Weber number \((24)\), various breakup regimes can be discerned: For values below a critical value of about 81, the Rayleigh-Taylor instabilities induce the gradual deformation of the droplet into a bag-like structure. Finally, the remaining thin layer in the centre is disrupted, resulting in the formation of small droplets with diameters on the scale of the thickness of the former rim of the bag. This mechanism is usually referred to as bag-breakup. For Weber numbers above the critical value, the Kelvin-Helmholtz instabilities and the associated stripping mechanism become dominant. With very high Weber numbers, this stripping mechanism turns into an almost instantaneous shattering, commonly classified as catastrophic breakup.

The modelling of breakup phenomena is commonly based on the consideration of these mechanisms and will be addressed in more detail in 3.2.1.

Interactions of the droplets with the system boundaries represent another type of discontinuous effect on \(f(\psi, t)d\psi\). The multiple possible outcomes of collisions of droplets with walls, including splashing, rebounding, film formation etc. pose real challenges to their modelling (see e.g. [38]). However, as for the application considered in the present work, the occurrence of droplets hitting on the combustion chamber walls can practically be excluded as a consequence of the geometrical configuration, these issues are neglected here.

Note that all the processes listed in this section only affect the droplet distribution function and do not involve any coupling terms to the gas phase solution.

### 2.5 Chemistry

An arbitrary system of chemical reactions is described by the general expression:
\[ \sum_{I} v_{i,f,r} \zeta_i \leftrightarrow \sum_{I} v_{i,b,r} \zeta_i, \quad r = 1, \ldots, R, \quad (39) \]

where \( v_{i,f,r} \) and \( v_{i,b,r} \) are the stoichiometric coefficients of the species \( i \) appearing as a reactant and as a product, respectively, in the individual reversible reaction \( r \). \( \zeta_i \) is the chemical symbol of species \( i \), representing one mole of this species. The rate of change of the concentration of species \( i \) due to chemical reaction is given by

\[
\frac{dc_i}{dt} \bigg|_{\text{reac}} = \sum_{R} (v_{i,b,r} - v_{i,f,r}) \omega_r, \quad (40)
\]

where \( \omega_r \) is the rate, at which reaction \( r \) proceeds. This specific reaction rate is related to the concentrations of the reactants via the phenomenological law of mass action applied to the forward and backward reactions:

\[
\omega_r = k_{\text{Arr},f,r} \prod_{I} c_i^{\nu_{i,f,r}^*} - k_{\text{Arr},b,r} \prod_{I} c_i^{\nu_{i,b,r}^*} \quad (41)
\]

The asterisk indicates that the reaction orders \( \nu_{i,f,r}^* \) and \( \nu_{i,b,r}^* \) may be different from the stoichiometric coefficients \( v_{i,f,r} \) and \( v_{i,b,r} \) in (39), if the respective reaction is not an elementary reaction. Note that for reactions involving third bodies such as dissociation or recombination reactions, the concentrations of all the species acting as third bodies together with their third body efficiencies have to be considered additionally. In that case, the right hand side of (41) has to be multiplied with the resulting efficiency term \( \Upsilon \)

\[
\Upsilon = \sum_{I} \epsilon_{i,r} c_i \quad (42)
\]

The specific reaction rate constants are mainly functions of temperature, expressed in the Arrhenius relation:

\[
k_{\text{Arr},f \text{ or } b,r} = A_{f \text{ or } b,r} T_{f \text{ or } b,r}^{b_{f \text{ or } b,r}} \exp \left[ -\frac{T_{A,f \text{ or } b,r}}{T} \right] \quad (43)
\]
The range spanned by the rates of individual reactions in chemical systems easily covers several orders of magnitude, which results in a stiff system of differential equations. Therefore, in order to reduce the associated high numerical effort, it is common practice to separate slow and fast reactions. Slow reactions are handled applying equations (40) to (43), whereas concentration changes due to fast reactions are computed implicitly, making use of the algebraic expressions resulting from the application of the quasi-steady-state or partial equilibrium assumption to those reactions:

\[
\prod_{i} c^{(v_{i,b,r} - v_{i,f,r})} = K_{c,r}(T) \tag{44}
\]

If the partial equilibrium assumption is applied to multiple reactions, the resulting system of coupled differential-algebraic equations requires special solution techniques (see e.g. [39], [40], [41]). However, the solution of the dynamics of the entire system is usually accelerated substantially when compared to the purely kinetic solution procedure.

The above considerations apply well to ideal, homogenous reaction systems. In real, strongly non-homogeneous systems such as diesel engine combustion however, the rates of chemical processes are no longer determined by the reaction rates alone. In fact, physical processes associated with the mixing of the reactants are mostly slow in comparison with the reaction itself. Generally, in a system of serial processes, the rate of change of the entire system is governed by the slowest individual process. Therefore, in most heterogeneous reaction systems the rates of chemical processes are governed by the rates of mixing rather than by the actual reaction rates. Therefore, the effective reaction rates have to be modelled appropriately taking into account the rate of the limiting upstream process.

This is commonly done by considering an overall characteristic time scale for the combined effects of mixing and chemical reaction. The concept is formally based on the expansion of a representative quantity \(\xi\), e.g. the concentration of a reactant, around its steady state value (in the case of a chemically reactive system this corre-
sponds to the local equilibrium condition). If higher order terms are neglected, the rate of change of $\xi$ is related to its instantaneous and its steady state values via

$$\frac{d\xi}{dt} = \frac{\xi_s - \xi}{\tau}. \quad (45)$$

The heat release term due to reaction in the energy conservation equation (see Table 1) is related to the rates of change of the individual concentrations computed from either (40), (44) or (45) via

$$Q_{\text{reac}} = \sum_i \left. \frac{d c_i}{dt} \right|_{\text{reac}} \Delta h_{f,i}, \quad (46)$$

where $\Delta h_{f,i}$ represents the heat of formation of species $i$.

2.6 Phenomenological Aspects

Basically, the correlations listed above should be sufficient to model combustion and pollutant formation in a diesel engine or, more generally, multi-phase turbulent reaction systems. For several reasons, however, the effective modelling additionally involves phenomenological considerations:

First, the individual processes are associated with different time and length scales. As already noted in the previous section, combustion is characterized by time and length scales substantially smaller than typical scales of the flow. Since the chemical scales can generally not be resolved for technical applications, the gap has to be bridged by means of modelling approaches based on, for instance, combustion phenomenology.

Second, most of the correlations given in the previous sections were derived by considering each process separately and undisturbed by other phenomena. In real systems, however, the individual processes appear strongly coupled, which may severely alter their characteristics. This requires more insight into how the various pro-
cesses interact, which, to present, is also mainly based on phenomenological considerations.

Third, since several processes involve statistical methods for their description, the derivation of the respective correlations must rely heavily on their phenomenology. Especially for spray processes such as the spray and individual droplet breakup and the collision of individual droplets, closed and exact solutions are not yet available. Note that the big number of simplifying assumptions required for the derivation of the fundamental equations for droplet evaporation clearly reveals the phenomenological nature of this approach as well.

The following section is intended to identify the modelling priorities with respect to simulation of combustion and nitric oxide formation in diesel engines on the basis of the phenomenology of the relevant in-cylinder processes.

**2.6.1 Injection and Spray Formation**

The liquid fuel is introduced into the combustion chamber through small orifices at high initial velocity, which is mainly the result of the pressure difference between the fuel injection system and the combustion chamber. An additional effect arises from the geometry of the nozzle holes, which determines the effective cross-section of the orifice. The overall spray behaviour is usually characterized by three parameters: The spray tip penetration, the spray angle and the Sauter mean diameter, a quantity representative of the drop size distribution (For an overview see e.g. [42], [43]).

The spray tip is propagating at almost constant speed during an initial phase whose duration is determined by the Levich-correlation [44] to

\[
t_{bu} = C \sqrt{\frac{\rho_{dr, ini}}{\rho_g}} \frac{d_o}{v_{ini}}.
\]  

The breakup-time \( t_{bu} \) can be interpreted as the time required for complete disintegration of the spray into primary droplets, which then undergo further breakup due to the action of aerodynamic
forces. The structure of the spray in the region close to the nozzle exit, however, is not well understood. Originally, this behaviour was attributed to the existence of an intact liquid core surrounded by a growing layer of small droplets stripped from its surface. This structure was observed in continuous sprays by means of experiments based on the measurement of conductivity (e.g. [45], [46]). The relevance of these observations to highly transient diesel sprays however, remains questionable. More recent investigations utilizing various techniques indicated that the liquid jets are broken into fragments of various size and shape already at or shortly after the nozzle exit ([47], [48], [49]). However, irrespective of the exact mechanism governing the breakup into primary droplets, appropriate methods have to be applied to its modelling. In fact, considering this process as purely aerodynamic would result in the erroneous prediction of immediate atomization at the nozzle exit as a consequence of the high initial Weber numbers.

After the breakup-time, the spray tip penetration increases with $\sqrt{t}$. This quantity is measured as the distance from the injector of the leading droplets for non-evaporating sprays, respectively of the tip of an iso-surface of non-negligible vapour mass fraction for evaporating sprays. The radial expansion of the spray leads to the observation of a spray angle, which is usually correlated to the density ratio via

$$\tan\left(\frac{\alpha}{2}\right) \sim \sqrt{\frac{\rho_g}{\rho_{dr, ini}}}.$$  \hspace{1cm} (48)

The spectrum of droplet diameters ranges from the size of the injector orifice to close to zero shortly before evaporation is completed. The Sauter mean diameter is usually employed to characterize this spectrum; it is defined as the diameter of the droplet with the same volume to surface ratio as the entire spray or of all the droplets at a certain location in the spray. The spatial distribution is mainly determined by two effects: The aerodynamically induced breakup and the evaporation.
A rough estimate of droplet life times under the influence of these two processes at typical engine conditions before the start of combustion shows that breakup is predominant: According to [50], the characteristic drop breakup time scale $\tau_{bu}$ for an inviscid droplet is determined by:

$$
\tau_{bu} = \begin{cases} 
  \frac{4.5}{\sqrt{8}N} \frac{\rho_{dr} r^3}{\sigma} & \text{if } \text{We} \leq 81 \\
  \frac{4.5}{\sqrt{8}N} \frac{\rho_g}{\rho_{dr}} \frac{r}{|v-u|} & \text{if } \text{We} > 81 
\end{cases}
$$

(49)

Considering a droplet in the bag breakup regime ($\text{We} \leq 81$, compare 2.4.3), where the breakup time is a function of the droplet radius alone, the resulting values of $\tau_{bu}$ are in the order $10^{-4}$ to $10^{-3}$ s. In the limiting case of $\text{We} = 81$, the corresponding droplet Reynolds number is in the $10^3$ range. Inserting this upper limit into the rate of change equation for the droplet radius (31), assuming constant gas properties and that the droplet is at its wet-bulb temperature, gives a rough estimate for the corresponding evaporation times.

$$
\tau_{evap} = \frac{2\rho_{dr} r^2}{(\rho D)_{g}(T)} \frac{1}{S\lambda \ln(1 + B)}
$$

(50)

The resulting values are typically one order of magnitude higher than the breakup times. In the case of larger Weber numbers, i.e. higher relative velocities, the breakup time is inversely proportional to the relative velocity, whereas the evaporation time scales approximately with $1/\sqrt{\text{Re}}$. Here, the predominance of breakup is even more obvious. It has to be noted, however, that droplet relaxation time scales, which reflect the droplet deceleration to the velocity of the mean flow, also scale with the square of the droplet diameter [51]. Consequently, Weber numbers are eventually decreasing due to both, reduction of droplet diameters and relative velocity. Finally, $\text{We}$ falls below the instability limit of 6 and hence, evaporation is becoming predominant and proceeds rapidly. This is even more the
case with combustion, when heat and mass transfer are enhanced by the increased temperature and concentration gradients.

2.6.2 Ignition

Autoignition in diesel engines is the result of the complex interaction of many individual processes including the dispersion and phase change of the fuel, its mixing with the oxidizer and the chemistry of the actual combustion-initiating reactions. For this reason, the ignition delay, which is considered as the quantity best characterizing the ignition process, is often subdivided into physical and chemical portions.

Whereas the physical contributions to the total ignition delay are mainly related to the two-phase phenomena described in the previous section, the chemical ignition process involves a complex reaction system associated with the oxidation of the fuel. Detailed combustion reaction mechanisms including the low- to medium-temperature regime relevant to ignition typically consist of thousands of reactions between hundreds of individual species, even for single component fuels. To present, only for a limited number of model fuels the associated reaction mechanisms are known in sufficient detail. Therefore, the current understanding of ignition is still largely based on phenomenological considerations of thermal and chain-branching effects (for an overview, see e.g. [52]).

The autoignition process of hydrocarbons is characterized by a number of regimes, which can be identified as a function of temperature and pressure considering the respective explosion diagrams (see e.g. [52]). The different regimes basically represent shifted weights between the various chain-branching and the thermal effects. In the ignition of higher hydrocarbons under engine-relevant conditions three regimes can be discerned ([53], [54]):

- The high-temperature regime, where the ignition delay is determined by the induction time of the chain-branching process, mainly via the reaction:

\[ H + O_2 \rightarrow OH + O \]
• The medium-temperature regime, where concentrations of $O, H$ and $OH$ are lower, whereas $HO_2$ concentrations are higher than in the high-temperature regime. This results in the predominance of another chain-branching mechanism starting with the abstraction of $H$ from the fuel through $HO_2$ and the subsequent dissociation of the resulting peroxides:

$$H_2O_2 + M \rightarrow 2 \ OH + M$$

• The low-temperature regime, where ignition proceeds through multiple stages in a degenerate branching process: Initiated by (external) $H$-abstraction by $H$-radicals, then followed by two subsequent series of $O_2$-addition and internal $H$-abstraction and concluded by propagation as well as branching steps involving again the formation of $OH$ (for details, see [53]).

Thermal effects also play a role in these regimes in that they enhance or inhibit individual steps, depending on the exo- or endothermic nature of the associated reactions. Note that, in specific situations, the confinement may act as sink for radicals and thus affect the ignition process additionally.

Considering the nature of the relevant reaction, the medium-temperature regime obviously has to exhibit a pressure (and composition) dependence: Dissociation as well as addition reactions are inherently pressure-dependent as a consequence of the different numbers of products and reactants, which has an effect on the specific reaction rate (41). The same applies to the high-temperature region, where, apart from the mainly determining reaction, various (pyrolytic) dissociation reactions are involved in the precombustion chemistry. Only in the low-temperature regime, the mechanism includes both (chain branching) dissociation and addition reactions, which, globally, balances potential pressure effects introduced by the individual reactions.

This behaviour is reflected in Figure 2, where ignition delays for homogeneous stoichiometric mixtures of n-heptane with air, computed using a detailed reaction mechanism, are shown as a function of temperature and for various pressures (c.f [55]). Note that n-hep-
n-heptane is usually regarded as the model fuel best representing diesel ignition behaviour, as indicated by the similar cetane numbers of n-heptane and customary diesel fuels.

Shock-tube measurements (e.g. [54]), where the ignition delay is measured after inducing a shock-wave in a homogeneous mixture of the fuel and oxidant, confirm these data. In particular, the existence of a region in the Arrhenius plot, where the gradient with respect to the inverse temperature is negative, was observed there as well. In ignition experiments for non-homogeneous situations, however, as found e.g. in spray combustion chambers, this effect is less pronounced [56]. This is clearly a consequence of the temperature and concentration inhomogeneities, which tend to blur the extrema. It is even more so for real, multi-component fuels as a consequence of partially sequential evaporation and transition temperatures between the individual temperature regimes varying between the individual components. In fact, numerous investigators correlated their ignition

**Figure 2:** Ignition delay of stoichiometric n-heptane/air mixtures computed by means of a detailed reaction mechanism (c.f. [55]).
delay data for diesel fuel to temperature by means of a single exponential relation applicable throughout the entire domain – for an overview, see e.g. ([42], [43]).

2.6.3 Combustion

The character of the combustion process in diesel engines is mainly determined by the progress of mixture formation at ignition [43]:

In case a large fraction of the fuel is sufficiently well mixed with the fresh gas already before ignition, the combustion is predominantly proceeding in the premixed mode. This is observed mainly in small engines running at high speed or engines up to medium-size operated at very low load, where ignition occurs in the late injection phase or even after the end of injection. They are characterized by a steep pressure increase resulting from the fast consumption of the fuel.

In contrast, in large low-speed engines, the amount of fuel already present in flammable mixture at start of combustion is negligible compared to the total mass of fuel injected per cycle. Therefore, after this small flammable mixture has been consumed, the mixing-controlled mode of combustion is predominant during the remainder of the combustion phase.

For intermediate cases, the combustion process is characterized by two phases: A premixed phase, discernable from a sharp initial pressure rise, and the mixing-controlled phase, during which the fuel is consumed in a diffusion or non-premixed flame.

It has to be pointed out that the combustion process during the premixed phase is substantially different from the one in spark-ignited engines. In those engines, a premixed flame front originating at the ignition source is sweeping through the combustion chamber. Turbulence enhances the combustion process by increasing the flame surface density through convolution and wrinkling of the locally laminar flame sheet. Only in the undesirable case of engine knock, autoignition in locations ahead of the flame front superimposes the fuel consumption in the propagating flame.
This effect is, however, believed to be more relevant during the premixed phase of combustion in diesel engines: On the one hand, the progress of the combustion-initiating reactions is similar in regions of similar thermodynamic state, which leads to the fact that already small disturbances lead to ignition. On the other hand, due to the non-homogeneous mixture formation, the propagation of a premixed flame is practically restricted to the close vicinity of the stoichiometric iso-surface, as towards the fuel-rich and fuel-lean sides, respectively, the flame is soon extinguished as a consequence of local compositions outside the flammability limits.

The premixed combustion mode in diesel engines can thus be interpreted as the result of the combination of two competing effects: The propagation of premixed flames from already ignited regions and the formation of new ignition sites. There are indications that the propagation is occurring via so-called triple flames forming at the edges of already established diffusion flames [57]; however, the mechanism is not fully understood. Obviously, both processes, the formation of new ignition sites as well as the propagation, are not substantially affected by turbulence, since the associated length scales are comparatively small. Note that a further prerequisite for local ignition is given by the condition of the strain rate level being below the limiting values for ignition, which, however, is not always the case in practical applications.

In the mixing-controlled combustion mode, the fuel is consumed in a non-premixed or diffusion flame, where the reactants are spatially separated and the combustion occurs in a thin layer at the stoichiometric interface of the fuel and oxidizer regions. The diffusion of the reactants to this interface is hence limiting the combustion rates in this type of flame. In diesel engines, the diffusion is enhanced by the turbulence generated both by the air charge motion originating from the intake process or the squish regions and by fuel injection.

Depending on the values of the velocity and length scales of the combustion system, various regimes of turbulent non-premixed combustion can be identified. The Borghi-diagram ([58], [59]), plotting the ratio of turbulent and flame velocity over the ratio of
turbulence and flame length scale, is commonly employed for this purpose. The individual regions in this diagram are separated by lines of constant value of various non-dimensional parameters, in particular: The Damköhler number $Da$, defined as the quotient of the turbulent and the chemical time scales, and the Karlovitz number $Ka$, which is the quotient from the laminar and the Kolmogorov time scale. $Da = 1$ separates the regions of thickened flames or stirred reactors from the flamelet regime. $Ka = 1$ marks the transition from wrinkled and stretched flamelets to perturbed or corrugated flamelets.

The regime applicable to combustion in medium-speed diesel engines can be identified as follows: As a consequence of the high temperatures after compression and the preceding ignition and premixed combustion phases, flame temperatures in the once established diffusion flames are relatively high. Estimating the flame time scale on the basis of the chemical time scale resulting from the kinetic data for the global reaction of a representative model fuel (e.g. from [60]) yields a value in the order $10^{-7}$ s. This is approximately an order of magnitude below minimum values of a corresponding estimate for the turbulent time scale based on the assumption of a turbulent length scale equivalent to the nozzle hole diameter and a representative fluctuating velocity proportional to the maximum injection velocity. The Damköhler number $Da$ is therefore well above the critical value of 1, whereas the Karlovitz number $Ka$ is slightly below one, based on the above estimates. This indicates that the flame type encountered in these engines has to be considered as consisting of wrinkled and stretched flamelets, however in the transition region to the perturbed flamelet regime.

### 2.6.4 NO Formation

Three main forms of oxygenated nitrogen compounds have to be considered in combustion processes [61]: $N_2O$, $NO$ and $NO_2$.

Nitrous oxide, $N_2O$, usually represents a trace species; however, it can play an important role as an intermediate in the formation and destruction of the two other oxides. Nitric oxide, $NO$, is the pre-
dominantly formed species (typically between 98 and 99% for spark ignition engines and 70 to 90% for diesel engines, c.f. [43]). However, as it is almost entirely converted into nitrogen dioxide, $NO_2$, in the atmosphere, emissions are often related to the latter species, in particular when specified in mass-related units.

Nitric oxide formation can follow three main pathways, illustrated in Figure 3, depending on the source of the nitrogen and the location of the formation process [61].

**Figure 3:** Nitric oxide formation pathways (according to [61]).

The formation of nitric oxides from molecular nitrogen requires to break the very stable triple bond in these molecules. This can be achieved by attack of either oxygen radicals or highly reactive low-molecular hydrocarbon compounds formed as intermediate species during the combustion process. Accordingly, two mechanisms are distinguished: The Thermal and the Prompt $NO$ mechanisms.

The Thermal $NO$ mechanism, describing the formation of $NO$ as a consequence of the attack of oxygen radicals, was first postulated by Zeldovich ([62], reactions (51) and (52)). It was later extended by Lavoie et al. [63], allowing for $NO$ formation under fuel-rich conditions as well, by introducing reaction (53):

\[
N_2 + O \leftrightarrow NO + N \tag{51}
\]

\[
N + O_2 \leftrightarrow NO + O \tag{52}
\]

\[
N + OH \leftrightarrow NO + H \tag{53}
\]

2.6 Phenomenological Aspects
Reaction (51) is the initiating step, which is characterized by a very high activation energy. Therefore, $NO$ formation rates due to reactions (51) through (53) are significant only at high temperatures. However, even then, they are very slow in comparison with the rates of fuel oxidation. It is common practice therefore, following the suggestion of Zeldovich, to decouple $NO$ formation from the fuel oxidation process and to apply an equilibrium assumption for determining the $O$ and $OH$ radical concentrations in the post-flame zone. However, Miller and Bowman [64] showed that superequilibrium concentrations of $O$ in the vicinity of the flame can lead to a substantial increase of $NO$ formation rates when compared to the results obtained with the equilibrium assumption for $O$ and $OH$. The superequilibrium concentrations result from fast radical formation in the flame in combination with comparatively slow recombination reactions when moving away from the reaction zone.

An alternate pathway was proposed by Wolfrum [65] and Malte and Pratt [66], considering nitrous oxide as the result of a three-body reaction of molecular nitrogen and the oxygen radical instead of (or additionally to) reaction (51):

$$N_2 + O + M \leftrightarrow N_2O + M \quad (54)$$

$NO_2$ is then subject to further oxidation via

$$H + N_2O \leftrightarrow NO + NH \quad (55)$$

$$O + N_2O \leftrightarrow 2 \ NO \quad (56)$$

or reduction via

$$H + N_2O \leftrightarrow N_2 + OH \quad (57)$$

$$O + N_2O \leftrightarrow N_2 + O_2, \quad (58)$$

depending on thermodynamic conditions. As a consequence of the three-body nature of reaction (54), the $NO$ formation rate associated with this mechanism is pressure-dependent. As discussed above for the original Thermal $NO$ mechanism, superequilibrium concentra-
tions of the oxygen radical in vicinity of the flame enhance $NO$ formation via reactions (54) to (56).

In the Prompt $NO$ mechanism, also known as the Fenimore mechanism [67], the $N_2$ chemical bond is broken after attack of fuel radicals in the flame, e.g. via

$$N_2 + CH \leftrightarrow HCN + N.$$  \hspace{1cm} (59)

The $C-N$ species formed in these reactions, e.g. the hydrogen cyanide, $HCN$, resulting from reaction (59), are subsequently, like the same species formed from fuel-bound nitrogen, partially converted into nitric oxide (see Figure 4 below). The $N$-radicals generated in (59) again react with oxygen or hydroxyl radicals to form $NO$ via reactions (52) and (53).

Nitrogen compounds in fuels can take on various forms and are present in noticeable amounts mainly in solid and heavier liquid fuels [61]. Experiments showed that the conversion of fuel-bound nitrogen is almost independent of the identity of the nitrogen-containing species. However, it depends strongly on the combustion conditions and the initial nitrogen compound concentration in the fuel-air mixture (c.f. [64]).

In fact, the fuel nitrogen compounds are rapidly and almost entirely converted into hydrogen cyanide and ammonia (the latter mainly in the case of amine compounds). The cyanide formed is then converted to $NH$, either directly or via partially oxidated intermediate species. $NH$, like any ammonia or $NH_2$ present, undergoes $H$-abstractions resulting in the formation of nitrogen radicals. These radicals then react to form either $NO$ via reactions (52) and (53) or $N_2$ via the reverse of reaction (51).

Figure 4 shows schematically the main reaction paths in the conversion process of fuel-bound nitrogen as described in ([59], [64]).

Included in this scheme are the Prompt-$NO$ start reaction (59), represented by the dashed line, and the so-called $NO$-recycle reactions related to the conversion of $NO$ into $HCN$ or $CN$ after the attack of fuel radicals, symbolized by the dotted lines.
Typical nitrogen content levels of customary diesel fuels are in the 0.1% by mass range or below. Even if complete conversion to $NO$ is assumed, the resulting emission level is typically less than 10% of the total nitric oxide emissions, which corresponds to the minimum prediction uncertainty of Thermal $NO$ formation. Therefore, the Fuel $NO$ mechanism is usually neglected in the simulation of diesel engines. The associated necessary detail in the modelling of the combustion chemistry is a further grave argument against its inclusion in these simulations. Note that the nitrogen content of fuels burnt in diesel engines can vary considerably, depending on provenance and the degree of refinement of the fuel. This uncertainty adds to the above reservations towards the consideration of the Fuel $NO$ mechanism in diesel engine simulations.

The same order of magnitude argument as above applies to the fraction of $NO$ formed via the Prompt $NO$ mechanism. As a consequence of the very thin reaction zone found in a diffusion flame and the corresponding short residence times in this reaction zone, the contribution of Prompt $NO$ to total emissions is considered of minor relevance. Additionally, it can be expected to be less sensitive to in-

Figure 4: Reaction path diagram of the conversion of fuel nitrogen to $NO$ after ([59], [64]).
initial and boundary condition variations than the $NO$ formed via the Thermal $NO$ mechanism.

Drake and Blint [68] showed in their numerical investigation of laminar premixed methane flames that the importance of superequilibrium concentrations of oxygen radicals in Thermal $NO$ formation decreases with increasing pressure. In their calculations, the fraction of $NO$ formed due to superequilibrium concentrations of $O$ fell from 36.8% at 1 atm to 12.9% at 20 atm. It is therefore assumed that in view of the substantially higher pressure levels observed in diesel engines during combustion (typically above 100 bar), this effect may be neglected.

In the same investigation, it was observed that the contribution due to reactions (54) through (58) increased from 4.7% to 11.9% as the pressure was increased from 1 to 20 atmospheres. In view of the pressure dependence already noted previously, this pathway is expected to be of significance in $NO$ formation in diesel engines.

In summary, we can state that a more detailed mechanism than the simple extended Zeldovich mechanism is required in order to model $NO$ formation in diesel engines appropriately. However, for engine process optimization purposes, the consideration of neither the Fuel $NO$ nor the Prompt $NO$ mechanisms appears necessary. Superequilibrium concentration effects may also be neglected.
3 State of the Art

First attempts to predict combustion in DI diesel engines, partly already including approaches towards pollutant formation modelling, were reported in the late sixties and early seventies ([69] - [72]). The first comprehensive modelling approach dates back to 1976 [73]. Though these models were extended and enhanced continuously, substantial progress was achieved only in recent years, mainly as a consequence of the following developments: On the one hand, growing environmental concerns stipulated intense research in this field. On the other hand, the continuous expansion of computational resources eventually enabled the application of Computational Fluid Dynamics in this context.

Generally, following Bracco [74], combustion (and emission) models are classified by the number of dimensions they account for as zero-, quasi- or three-dimensional. In contrast to the purely thermodynamic character of zero-dimensional models, quasi-dimensional models include, although not spatially resolved, fluid-dynamic effects in the determination of the rate of heat release. Other reviewers (e.g. [42]) refer to the latter models as phenomenological ones; however, in view of the largely phenomenological nature of the three-dimensional models as well (see preceding chapter), the former classification is preferred by the author and will be employed throughout the following discussion.

3.1 Zero- and Quasi-Dimensional Models

Various researchers ([69], [70]) attempted to correlate the rate of heat release and the injection rate. These approaches are typically based on an incrementation of the total amount of fuel injected. The ignition delay and burning rates of the individual increments are determined by means of empiric correlations fitted to experimental data, partially accounting for the different combustion regimes and the respective rate-determining effects.

The modelling approach of Woschni and Anisits [71] is a typical representative of the purely zero-dimensional models. It describes
the alteration of the combustion characteristics of an engine as a function of operating condition variations based on the semi-empiric method proposed by Wiebe [75]. Based on comprehensive experimental data, the authors identified rules for the variation of the model parameters as a function of changing operational parameters.

Khan et al. [72] proposed one of the first diesel engine combustion models including pollutant formation. It is based on the fuel spray jet model of Grigg and Syed [76], which predicts the rate of heat release mainly by calculating the rate of air entrainment of an airborne jet. After the ignition delay has been determined from experimental data, a premixed combustion peak of triangular shape is prescribed, its extent depending on the amount of fuel and air mixed at that stage. It is followed by the main part of combustion, where the micromixing of fuel and oxygen is assumed to determine the instantaneous burning rate. The NO formation is computed for a single product zone on the basis of the Zeldovich mechanism; however, in order to achieve agreement with the experimental data, the rate constants had to be adjusted to compensate for the deficiencies of the thermodynamic model.

After detailed studies of the individual phenomena associated with the combustion process in diesel engines, Hiroyasu and Kadota [73] proposed a multi-zone model based on the consideration of a liquid fuel jet. Its disintegration as well as the entrainment of the surrounding air and the associated mixture formation are modelled based on empiric correlations. The spray is discretized axially and radially into ring-type packages assumed to contain the same fuel mass in liquid form, initially. Each package experiences its own temperature, evaporation, mixing, ignition and burning history without interfering with the other ones. After ignition in each package, the combustible mixture is assumed to burn rapidly under stoichiometric conditions. In the following, either the entrainment or the evaporation rate are considered rate-limiting, depending on the local fuel/air ratio. Nitric oxide formation is computed in each package, applying the extended Zeldovich mechanism. When compared to experimental data, both cylinder pressure histories and NO emissions from simulation showed noticeable deviations; however, trends could be predicted.
fairly well at this early stage already. The model was further de-
veloped and extended to account for the influence of swirl and spray-
wall interaction ([77], [42]) and is still considered as the reference in
the field. Both commercial diesel engine simulation codes like GT-
Power [78] and combustion models proposed even most recently
(e.g. [79]) are, to a large extent, based on the developments of
Hiroyasu and co-workers.

Previous investigations conducted at the Internal Combustion En-
gines Laboratory of the Swiss Federal Institute of Technology ([80],
[81]) also employed similarity laws in combination with empiric
correlations to determine spray propagation. Burning rates are com-
puted after the determination of evaporation and mixing, by applying
global reaction rates with parameters fitted to match experimental
data. In Papadopoulos’ model [81], the nitric oxide emission is then
computed considering discrete burnt gas zones, subject to mixing
with fresh air, applying the extended Zeldovich mechanism. The
mixing process is assumed to be controlled by a characteristic time
scale relating to the mean gas motion inside the cylinder.

The more recent NO emission models of Hohlbaum [82] and
Heider [83] are classical two-zone models. The latter uses the
Woschni-Anisits correlation [71] for determining the heat release
rate, whereas the former includes, besides an empiric approach, a
phenomenological spray model. This combustion model employs a
bimolecular combustion reaction proceeding at initially fuel-rich
conditions. The transition of the flame stoichiometry to lean con-
ditions is modelled to match experimental heat release rates. Nitric
oxide formation is computed in the burnt gas zone, which is event-
ually mixed with the residual fresh air, by means of the extended
Zeldovich mechanism. The same mechanism is employed in the
model of Heider [83], which is based on the assumption of reactant
(and product) zones of constant air/fuel ratio, where the temperature
difference between the zones is modelled empirically.

The predictive quality of the presented models in terms of NO
emissions is mainly dictated by two effects: The accuracy of the heat
release rate predictions and the type and detail of the NO formation
model. In order to accurately model the heat release, either a purely empiric approach or the detailed consideration of spray and mixture formation phenomena can be employed. It is believed, however, that the latter approach allows more reliable predictions for conditions outside the range applied in the determination of the empiric correlations of the former approach. The predictive quality of a NO formation model in turn is both determined by the modelling concept in order to resolve the spatial inhomogeneities and the underlying chemistry model. In view of the discussion in 2.6.4, the latter effect must not be neglected. To our best knowledge, so far no zero-dimensional model has been proposed that includes both the detailed consideration of spray and mixture formation processes in the determination of the heat release rate and a multi-zone approach for modelling NO formation on the basis of more detailed chemistry.

### 3.2 Three-Dimensional Models

In the context of internal combustion engines, fluid dynamics based models were introduced in the early eighties. First attempts to model combustion processes - mainly for spark ignited engines - were made right from the start. The first years however, were mainly dedicated to the modelling of gas exchange processes and in-cylinder flow including turbulence (for an overview, see e.g. [43]).

The introduction of KIVA in 1985 [84], providing a common, open platform for researchers in the field of internal combustion engine modelling, marks an important step in the development of simulation methods for in-cylinder processes. The same applies to its successors, KIVA-II ([33], 1989), which includes an advanced spray model, and KIVA-3 ([85], 1993), which is adapted for block-structured grids. Since then, the number of publications related to three-dimensional simulations of internal combustion engines has increased tremendously. Therefore, in the following sections, only the major contributions to the modelling of the key processes identified in the previous chapter will be presented.
3.2.1 Spray and Individual Droplet Breakup Modelling

As already discussed previously in 2.4.3 and 2.6.1, two main phases have to be distinguished in the disintegration of the liquid fuel jet: The initial phase, which is associated with the breakup of the liquid, though possibly already fragmented jet into primary droplets, and the second phase, where these primary droplets undergo sequences of further breakup into smaller droplets. Finally, this results in the formation of small, stable droplets.

Based on the fundamental study of Reitz and Bracco [37], Reitz and Diwakar [86] and Reitz [87] derived a general breakup model describing the stripping of small droplets from the surface of larger droplets. This approach is inherently capable of simulating the primary breakup of the liquid core as well when modelling the liquid core as an ensemble of large drops with the initial diameter of the injector orifice. However, a more recent investigation [88] showed that, for the description of secondary breakup, it may be advantageous to use a different approach.

A second, equally popular model for droplet breakup is the one proposed by O’Rourke and Amsden (TAB - Taylor Analogy Breakup model, [89]). In this model, droplets are considered as damped, harmonic oscillators excited by the relative velocity. Breakup is assumed to occur when the nondimensionalized distortion of a droplet exceeds a critical value. Since this is achieved very fast for the large droplets entering the combustion chamber at high speed, this model cannot reproduce the primary breakup and hence results in rather poor predictions of the global spray propagation.

An enhanced version of the TAB model was introduced by Tanner [50], allowing both the modelling of primary breakup and an improved description of the secondary breakup. The former is achieved by artificially delaying the first breakup of the initial droplets, modelled again as drops of the size of the injector orifice, in order to match experimentally observed values for the spray breakup time (47). The latter is based on the consideration of a breakup cascade, where the diameter of the resulting droplets is determined from a regime-dependent breakup law and the radial velocity component
from energy conservation. This model showed drastically improved predictions of overall spray propagation over the original TAB model both for non-evaporating and evaporating sprays [90].

### 3.2.2 Ignition Modelling

Two major groups of ignition models can be distinguished: Empiric models based on experiments with diesel fuel ([91]-[93]) and models deduced from detailed mechanisms using reduction techniques ([53], [94]). There also exist hybrid approaches, including the Shell-model [95], which is probably the most popular ignition model utilized in engine simulations.

The first group of models is commonly based on the consideration of a progress variable for ignition. This variable is often modelled similar to the ignition integral, well-known from zero-dimensional modelling approaches, now applied to each individual cell separately:

\[
\int_{t_0}^{t} \frac{dt}{\tau_{ig}(p, T, c_i)}.
\]

where \( t \) denotes time after start of injection. As soon as the progress variable exceeds the critical value of one, the combustion model is activated. Abraham and Bracco [93] introduced an additional conservation equation for the evolution of the ignition integral and again applied empiric correlations for the determination of the instantaneous ignition delay.

The second group of models considers a reduced reaction scheme for a model fuel. The underlying detailed mechanism is systematically reduced to a set of rate-determining steps, including the formation and consumption of some intermediate species, which can either be representative “real” species or generic ones combining various species with equivalent functional behaviour. Obviously, such an approach requires a more detailed treatment of the transport phenomena as well, resulting in additional conservation equations for each
intermediate species. The criterion for ignition can be defined either in the form of a critical temperature, in case a heat release is associated with individual reactions, or simply by comparing the fuel consumption rate computed from the ignition model with the corresponding value of the combustion model. To overcome the problem of increased computational expense, Elsden et al. [94] devised a method, where only a single representative species (CO) is tracked in the fluiddynamic solver and the conservation equation is closed by means of a presumed PDF approach applying lookup tables for the precalculated laminar ignition chemistry. However, the calculation of the PDF’s requires one additional conservation equation for the variance of CO. The ignition criterion in their case is basically a critical value of the concentration of H₂O, which, in their approach, is uniquely related to the CO concentration.

The Shell-model [95] and its numerous derivatives (e.g. [96]-[98]) have to be considered as a hybrid approach in the sense that they are based on a scheme of 8 generic reactions involving 6 equally generic species. The associated kinetic parameters, however, were determined by means of fitting to experimental ignition delay data. The introduction of generic species again involves the solution of additional conservation equations. One of the reactions is associated with a heat release and the excess of a critical temperature (or a critical temporal temperature gradient) serves as the criterion for ignition.

### 3.2.3 Combustion Modelling

The combustion models proposed and applied to diesel engines in recent years can be grouped as follows:

The first models applied in this context were based on characteristic time scales, the most popular one among them being the Magnussen model [99]. It describes the combustion process as a single-step reaction, where the consumption of the fuel is determined by the following expression:

\[ \frac{dc_{\text{fuel}}}{dt} = C_1 \min \left[ c_{\text{fuel}} \frac{c_{O_2}}{a_{st}} \right. \left. C_2 \frac{c_{\text{prod}}}{1 + a_{st}} \right] \frac{\varepsilon}{k} \]  

\[ (61) \]
The basic idea behind this approach is that, in diffusion flames, the reactants are intermittent, i.e. confined to separate eddies. Therefore, the dissipation rate of these eddies, modelled as $\frac{\varepsilon}{k}$, is assumed to be responsible for the mixing of fuel and oxygen on a molecular scale, hence combustion. On the micro-scale, the reaction rate is additionally affected by the local stoichiometry, represented by the first two arguments of the min-term in (61). The last argument in this term applies to premixed flames rather, where the mixing of hot product eddies with cold reactant eddies is assumed to be controlling. However, it also has an effect in non-premixed cases by keeping reaction rates low in the initial combustion phase, when product concentrations are not yet significant.

This model, also known by the name of eddy dissipation concept (EDC), exhibits some similarity to the eddy breakup model (EBU) proposed earlier by Spalding [100]. For this reason, it is often grouped among the eddy breakup type models.

The model was further developed [101] in order to account for the small structures in which the reaction is assumed to proceed and even by applying detailed [102] or generic [103] reaction schemes in these small scale ‘reactors’. The problems in this approach lie in the estimation of the size of the ‘reactors’ and the modelling of their interaction with the mean flow.

Another type of characteristic time scale model was proposed by Kong et al. [104]. It relates the instantaneous rate of change of species mass fractions due to combustion to the difference of the local mass fractions and their equilibrium values, divided by a characteristic time scale of the combustion process (compare Eq. (45)) as

$$\frac{dY_i}{dt} = \frac{Y_{i,eq} - Y_i}{\tau_{comb}}.$$  \hspace{1cm} (62)

This time scale $\tau_{comb}$ is computed from the laminar and turbulent time scales using the expression

$$\tau_{comb} = \tau_{lam} + \zeta_{prog} \tau_{turb}.$$  \hspace{1cm} (63)
In (63), the laminar time scale \( \tau_{lam} \) is determined from the Arrhenius formulation of the global combustion reaction, the turbulent time scale is modelled as proportional to \( k/\varepsilon \). The weighting function \( \zeta_{prog} \) may take on values between zero and one and its instantaneous value is related to the ratio of product mass fractions to reactant plus product mass fractions. As \( \zeta_{prog} \) varies from zero to one, it shifts the dependence of the combustion rate from a purely chemistry-related state shortly after ignition to the mixing-controlled regime.

In this approach, a local equilibrium assumption is applied: The combustion process is thus inherently modelled as a multi-step reaction scheme through the consideration of combustion products other than \( CO_2 \) and \( H_2O \). The model was tested against various engines of different sizes and at different operating conditions; the simulation results presented show good agreement with experimentally observed trends.

A second group of models is based on the flamelet approach of Peters ([105], [106]) for non-premixed turbulent combustion.

This concept is based on the transformation of the conservation equations for energy and species into mixture fraction space, thereby assuming a one-dimensional flame structure on a coordinate perpendicular to the flame surface. This procedure involves the introduction of the scalar dissipation rate \( \chi \) as a new quantity representative of the local turbulence effects on the flame. Formally, \( \chi \) is equivalent to the differential of the mixture fraction \( Z \) with respect to the coordinates on the flame surface.

The flamelet structure can then be resolved in one-dimensional, time-dependent calculations as a function of prescribed parameters. This can be done either prior to the solution of the flow field or in parallel. In the first approach, the results are then either analysed in order to obtain algebraic laws for fuel consumption ([107] - [109]) or so-called flamelet libraries are generated [110], which are subsequently employed as look-up tables in the combustion simulation. In contrast to these decoupled solution approaches, Pitsch et al. [111] proposed a concept, where the flamelet code is coupled directly to

3.2 Three-Dimensional Models
the solution of the flow field. In their approach, the combustion rates are determined interactively for representative flamelets.

In the coherent flame(let) models of Dillies et al. [107] and Musculus and Rutland [108], the local combustion rate is computed from the algebraic laws for fuel consumption per unit flame surface in combination with a local flame surface density. For this latter quantity, an additional conservation equation is solved. The modelling of the flame surface evolution represents a major challenge: On the one hand, because of the complex interaction of the flame and the turbulent flow field; on the other hand, as the premixed part of combustion and the evolution of the turbulent diffusion flame have to be modelled appropriately (see also 2.6.3). Consequently, the results obtained with this type of model that were presented so far do not agree as well with experimental data as do those based on the previously discussed characteristic time scale models.

In the actual flamelet approach as employed by Gill [110] and the various members of the Peters group ([111] - [113]), the chemistry closure problem is largely decoupled from the solution of the flow field. The source terms due to reaction are given implicitly by the equation

\[
\bar{\phi} = \int_{0}^{1} \int_{0}^{\infty} \varphi(Z, \chi) P(Z, \chi) d\chi dZ, \quad \phi = Y_i, T, \quad (64)
\]

where the first term in the integral represents any flow variable (e.g. \(Y_i, T\)) and the second term the probability density function (PDF) of \(Z\) and \(\chi\). This is based on the assumption that only one single chemical time scale is relevant. Thus, all flow variables are uniquely correlated to one single reaction progress variable and the solution of the flow field can be simplified accordingly to only solve for this variable. Additionally, one solves for \(Z\) and \(\chi\) (and any additional parameters defining the PDF), which are fed into the flamelet calculation. In turn, the flamelet model determines density and viscosity of the flow field, which effectively completes the coupling of thermochemistry and fluid dynamics in this approach.
This approach is quite well established for stationary, non-premixed applications. However, for partially premixed and highly transient situations, substantial additional modelling effort is required ([114], [115]). The interaction between the flamelet and the spray model is not yet well understood, either. Therefore, flamelet models are still considered to be in the development stage with respect to their application in diesel engine combustion simulations.

Only recently, preliminary results of the application of a PDF model for diesel spray combustion were reported [116]. In the long term, this type of model is, because of its universality, expected to become more and more widespread. At present, the associated enormous computational expense for reasonably detailed chemistry still excludes its use for practical applications.

3.2.4 Nitric Oxide Formation Models

In spite of the deficiencies discussed in 2.6.4, the extended Zeldovich mechanism, applied to cell-averaged quantities, is still employed almost exclusively in the investigations of NO formation in diesel engines reported to present (e.g. [104], [117], [118]). This is commonly justified by referring to the additional expense for more detailed models in relation to the assumed modest increase in accuracy. Furthermore, before the upstream processes, mixture formation and combustion in particular, are not reproduced with adequate accuracy, the dependence of the obtained results on the detail of the NO formation model is negligible in comparison with the effect of poor predictions of the preceding phenomena. More detailed models including the complex interaction of NO formation and turbulence are the subject of current research for stationary applications (see e.g. [119]) and not yet an issue in the context of diesel engines. Note that the flamelet approach discussed in the previous section inherently models this interaction in a form similar to the interaction of turbulence and combustion.

The extended Zeldovich mechanism was reported to yield good results with respect to the nitric oxide emission trends for e.g. variations of injection timing [104]. It was also applied successfully to
explain the experimentally observed effect of multiple injections on engine emissions [120]. Note that, in these simulations, a weighting factor for the reaction rates relating to NO formation is commonly applied in order to quantitatively match the experimental data. This can be considered common practice; however, it underlines the deficiencies of this approach.

As noted above, the flamelet models offer the possibility to include detailed mechanisms for NO formation and therefore the opportunity to account for Prompt-NO and the contribution of the nitrous oxide pathways (compare 2.6.4) as well. Results obtained for e.g. variations in exhaust gas recirculation rate are in good agreement with experimental data [112]. However, since the flamelet approach actually models the fast chemistry occurring on a thin flame sheet, whereas Thermal NO formation proceeds at comparatively low rates and on larger scales, the validity of the flamelet solution for Thermal NO formation remains unclear.

A specific “flame sheet model” for NO formation was presented by Akinyemi and Cheng [109]. They argue that, due to the high temperatures in the close vicinity of the flame, the NO production is substantially increased. Therefore, they devised a model to account for the associated excess NO formation. However, in view of the typical length scales of flames and the corresponding short residence times, their resulting contribution from this effect appears excessively high (see also discussion in 2.6.4). Also, their computed pressure histories are significantly below the experimental ones, which indicates an underestimation of the local (cell-mean) temperatures already, which is expected to have a much higher effect than the neglect of temperature inhomogeneities. Therefore, the validity of this approach is considered rather questionable.
4 The Zero-Dimensional Model

In view of the classification introduced at the beginning of the previous chapter, the model presented here has to be considered rather quasi- than zero-dimensional: It employs dimensional considerations in the determination of the spray propagation, which influences downstream processes such as turbulence evolution, mixing and combustion. The multi-zone approach applied here, however, does not involve any spatial discretization with respect to the location of the individual zones. The core of the model is, therefore, truly zero-dimensional.

4.1 The Multi-Zone Concept

In order to model the spatial inhomogeneity of the combustion chamber content during the relevant phases (injection and combustion), a multi-zone concept is utilized: A single fresh gas zone is considered during the compression stroke until start of injection (SOI), when a mixture zone is introduced additionally. After combustion has started, various exhaust gas zones are formed subsequently, which are then subject to mixing with the residual fresh air until exhaust valve opening (EVO). The individual zones are regarded as internally homogeneous; note that this assumption is also employed for the fresh gas zone at inlet valve closing (IVC), where the computation starts. We thereby assume perfect mixing of the fresh air with potential exhaust gas recirculated either internally or externally.

On the one hand, the limitation to the period between IVC and EVO allows to circumvent the problem of modelling the gas exchange process, especially in view of the multiple zones, which otherwise had to be accounted for during exhaust. However, on the other hand, this approach requires the coupling of the present model with a cycle simulation tool such as CIRCE [121] in order to properly define the initial conditions at IVC.

As already stated in the introductory paragraph, the individual zones are defined by the period during which they are formed rather than by their spatial position. This reflects the basic idea that mixture
segments burning at the same time will experience similar processes of mixing and zone-internal chemistry later on. The spatial inhomogeneity is thus traced back to differences in the progress of the evolution of a temporal discretization. Correspondingly, the individual zones cannot be uniquely localized and they are not necessarily spatially coherent either, since they are not associated with individual sprays.

For each active zone, the conservation equations of mass (3), species mass fractions (2) and energy (6) are solved simultaneously. In the energy equation, kinetic energy as well as any effects of body forces and surface stresses are neglected, whereas the energy required to heat up and evaporate the droplets is considered as additional heat exchange term. This is done in order to assure full coupling with the liquid phase. The solutions of the individual zones are interdependent since constant pressure throughout the domain can be assumed and the total temporal volume gradient at every time is uniquely defined by the piston motion. Therefore, the distribution of the total volume change among the active zones has to be performed appropriately in order to comply with the constant pressure condition at the end of each individual timestep. For this purpose, a specific solution procedure was devised, which will be presented below.

4.2 Spray Model

The modelling of spray processes is based on the concepts discussed in 2.4 and 2.6.1. We consider a representative spray, which is discretized in individual particles consisting of droplets of equal diameter, temperature, penetration (i.e. distance from the nozzle) and velocity. These droplets are eventually evaporating and mixing with the surrounding fresh gas, forming a new, homogeneous mixture zone.

4.2.1 Initial Conditions at the Nozzle Exit

The injection velocity is prescribed as a function of crank angle, which is determined from the analysis of experimental data for
pressure in the nozzle and in the combustion chamber as well as the valve needle lift, assuming a constant discharge coefficient of the injector holes. For this purpose, hydraulic models of the various injection systems were applied ([122], [123]). The initial diameter of the droplets is determined by averaging the results from several empiric correlations for the Sauter mean diameter of atomized sprays ([42], [124], [125]), as proposed in [51]. The initial temperature of the fuel is assumed to be time-invariant during injection.

4.2.2 Spray Propagation

The individual particles resulting from temporal discretization of the fuel mass injected are assumed to penetrate independent of each other into the combustion chamber. For the late phase, after the breakup time \( t_{bu} \) (47), the empiric correlation of Dent [126] is applied, which, according to [43], yields the best predictions here. Initially, a linear correlation with time since start of injection of the particle under consideration is employed.

\[
X = \min \left[ C_1 \sqrt{\frac{2\Delta p}{\rho_{dr, inj}}} t, C_2 \left( \frac{2\Delta p}{\rho_g} \right)^{\frac{1}{4}} \left( \frac{C_3}{T} \right)^{\frac{1}{4}} \sqrt{d_o t} \right]
\]  

(65)

Differentiation of (65) yields the corresponding correlations for the instantaneous particle velocity \( v \). The effective relative velocity with respect to the air in the vicinity of the spray is taken to be a constant fraction of the absolute velocity of the particle.

4.2.3 Evaporation and Mixture Formation

The evaporation model is based on the set of governing equations presented in 2.4.2; however, it additionally accounts for the effect of the liquid density changes as a consequence of droplet heating. For this purpose, the evolution equations (31) and (32) are regrouped as (see e.g. [127]):

\[
\frac{dm_{dr}}{dt} = -2\pi r((\rho D)_g(\hat{T}))B Sh
\]  

(66)
This approach allows the reproduction of the experimentally observed behaviour that droplet sizes are actually increasing in the initial phase of the evaporation process. This effect is due to the density decrease as a consequence of heating, which, initially, overcompensates the radius decrease associated with mass transfer. Note that this has a non-negligible effect on the predictions of droplet lifetimes.

The convective enhancement of heat and mass transfer is modelled via equation (34), where the effective relative velocity of each particle with respect to the surrounding air, mentioned in the previous section, is used in the determination of the Reynolds number.

One of the major assumptions of the present model relates to the character of combustion in medium size diesel engines: Since most of the fuel is consumed in a turbulent diffusion flame and even the premixed part of combustion is associated mainly with at least close-to-stoichiometric conditions, one can assume that combustion proceeds predominantly at $\Phi = 1$. This allows the definition of a mixture zone of constant stoichiometric composition and to pass the control of the actual fuel mixing and consumption process to the combustion model. Consequently, the second zone formed after injection is fed continuously with the evaporated fuel mass and the corresponding stoichiometric amount of fresh gas; it subsequently serves as the sole reservoir for combustion.

\[
\frac{dr}{dt} = \frac{1}{4\pi r^2 \rho_{dr}} \frac{dm_{dr}}{dt} - \frac{r}{3 \rho_{dr}} \frac{d\rho_{dr}}{dt} \tag{67}
\]

\[
\frac{dT_{dr}}{dt} = \frac{1}{c_{dr}} \left( \frac{\dot{Q}_{dr}}{\rho_{dr} r} - \frac{dm_{dr}}{dt} L(T_{dr}) \right) \tag{68}
\]
4.3 Turbulence Model

The turbulence inside the combustion chamber is characterized by solving the evolution equations for the turbulence intensity and the integral length scale as presented in 2.3. However, the existence of different length scales characterizing the various turbulence generating effects has to be accounted for. In the present approach, this is done by considering the effects of piston motion and injection separately and superimposing the resulting turbulence quantities.

For the charge air motion without injection, equations (22) and (23) are used without modification. The values of the integral length scale and the turbulence intensity are initialized as a fraction of the cylinder bore and the mean piston velocity, respectively, in accordance with experimental data presented in [43]. The instantaneous piston speed is employed as the representative mean velocity for turbulence generation. Since the engine under investigation has almost no swirl, a flat cylinder head and only a very shallow piston bowl, any potential effects of swirl and squish flows on turbulence were neglected in this work.

For injection-generated turbulence, the situation is more complex: On the one hand, the turbulent structures are again subject to compression or expansion, as reflected in equation (22). On the other hand, their dimension also varies along the spray axis and is therefore time-variant as well, when cylinder-averaged quantities are considered. The same applies to the velocity representative of turbulence generation. In order to account for both these effects, the evolution equation of the integral length scale is reformulated:

\[ l_{I, S}(t) = l_{I, S}(t - dt) \left( \left( \frac{\rho(t - dt)}{\rho(t)} \right)^\frac{1}{3} + \frac{\bar{l}_p(t) - \bar{l}_p(t - dt)}{\bar{l}_p(t - dt)} \right) \]  \hspace{1cm} (69)

At start of injection, \( l_{I, S} \) is initialized with the orifice diameter \( d_o \). The quantity \( \bar{l}_p \) represents an average characteristic dimension of the spray, where the averaging is performed over all particles by weighting with the axial thickness of each particle, which is defined...
as the product of its initial velocity $v_{l, ini}$ and the time increment $\Delta t_{inj, l}$, during which it was formed:

$$
\bar{l}_p = \frac{\sum l_{p, l} v_{l, ini} \Delta t_{inj, l}}{\sum v_{l, ini} \Delta t_{inj, l}}
$$

(70)

The individual values of $l_p$ are related to the radial expansion of the spray, which defines the outer radius of the individual particles and is reflected in the empirical correlation for the spray angle (48). Before the individual particle reaches its breakup time, $l_p$ is set to the nozzle hole diameter; subsequently, a linear increase with the further penetration of the particle is assumed, in agreement with the similar analysis in [30] for free, axisymmetric, single-phase jets.

$$
l_{p, l} = d_o \left( 1 + C \sqrt{\frac{\rho_g}{\rho_{dr, ini}}} \max \left[ 0, \frac{X - v_{l, ini} t_{l, bu}}{v_{l, ini} t_{l, bu}} \right] \right)
$$

(71)

The representative mean velocity for turbulence generation, $\bar{v}_p$, is determined in analogy to (70) by averaging over the effective relative velocities with respect to the surrounding air. However, we have to account for the fact that, in the early injection phase, only a small fraction of the volume is affected, whereas the turbulence quantities are related to the entire combustion chamber. In order to compensate for this effect, a correction factor depending linearly on the penetration progress is applied additionally:

$$
\bar{v}_p = \min \left[ \frac{X_{p, max}}{R}, 1 \right] \frac{\sum v_l v_{l, ini} \Delta t_{inj, l}}{\sum v_{l, ini} \Delta t_{inj, l}}
$$

(72)

The two contributions to turbulence are superimposed linearly to obtain cylinder-averaged quantities. In order to assess the validity of
this approach, a comparison with data from a 3-dimensional simulation with KIVA-3 using the $k-\varepsilon$ model was performed. Figure 5 shows a comparison of turbulence intensity histories during injection, computed by means of the two simulation tools. Initial conditions at IVC were identical in both calculations, which refer to the engine specified in 4.4.3 below, operated at full load.

Figure 5: Comparison of predictions for turbulence intensity evolution during combustion by means of the present model (NOEMI) and three-dimensional simulation based on a $k-\varepsilon$ model for turbulence (KIVA-3).

After compression, the values just before start of injection are still in quite good agreement. With the present model (NOEMI), the turbulence intensity increases more sharply than in the three-dimensional simulation and reaches a slightly lower maximum value at an earlier time. In the later phase, after a coincident steep decrease, the values remain at a higher level. Generally, we can state that, in spite of these discrepancies in absolute values, the global trend is reproduced in a satisfactory manner.

4.3 Turbulence Model
4.4 Combustion Model

As already noted above, the present model is based on the assumption that the fuel is burnt predominantly under stoichiometric conditions. This allows to model the combustion process as the consumption of a homogeneous, stoichiometric mixture zone, where any effects related to the mixing of the reactants as present in the actual combustion process are accounted for by the modelling approach for the burning rates.

The approach consists of four parts: An ignition model, a model for premixed combustion, a model for mixing-controlled combustion and a model for the distribution of the fuel among the two combustion modes. Combustion chemistry is assumed to proceed infinitely fast at the adiabatic flame temperature associated with the instantaneous mixture zone conditions and to yield products corresponding to the equilibrium composition at that temperature.

4.4.1 Ignition

The ignition process is modelled applying the well-known empiric integral relation

$$\int_{t_{ig}}^{1} \frac{1}{\tau_{ig}} dt = 1$$  \hspace{1cm} (73)

as the criterion for ignition [43]. The instantaneous ignition time scale $\tau_{ig}$ is computed as a function of pressure and temperature employing an empiric correlation similar to Stringer’s [128]:

$$\tau_{ig} = C p^{-0.75} \exp\left[\frac{5473}{T}\right] \hspace{1cm} (74)$$

The above relation is applied to the mixture zone. Note that the mixture zone is cooler than the fresh gas zone, because the heat required for the evaporation of the fuel is extracted from this zone, exclusively. As soon as the ignition integral exceeds the value of 1, the combustion model is activated.
4.4.2 Combustion

Combustion is modelled by means of a characteristic time scale approach as presented in 2.5. The fuel consumption rates with respect to both combustion modes are related to the amount of fuel prepared for combustion and the reciprocal of a characteristic time scale of the underlying physical process.

For premixed combustion, the rate of fuel consumption is dependent on the rate of the associated chemical reactions, where the initiating steps are dominant. Therefore, the instantaneous ignition delay is considered an appropriate choice for the characteristic time scale in this mode.

\[
\frac{dm_{\text{prem}}}{dt}_{\text{comb}} = -C \frac{1}{\tau_{\text{ig}}} \zeta_{\text{prem, prem}} m_{\text{prem}}
\]

(75)

The product \( \zeta_{\text{prem, prem}} m_{\text{prem}} \) represents the instantaneous fuel amount available and ‘prepared’ for premixed combustion. Before onset of combustion, the major part of the fuel evaporating is defined available for premixed combustion (compare (77) below). However, after ignition, only a fraction of this theoretically available fuel mass is effectively ‘prepared’ for combustion. We use this concept in order to account for the fact that, in practice, not all of the fuel evaporated is already mixed with air within ignitable limits as well as to account for the additional spatial inhomogeneities with respect to the ignition progress. For this purpose, the preparation factor \( \zeta_{\text{prem, prem}} \) is introduced, which is linearly related to the further increase of the ignition integral:

\[
\zeta_{\text{prem, prem}} = \min\left[\int \frac{1}{\tau_{\text{ig}}} dt - 1, 1\right]
\]

(76)

This relation can be interpreted such that only after the fraction of fuel evaporated just before onset of combustion has also reached the ignition criterion, it is also ‘prepared’ for premixed combustion.

The fuel evaporating during the ignition delay is only partly mixed within the ignition limits at start of combustion and can therefore not
be expected to be entirely consumed in the premixed mode. This effect is modelled by distributing the evaporating fuel according to

$$\frac{dm_{\text{prem}}}{dt}\bigg|_{\text{evap}} = \max\left[1 - \left(\int_0^{\tau_{ig}} \frac{1}{\tau_{ig}} dt\right)^3, 0\right] \frac{dm_{\text{evap}}}{dt} \quad (77)$$

$$\frac{dm_{\text{diff}}}{dt}\bigg|_{\text{evap}} = \min\left(\left(\int_0^{\tau_{ig}} \frac{1}{\tau_{ig}} dt\right)^3, 1\right) \frac{dm_{\text{evap}}}{dt} \quad (78)$$

The diffusion burning part is assumed to be controlled by the turbulent mixing of the reactants. Therefore, the corresponding characteristic time scale is related to the turbulent diffusivity, or the turbulent viscosity $u' l_I$ when assuming a turbulent Schmidt number of 1, in combination with a typical length scale $s$ of the process.

$$\frac{dm_{\text{diff}}}{dt}\bigg|_{\text{comb}} = -C \frac{u' l_I}{s^2} \zeta_{V, \text{turb}} \zeta_{\text{prep, diff}} m_{\text{diff}} \quad (79)$$

Here, the preparation factor accounts for the fact that the diffusion flame can only be established after local ignition or the propagation of a premixed flame has provided the necessary conditions. It is therefore modelled as a function of the progress of premixed combustion.

$$\zeta_{\text{prep, diff}} = \frac{-\int_0^t \frac{dm_{\text{prem}}}{dt}\bigg|_{\text{comb}} dt}{\int_0^t \frac{dm_{\text{prem}}}{dt}\bigg|_{\text{evap}} dt} \quad (80)$$

The typical length scale $s$ represents, according to the derivation of (79) from the governing equation for one-dimensional diffusion, basically a surface-to-volume ratio. It is modelled as a typical dimension of the system, here as the spray breakup length during injection derived from (47), later reducing gradually to a constant multiple of the nozzle diameter.
This quantity generally represents the ratio of the volume relevant to the diffusion process and the corresponding, non-distorted transfer area. In turbulent systems, however, iso-surfaces of scalars are strongly wrinkled and therefore believed to exhibit fractal character ([129], [130]). In order to allow for this effect, a correction factor \( \zeta_{V, turb} \) is introduced, which employs the fractal dimension of the iso-surface, selected as 8/3 according to [129], to describe the surface increase due to turbulence between the limits of the inertial range, \( l_I \) and \( l_K \). The Kolmogorov microscale \( l_K \) is given by

\[
l_K = \left( \frac{\left( \frac{\mu}{\rho} \right)^3}{\epsilon} \right)^{\frac{1}{4}}.
\]

Additionally making use of the relation \( \epsilon \sim u'^3/l_I \), this results in

\[
\zeta_{V, turb} = \frac{u'l_I}{\mu/\rho}
\]

### 4.4.3 Model Test

The present model was validated by simulating various operating conditions of a Sulzer A20S engine and comparing computed pressure and rate of heat release histories with experimental data. Table 2 lists the main data of the engine under consideration.

<table>
<thead>
<tr>
<th>bore, m</th>
<th>0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>stroke, m</td>
<td>0.3</td>
</tr>
<tr>
<td>compression ratio, -</td>
<td>14</td>
</tr>
<tr>
<td>speed, rpm</td>
<td>1000</td>
</tr>
<tr>
<td>rated power output, kW/cyl</td>
<td>130</td>
</tr>
</tbody>
</table>
Figure 6 shows the imposed boundary conditions as derived from the measurements with respect to injection velocity for the four different operating conditions investigated.

![Injection velocity patterns for different loads at constant speed for the Sulzer A20S, determined from experimental data.](image)

**Figure 6:** Injection velocity patterns for different loads at constant speed for the Sulzer A20S, determined from experimental data.

The resulting pressure and heat release curves are presented in Figure 7 in comparison with the results from the experiments.

In all cases, the onset of combustion is in excellent agreement between measurement and experiment, thus indicating the validity of the ignition modelling approach.

The peak pressure at high loads is in excellent agreement for both the absolute value and the time in the cycle when it is reached. The latter is still well predicted at lower loads, the peak value is, however, slightly overestimated at half load and underpredicted at low part load.
Figure 7: Comparison of pressure and rate of heat release (ROHR) histories from measurement and simulation for four different loads at constant speed for the Sulzer A20S.

4.4 Combustion Model

65
A premixed peak can be discerned in all the rate of heat release histories from simulation, located at the same time as in the experimental data; however, the height is different in most cases. Whereas it is in very good agreement for the 50% case, it is slightly underpredicted at the high loads and specifically at low part load, where the premixed part makes up almost half of the entire combustion process.

The peak in the diffusion burning phase, though quantitatively in good agreement in all cases, occurs generally earlier in the simulations than in the experiments, the deviation increasing with decreasing amount of fuel burning in the diffusion mode. The resulting underprediction of burning rates in the late main combustion phase is then compensated by an extended burnout phase. This effect has been observed in all simulations, be they zero- or three-dimensional and is attributed to the turbulence model - note that the model applied here is sort of a derivative of the $k-\varepsilon$ model usually employed in three-dimensional simulation. This issue will be discussed in more detail in 5.4.2.b.

Both effects, the underprediction of the premixed peak at very low load and the increasing shift of the peak of diffusion burning with decreasing amount of fuel subject to burning in this mode have to be taken as an indication that the model may be less suitable under conditions where premixed combustion is predominant.

### 4.5 Heat and Mass Transfer Models

The challenge in modelling the heat transfer from multi-zone models lies in the distribution of the heat losses among the individual zones. The general modelling effort with respect to mass transfer is obviously reduced as the gas exchange is excluded from the model. However, the exchange of mass between the individual zones still represents an essential feature of the model through the associated determination of the temperature and oxygen concentration evolutions of the combustion product zones, which in turn define the local nitric oxide formation rates.
4.5.1 Heat Transfer

Generally, various concepts are conceivable for modelling heat transfer from multi-zone models. One approach typically used is to employ a single-zone model in parallel and compute the overall heat loss on the basis of the cylinder-mean temperature from correlations well-proven in cycle simulation and then distribute it in a rather arbitrary manner among the zones (e.g. [83]). In the present model, the opposite approach is used: The heat transfer is modelled for each zone individually, assuming a distribution of the instantaneous effective heat exchange surface among the zones.

For the modelling of engine heat transfer, numerous models of varying complexity were proposed - for an overview, see e.g. [131]. In the present model, the approach of Annand [132] was adopted and reformulated for the multi-zone concept:

\[
\dot{Q}_{j \rightarrow w} = -\frac{V_j}{V_{cyl}} G_{cyl} \left( C_{conv} \frac{\lambda}{2R_{cyl}} Re^{0.7} (T_j - T_W) \right) + C_{rad} \left( T_j^4 - T_W^4 \right)
\]

(83)

The main reasons for this selection are twofold: On the one hand, the simplicity of its application related to its direct derivation from the fundamental laws of heat transfer - the application does not include any phenomenological considerations of the deviation from the theoretical motored engine cycle. On the other hand, it allows for contributions to heat transfer due to radiation. Considering the fact that radiation, mainly due to soot incandescence, can be in the order 25 to 40% of the total heat transfer at high loads ([43], [133]), makes its inclusion indispensable, specifically for the high-temperature zones during and after combustion, where soot also prevails.

The total combustion chamber surface area is distributed among the zones according to their fraction of the total volume. This does not reflect the real situation characterized by a marked spatial distribution of the flames and hence, temperature and composition. However, a detailed consideration of this spatial structure would in-
volve substantial additional modelling, if not require a three-dimen-
sional simulation and must therefore be considered beyond the scope
of the present type of model.

Figure 8 shows a comparison of the wall heat transfer rates com-
puted with the present model with the results of cycle simulation for
the engine under consideration. The cycle simulation tool CIRCE
[121] employed and assessed in the layout of the process modifica-
tions for the given engine [134], applies Woschni’s correlation [135]
for the description of heat transfer, well established in this context.

![Figure 8](image_url)

**Figure 8:** Comparison of wall heat transfer rates computed by
means of an established cycle-simulation tool applying
Woschni’s correlation (CIRCE) and the present model
(NOEMI).

The data are in good agreement; only in the later expansion phase,
the model employed here yields higher values of the instantaneous
heat transfer rates as a consequence of the radiative contributions.
These also determine the peak value, in contrast to Woschni’s corre-
lation, where the peak is basically the result of the assumed increased turbulence during combustion.

### 4.5.2 Mass Transfer

The basic concept of the mass transfer model is illustrated in Figure 9:

![Diagram of mass transfer pathways](image)

**Figure 9:** Scheme of mass transfer pathways between the individual zones.

Fresh gas is mixing with the fuel injected and evaporated, forming the stoichiometric mixture zone. This latter zone is depleted in the course of combustion, the combustion products always feeding the latest-built exhaust gas zone. All the exhaust gas zones are subject to mixing with the residual fresh gas. For consistency with the combustion modelling approach, only mixing of the residual fresh gas to the
individual exhaust gas zones is considered and any interaction between exhaust gas zones is neglected. Any more detailed consideration of the actual mass transfer between the fuel- and oxidizer-rich parts of the volume separated by the flame would again result in three-dimensional modelling approaches.

The rate of mixing is assumed, for reasons of consistency again, to be controlled by the same processes as is the diffusion combustion mode. A correlation similar to (79) is employed for the determination of the instantaneous mass transfer rate from the fresh gas zone to the exhaust gas zone with index $j$:

$$\frac{dm_{mix, FG \rightarrow j}}{dt} = -\min \left[ C \frac{u'l}{s_{mix}^2} \zeta_{V,turb} q_{st} \frac{m_{diff}}{J}, \right]$$

$$\frac{m_{rest, mix, FG \rightarrow j}}{dt}$$

Note that the proportionality constant as well as the typical length scale are different from (79). Detailed investigations showed that the length scales for mixing and combustion are best related as $s_{mix} = s/\Phi$. The fuel preparation factor does not play a role in mixing and a minimum condition is applied in order to achieve a practically uniform distribution of the residual fresh gas among the exhaust gas zones at EVO. Accordingly, the total mass available for mixing, modelled as $q_{st} m_{diff}$, has to be distributed among the total number of zones $J$.

### 4.6 Nitric Oxide Formation Model

Nitric oxide emissions are determined from the cylinder-average concentration of $NO$ and $NO_2$ at EVO, taking into consideration the effect of scavenging efficiencies exceeding 1.0. The concentrations of the individual species in each zone are solved for applying a detailed kinetic scheme for Thermal $NO$ formation [64]. The basic mechanism consists of 77 reactions involving 23 species including the oxidation of $CO$ and is listed in Appendix A.1.
For each individual zone, the concentration changes due to the individual reactions are determined from their reaction rates according to equations (40) through (43). For this purpose, the CHEMKIN code [136] is employed together with a specific solver for stiff ordinary differential equation (ODE) systems [137]. The latter uses an adaptive timestep technique based on the assessment of the residuals of the individual equations to be solved.

CHEMKIN was extended to enable the simultaneous consideration of various mechanisms. Note that the detailed chemistry is only applied where necessary, viz. in the high-temperature exhaust gas zones. The fresh gas and mixture zones are treated as stationary with respect to composition, the ‘mechanism’ applied in their case does not involve any reactions. A third mechanism is employed in the computation of the adiabatic flame temperature and the equilibrium composition of the combustion products: Recirculated nitric oxides are modelled as inert species in this context.

4.7 Solution Procedure

The solution for the individual zones is based on standard procedures as described in [138]. The problem lies in the coupling of the solutions of the various zones and the tailoring of the adaptive timestep technique to the multi-zone concept.

The latter is performed by adapting the solution process. The timestep adaptation is transferred from the actual solver to the module driving the solution of all zones: In case the timestep proves too large in the solution of an individual zone, the solver returns the proposal for a reduced timestep to the driving module. There, the solution is reinitialized with the results of the previous timestep for all zones present with the now reduced timestep. Since convergence problems leading to timestep reductions can predominantly be expected in the zones at highest temperature due to the corresponding high reaction rates, the order of solving for the individual zones is selected appropriately to avoid idling.
The distribution of the total volume change due to compression or expansion among the individual zones is unknown before an individual timestep. Additionally, mass transfer due to evaporation and the mixing between individual zones affects the volume distribution. And finally, the cold zones experience additional compression due to the expansion of the combustion products. In order to account for all these effects, a specific predictor-corrector scheme was devised.

The effects of mass transfer due to evaporation and of expansion as a consequence of combustion are modelled by means of virtual volumes. At the start of each timestep, the incremental isobaric expansion associated with the two effects is determined, which is then added to the incremental volume change as a consequence of piston motion.

In each timestep, the initial prediction for the distribution of the incremental volume change is based on the one from the previous timestep. After the solution for all zones, convergence is checked by comparison of the resulting pressure values of the individual zones. If the deviation of the maximum and minimum values exceeds the convergence criterion, the volume change increment is corrected on the basis of the deviation of the individual zone pressure from the mean and the solution reinitialized with the results of the previous timestep. This procedure is repeated until convergence is achieved. After optimization of the correction term and the additional introduction of a relaxation scheme to prevent solution oscillations, the scheme proved efficient and robust.
5 The Three-Dimensional Model

The model presented here is based on KIVA-3, a simulation tool developed at Los Alamos National Laboratories for the numerical solution of transient, chemically reactive fluid dynamic problems involving sprays ([33], [85]). The following two sections briefly summarize the main features of this basis and previous enhancements, whereas the remainder of this chapter focuses on the recent modifications relating to the modelling of chemical processes, which were introduced in the course of the present work.

5.1 The KIVA-3 Basis

KIVA-3 solves the transport equations describing the laminar or turbulent flow of a chemically reactive mixture of ideal gases as presented in the various sections of Chapter 2. The gas phase solution is coupled to the solution of the spray evolution equation in the manner discussed in 2.4. The chemistry model allows the consideration of both kinetically controlled and equilibrium reactions.

5.1.1 Gas Phase Solution

The conservation equations of species mass fractions, total mass, momentum, specific internal energy ((7), respectively Table 1) as well as of turbulent kinetic energy (17) and its dissipation rate (21) are solved by means of a finite volume technique: The arbitrary Lagrangian Eulerian (ALE) method employed in KIVA-3 is formulated for all-hexahedral, block-structured meshes.

This solution procedure allows the use of arbitrarily shaped hexahedrons and consists of two phases within each individual timestep: A Lagrangian phase, in which the motion of the individual vertices is computed, and a second phase, in which the solution of the first phase is remapped to the original (or an user-prescribed new) mesh. Accordingly, convective terms are neglected in the first phase and the remapping is accomplished through convection across the cell boundaries. The option for prescribing the mesh as a function of time allows the handling of moving boundaries such as the piston. For
that purpose, a method for the activation and deactivation of cell layers is provided additionally.

Boundary condition options available include both periodicity and symmetry, open boundaries with either pressure or velocity specified and solid as well as moving walls. Wall functions are employed to describe the turbulent boundary layer, including a model for the heat transfer across the turbulent boundary layer to a wall at constant temperature. Adiabatic walls are the second option with respect to heat transfer.

Initial conditions in terms of the thermodynamic state are commonly prescribed as uniform values inside the computational domain and at any open boundaries. The flow field is initialized either at rest or by specifying a swirling motion. Initial values of the turbulent kinetic energy and of the dissipation rate are additionally required to define the initial state of turbulent flows. The latter may be initialized based on common assumptions for the associated length scale.

5.1.2 Spray Model

A discrete droplet model (DDM) is applied to describe the dynamics of the liquid phase. For this purpose, the spray evolution equation (25) is discretized and applied to a prescribed number of representative droplets characterized by identical properties. The initial values of the droplet properties are defined through the injection boundary conditions.

Evaporation of the representative droplets is modelled by means of the standard technique presented in 2.4.2. The ambient state in the evaporation computations is selected as the state of the computational cells in which the individual representative droplets reside. Accordingly, the source terms in the gas phase equations resulting from evaporation ((35) - (37)) are assigned to the respective surrounding cells.

Collision of representative droplets is only permitted for droplets residing in the same computational cell. The probability and charac-
Droplet break-up is modelled by means of the TAB model (see 3.2.1). KIVA-3 in its basic state does not provide a model for jet disintegration, which, in view of the discussion in 2.6.1, constitutes a major drawback for the simulation of DI diesel engines.

Droplet/wall interaction effects are not accounted for in detail. KIVA-3 only considers sticking of droplets impinging on a wall. Interactions between the droplet and the wall, e.g. heat transfer, are neglected.

### 5.1.3 Chemistry Model

KIVA-3 allows the consideration of both kinetically controlled and equilibrium reactions between the fuel and 11 gaseous species included in the basic thermodynamic database. The fuel can be selected from a library containing the data of both the liquid and gaseous phases of the 31 most common single component model fuels.

For the kinetically controlled reactions, the rate constants for both the forward and backward reactions have to be specified. The source terms due to those reactions are computed explicitly from equations (40) to (43), applying a numerical procedure preventing species mass fractions from being driven negative.

Equilibrium reactions are handled by means of a numerical technique solving iteratively for reaction progress increments until the equilibrium condition (44) is met. In contrast to standard procedures, this technique takes into account the heat release of the equilibrium reactions and is therefore considered more accurate.

KIVA-3 does not include actual combustion models. It provides an option for simulating spark ignition; however, models for the description of autoignition as well as both premixed and mixing-controlled combustion have to be implemented by the user.
5.2 Previous Enhancements

The model employed in this work is based on previous enhancements of KIVA-3 with respect to turbulence modelling and both individual droplet and spray breakup (see e.g. [90], [139]).

5.2.1 Turbulence Model

As reported by various investigators ([140], [141]), the predictions of turbulent diffusivities and large flow structures can be improved by applying a modified version of the $k - \varepsilon$ turbulence model as presented in 2.3.

The RNG $k - \varepsilon$ model as proposed by Yakhot and Orszag [142] was derived by means of the application of the renormalization group technique to the turbulence spectrum. This resulted in the formulation of conservation equations for the turbulent kinetic energy $k$ and its dissipation $\varepsilon$ of a form very similar to (17) and (21). However, the $\varepsilon$ equation contains an additional term $-\rho \Xi$ on the right hand side, formulated as a function of the mean strain rate $U = \sqrt{2S_{ij}S_{ij}}$, with $S_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$:

$$\rho \Xi = \rho \frac{C_\mu \eta^3 (1 - \eta/C_{\eta 1}) \varepsilon^2}{1 - C_{\eta 2} \eta^3} \frac{k}{k},$$

(85)

where

$$\eta = U \frac{k}{\varepsilon}.$$

(86)

Note that the constants derived for the RNG $k - \varepsilon$ model take on slightly different values from the empirically determined ones of the standard $k - \varepsilon$ model. In the present investigation, the implementation of the model as well as the model constants were selected according to [143]. This includes the introduction of a strain-rate-dependent definition of $C_{\varepsilon 3}$ derived by means of rapid distortion analysis in order to allow for flow compressibility effects due to isotropic compression or expansion. This approach is claimed to im-
prove the prediction of the evolution of turbulence in the late compression phase. The additional term in the ε equation (85) arising from the RNG derivation is, on the other hand, believed to be responsible for a more realistic representation of the injection-generated turbulence and hence, the improved prediction of combustion and emission formation. More details on these considerations as well as on the model derivation and the underlying assumptions can be found in [144].

5.2.2 Breakup Model

In order to overcome the above-mentioned deficiency of the original TAB-model, as implemented in KIVA-3, with respect to the modelling of primary breakup of liquid fuel sprays, the cascade breakup model of Tanner and Weisser [90] was used in the present study. It is based on the Enhanced TAB (ETAB) model as proposed by Tanner [50].

This model employs the same droplet deformation dynamics and droplet breakup criterion as the original TAB model: The droplets are considered as damped, harmonic oscillators, whose non-dimensional deformation from sphericity \( y = 2\Delta r / r \) (\( \Delta r \) denoting the deviation from the spherical surface of radius \( r \), in the direction perpendicular to the relative velocity) is described by

\[
\ddot{y} + \frac{5\mu_{dr}}{\rho_{dr} r^2} \dot{y} + \frac{8\sigma}{\rho_{dr} r^3} = \frac{2\rho_g |u - v|^2}{3\rho_{dr} r^2}.
\]

The aerodynamic drag acts as the forcing term, whereas the restoring force and damping term are due to surface tension and liquid viscosity, respectively. Breakup is assumed to occur, when the value of the deformation parameter exceeds 1. It can be shown that this value is only reached if the droplet Weber number exceeds the critical value of 6.

In contrast to the original TAB model, the initial conditions at the nozzle exit, namely the initial droplet diameter and the initial deformation velocity, are pre-selected in order to control the first occur-
rence of breakup for each droplet. An initial droplet size distribution with a pronounced maximum at the diameter of the injector orifice is prescribed. The droplets at injection are equipped with a zero initial deformation in combination with a negative deformation velocity \( \dot{y} \). The initial value of \( \dot{y} \) is determined from the consideration of a corresponding, inviscid drop, reaching the breakup criterion at a time \( t_{bu} \) after entering the computational domain. This breakup time \( t_{bu} \) is computed from the empiric Levich-correlation given in (47), thus representing the time required for the primary breakup of the fuel jet. Note that, in this procedure, breakup is only allowed for positive values of \( \Delta r \), hence \( y \). Conceptually, the initial droplets first undergo a prolongation in their direction of flight, before eventually being flattened by the drag and finally breaking up.

The second major enhancement from the original TAB model is in the determination of product droplet sizes and velocity components perpendicular to the direction of flight of the parent droplets. The original TAB model computes the product droplet size on the basis of an energy balance between parent and product droplets. In contrast, the ETAB breakup law assumes a cascade-type sequence of breakup events for the individual droplet, reflected in an exponential decay of the droplet radius

\[
\frac{r}{r_{ini}} = \exp[-C_{bu}(t-t_{ini})].
\]  

(88)

The breakup constant \( C_{bu} \) is breakup-regime-dependent according to

\[
C_{bu} = \begin{cases} 
C_1 \Omega, & \text{if } We \leq We_{tr} \\
C_2 \Omega \sqrt{We}, & \text{if } We > We_{tr} 
\end{cases}, \quad \Omega = \sqrt{\frac{8\sigma}{\rho_{dr}r^3} - \frac{5\mu_{dr}}{2\rho_{dr}r^2}},
\]  

(89)

reflecting the experimentally observed variations in individual droplet breakup results between the bag (\( We \leq We_{tr} \)) and the stripping and catastrophic (\( We > We_{tr} \)) breakup regimes (compare 2.4.3). The Weber number \( We_{tr} \) marking the transition between the regimes was selected as 80 [50].
In the original TAB model, the velocity component of the product droplets perpendicular to the direction of flight of the parent droplets is set to \( v_\perp = \frac{\dot{y}}{2} \), where \( \dot{y} \) is the deformation velocity of the parent droplets at breakup. The ETAB model determines this velocity from an energy conservation consideration taking into account the surface energies of both parent and product droplets as well as the drop deformation energy of the parent droplets and the additional kinetic energy of the product droplet associated with the velocity in question. Note that both models assume full conservation of the velocity component in the direction of flight of the parent droplet. It can be shown that for an inviscid droplet at high Weber number the approach taken results in a scaling law for the ratio of perpendicular to direction of flight velocities as follows

\[
\frac{v_\perp}{v} \sim \sqrt{\frac{\rho_g \rho_d}{\rho}}.
\] (90)

Keeping in mind that the limiting assumption of large Weber number is hardly ever valid except for the initial, large drops traveling at their high initial velocity, this relation can be considered dominant for the radial expansion after the first breakup, hence for the spray angle. It exhibits a striking similarity with the empiric correlation for the initial spray angle (50), which suggests that this overall spray characteristic property is practically self-adjusting when the ETAB model is used. As a consequence, the initial spray angle needs not be prescribed appropriately, but can be selected as a small and rather arbitrary value.

### 5.3 Ignition Model

In view of the discussion in 3.2.2, the ignition model presented below has to be grouped among the hybrid approaches: It employs techniques known from the empiric models and attempts to combine their cost-effectiveness in terms of computational resources with the increased accuracy of kinetic analysis by using results obtained by means of the application of a detailed chemical scheme to the ignition of a model fuel.
5.3.1 Formal Derivation

Considering the fundamentals of autoignition in diesel engines as outlined in 2.6.2, the chemical ignition process throughout the various regimes is strongly related to the formation of a representative intermediate species. It can be assumed that a critical value of this intermediate has to be reached locally in order to initiate - either directly or indirectly via the associated sharp temperature rise - the actual combustion reactions. In view of the fact that the dominant chain-branching reactions of the individual regimes all involve the formation of the same radical (OH), the consideration of one single representative intermediate appears to be justified. The ignition progress can hence be described by means of a conservation equation of the mass fraction of this intermediate.

\[
\frac{\partial (\rho Y_\text{ig})}{\partial t} + (\nabla \cdot \mathbf{u}) \rho Y_\text{ig} = \nabla \cdot (\rho D \nabla Y_\text{ig}) + \frac{\partial}{\partial t} \left[ \frac{d c_1}{d t} \right]_{\text{rea}}
\]

This equation can be further simplified introducing the following additional assumptions relating to the critical value of the intermediate mass fraction, \(Y_{i, \text{ig}}\):

- \(Y_{i, \text{ig}}\) is very small in comparison with the mass fractions of the other species present.
- \(Y_{i, \text{ig}}\) is independent of the thermodynamic conditions.

The former assumption can easily be justified by considering typical values of radical concentrations: Mass fractions at thermodynamic equilibrium under the conditions in question (pressures around 100 bar and temperatures around 1000 K) are generally several orders of magnitude lower than those of the major species present. Even if, locally, as a consequence of the ignition process and the associated local temperature increase, the concentration of the intermediate may exceed the equilibrium value associated with cell-mean conditions, the cell-averaged concentration will remain far below the limit where it would have a noticeable impact on the other
species. Therefore, the solution of (91) may be decoupled from the solution for the major species.

The latter assumption is not that straightforward. Since the rate of progress of an arbitrary combustion reaction involving the intermediate is to leading order dependent on temperature ((41), (43)), a temperature dependence of the critical value appears more appropriate. However, in view of the very fast increase of both temperature and radical concentrations right after ignition, the error introduced by this assumption can be considered almost negligible. Note that a pressure effect can practically be excluded in view of the reaction orders of the typical elementary reactions involved in the actual combustion process.

Division of (91) by $Y_{1,\text{ig}}$ and expansion of the reaction source term according to the procedure outlined in 2.5 results in

$$\frac{\partial (\rho C_{ig})}{\partial t} + (\nabla \cdot \mathbf{u}) \rho C_{ig} = \nabla \cdot (\rho D \nabla C_{ig}) + \frac{\rho}{\tau_{ig}},$$

the conservation equation of the passive scalar $C_{ig} = Y_{1}/Y_{1,\text{ig}}$, which will furtheron be designated as ignition progress variable.

As a consequence of the definition of the ignition progress variable as the quotient of the instantaneous and the critical mass fractions of the intermediate, the condition for local ignition simplifies to $C_{ig} \geq 1$.

The determination of the source term is based on the detailed analysis of the ignition behaviour of the model fuel n-heptane, which was already addressed in 2.6.2. The ignition delay of a homogeneous mixture of n-heptane and air under quiescent conditions appears as the natural choice for the characteristic chemical timescale for ignition $\tau_{ig}$. As already discussed, the characteristic pressure and temperature dependence of the ignition delay, as represented in Figure 2, is the consequence of different rate-determining processes governing the various regimes. The chemical timescale for ignition can thus be determined from a combination of the timescales associated
with the individual rate-determining processes, modelling ignition by means of the following simplified system.

![Simplified system](image)

Figure 10: Simplified system employed for the description of the ignition process.

The characteristic time $\tau_{ig}$ of the entire system (symbolized by the dashed block in Figure 10) is then related to the individual characteristic timescales of the respective rate-determining processes as follows:

$$\frac{1}{\tau_{ig}} = \frac{1}{\tau_{ig,1} + \tau_{ig,2}} + \frac{1}{\tau_{ig,3}}, \quad (93)$$

where the individual timescales $\tau_{ig,1}$, $\tau_{ig,2}$ and $\tau_{ig,3}$ represent the low-, medium- and high-temperature regimes of ignition, respectively.

These timescales are evaluated from Arrhenius-type correlations (compare (43)) to

$$\tau_{ig,r} = A_r \Psi_r(\Phi) \left( \frac{p}{p_{ref}} \right)^{\beta_r} b_r T_r^{\beta_r} \exp \left[ \frac{T_{A,r}}{T} \right], \quad r = 1, 3, \quad (94)$$

with $A_r$, $\beta_r$, $b_r$ and $T_{A,r}$ as the parameters of the kinetic model. The function of the local fuel/air equivalence ratio $\Psi_r(\Phi)$ was additionally introduced in order to allow for the equivalence ratio dependence in the medium-temperature regime suggested by the results of Müller [53].
Fitting of the model constants to the available data from detailed analysis of n-heptane ignition ([55], [53]) yielded the parameter values listed in Table 3.

Table 3: Parameter values of the ignition model.

<table>
<thead>
<tr>
<th></th>
<th>$A_r$</th>
<th>$\beta_r$</th>
<th>$b_r$</th>
<th>$T_{A,r}$</th>
<th>$\Psi_r(\Phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r = 1$</td>
<td>2.39E-11</td>
<td>−0.1</td>
<td>0</td>
<td>14000</td>
<td>1</td>
</tr>
<tr>
<td>$r = 2$</td>
<td>1.33E+05</td>
<td>−2.125</td>
<td>0</td>
<td>−10000</td>
<td>$\Phi^{-1}$</td>
</tr>
<tr>
<td>$r = 3$</td>
<td>2.50E-08</td>
<td>−1</td>
<td>0</td>
<td>14000</td>
<td>1</td>
</tr>
</tbody>
</table>

Figure 11 shows a comparison of results for the ignition delay of a homogeneous, stoichiometric mixture of n-heptane with air under quiescent conditions, applying the above approximation, with the results of detailed chemical analysis presented previously in Figure 2. Especially in the high-pressure and -temperature range, relevant for diesel engine simulations, the approximation is excellent.

### 5.3.2 Implementation

The conservation equation of the ignition progress variable (92) is solved in accordance with the general numerical scheme of KIVA. The chemistry source term is determined in conjunction with the spray source terms. Note that, in the implementation, the source term is weighted with an adjustable model parameter in order to enable the compensation of any discretization or real fuel behaviour effects.

Since ignition is occurring on the sub-cellsizescale, cell-averaged quantities are not considered appropriate for the determination of these source terms. Therefore, an interpolation scheme is applied in order to determine the “closest to stoichiometric” condition inside each cell. The interpolation is performed both for the cell in question and all adjacent cells and between cell-mean quantities and conditions at the surface of each droplet residing in the present cell.
This “closest to stoichiometric” condition, i.e. the corresponding local equivalence ratio, is employed for two purposes: First, it is compared to the lower inflammability limit at the local pressure and temperature (approximated according to [145], [146]) - if it is below this limit, the source term is set to zero. Second, it is used for the determination of local composition effects on ignition, e.g. in the evaluation of the equivalence ratio dependence of the medium-temperature regime.

As soon as the ignition progress variable reaches a value above 1.0 in an individual cell, the combustion model is activated in this cell. The evaluation of the conservation equation - and of the chemistry source term - is, however, continued throughout the simulation. Hence, the ignition progress variable is allowed to increase far beyond its critical value. The reason for this procedure is to allow occurrence of ignition of the neighbouring cells not only indirectly through increased chemistry source terms as a consequence of en-

Figure 11: Comparison of approximated ignition delays for n-heptane with results of computations by means of a detailed mechanism (c.f. [55]).
thalpy transport from the already ignited cells, but also through convection as well as diffusion of the ignition progress variable.

Nevertheless, an upper limit of the ignition progress variable was introduced in order to avoid potential unphysical effects of discretization problems. After complete consumption of the fuel in an individual cell, the ignition progress variable is reinitialized to zero.

5.3.3 Validation

The model was validated against the experimental data of Reuter [147], conducted in a constant-pressure spray combustion chamber.

The setup of those experiments is shown in Figure 12 overleaf. The cylindrical combustion chamber of ca 200 mm height was equipped with four quartz glass windows of 40 mm width and 100 mm height distributed evenly on the circumference, such that the smallest diameter of the chamber between two opposing windows measured 90 mm.

The chamber was continuously fed with compressed air, thus generating a mean flow in the observation region at a velocity of approximately 0.1 m/s, in parallel to the direction of the injector nozzle. Recirculation at the outflow was prevented through the installation of appropriate flow restrictors. A conventional injection system was applied to deliver the diesel fuel to the single, central injector.

The pressure inside the test rig was controlled by means of a pressure-limiting valve at the outflow boundary. The required high gas temperatures were achieved by electrically pre-heating the inflowing gas in combination with thermal insulation of the non-glass chamber walls.

The experimental setup allowed the determination of both ignition delays and locations in a single diesel spray injected along the chamber centreline by means of luminosity detection from two perpendicular directions. A minimum rate of change of the global luminosity signal served as criterion for the ignition delay and the location
The Three-Dimensional Model

The three-dimensional model of the ignition region was detected by observing the development of local signals with a resolution of 4.2 mm.

The results of a series of realizations at one set of conditions were statistically analysed in terms of the axial distance of the ignition location from the nozzle. The radial position of the ignition region was not determined in a quantitative manner, as only for very few realizations an exact correlation of signals obtained from the two perpendicular directions was possible.

In the numerical validation tests, a corresponding constant-volume geometry with appropriately selected boundary conditions was employed: At the inflow boundary, corresponding to the exit of the flow-rectifying grid, a constant vertical velocity was prescribed. The outer walls as well as the injector were assumed to maintain their initial, uniform temperature and for the outflow boundary a constant-pressure condition, excluding backflow, was applied.

The injection rate histories were prescribed according to the experimental data. All comparisons shown below relate to an injector orifice diameter of 0.3 mm.

Figure 12: Spray combustion chamber setup in the experiments of Reuter [147], left: vertical section, right: cross-section.
The mesh, depicted in Figure 13, consisted of ca 5300 cells, concentrated around the nozzle exit. In the observation region of the experiment, the grid resolution was thus similar to the resolution of the luminosity detection apparatus.

In order to account for the potential effect of local combustion on the further evolution of ignition, the ignition model was coupled with a characteristic time scale model following Kong et al. [104]. Note that the abovementioned weighting parameter in the determination of the chemistry source term was fixed to 0.65 throughout this investigation.

The ignition delays were determined as the time after start of injection, when a minimum value of the rate of heat release was exceeded.

In order to achieve a similar information as in the experiment, where the ignition location results from various experiments under the same conditions were analysed statistically, the evaluation of the simulation results is based on the spatial distribution of burning rates at a short time after ignition. The mean distance of the ignition region from the nozzle exit was determined by weighted averaging over all cells with non-zero burning rate, employing the latter as weighting factor. Moreover, the range of cells with non-zero burning rate was,
in analogy to the experiment, considered as the region, where ignition is most likely to occur in case of small disturbances imposed.

5.3.3.a Effect of Temperature

The ignition behaviour of a diesel spray was studied in the range of initial temperatures between 700 and 900 K at a cell pressure of 45 bar and constant injected fuel mass.

Figure 14 shows the comparison of ignition delays from experiment and simulation, plotted as in Figures 2, 11 as a function of inverse temperature.

![Graph showing comparison of measured and computed ignition delays as a function of temperature at 45 bar.](image)

Figure 14: Comparison of measured and computed ignition delays as a function of temperature at 45 bar.

As with the homogeneous cases, in this representation an almost linear decrease is observed in the low-temperature region, eventually flattening towards higher temperatures, as a consequence of the transition to the medium-temperature regime. This effect could, however, partly also be attributed to the relatively growing contribution of the physical processes involved to the overall ignition delay - note
that the overall values are typically 30-60% higher than in the homogeneous system.

This effect, observed in the experiments, is well reproduced in the simulations. Both qualitatively and quantitatively, the computed results are in good agreement with the experimental data.

The same applies to the ignition locations, depicted in Figure 15. In the experiments, decreasing the temperature shifted ignition locations further away from the nozzle and increased the fluctuation range. Note that the average location was always observed at ca 40% of the spray length at ignition.

![Figure 15: Comparison of measured and computed ignition locations as a function of temperature at 45 bar, lines represent mean nozzle distances, shaded regions indicate range of experimental and computational values, respectively.](image)

These general trends are well reproduced by the simulations: The averaged computed values are slightly below the experimental ones and the fluctuation ranges broadly overlap. In view of the spatial res-
olution limitations in both the experiments and the simulations better agreement cannot be expected.

Though the radial positions of the ignition locations could not be exactly determined in the experiments, a general trend towards ignition closer to the spray axis with increasing temperature can be deduced from the results [147]. A similar trend was also observed in the computations.

5.3.3.b Effect of Pressure

The influence of a variation of chamber pressure between 40 and 50 bar was investigated for two distinct initial temperatures, again for otherwise unchanged conditions.

Figure 16 shows the comparison of measured and computed ignition delay data as a function of pressure for 786 and 892 K:

![Figure 16: Comparison of measured and computed ignition delays as a function of pressure at 786 and 892 K.](image)

A general trend of slightly decreasing ignition delay with increasing pressure is observed in both the experiments and the simulations.
However, the rather sudden, unexplained decrease in the experimental values between 45 and 47.5 bar at 786 K is not reflected in the simulations.

In Figure 17, the ignition locations for varying pressures obtained in the simulations are compared to the experimental data.

Figure 17: Comparison of measured and computed ignition locations as a function of pressure for 786 K (left) and 892 K (right), lines represent mean nozzle distances, shaded regions indicate range of experimental and computational values, respectively.

The agreement between measurements and simulations is again good, especially in the high-temperature case. As already observed in the investigation of the temperature influence, the absolute values obtained from the simulations are slightly lower than the experimental ones. However, for the range of conditions, where the computed ignition delays exceed the experimental values (i.e. p > 45 bar at 786 K), the computed nozzle distances of the ignition regions are also higher than the ones in the experiment.
It is interesting to note that, for both temperatures, the deviation between computed and experimental values decreases with increasing pressure.

5.4 Combustion Model

With respect to the classification introduced in 3.2.3, the model applied in this study has to be grouped among the characteristic time scale models. It basically represents a further development stage of the model proposed by Kong et al. [104].

5.4.1 Formulation

In case the local value of the ignition progress variable exceeds 1.0, the rate of change of species mass fractions due to combustion is computed according to equations (62) and (63), repeated below for simplicity:

\[
\frac{dY_i}{dt} = \frac{Y_{i,eq} - Y_i}{\tau_{comb}}, \tag{95}
\]

where the characteristic time scale of the combustion process, \(\tau_{comb}\), is determined from linear, weighted superposition of the laminar and turbulent time scales:

\[
\tau_{comb} = \tau_{lam} + \zeta_{prog} \tau_{turb}. \tag{96}
\]

The laminar time scale \(\tau_{lam}\) is related to the kinetics of the global reaction of the model fuel n-tetradecane, determined in a single droplet autoignition experiment [148] to

\[
\tau_{lam} = 1.54\times10^{-10} c_{fuel}^{0.75} c_{O_2}^{-1.5} \exp\left[\frac{9297\text{K}}{T}\right]. \tag{97}
\]

The turbulent time scale is selected as the eddy turnover time:

\[
\tau_{turb} = C_{\varepsilon^2z}. \tag{98}
\]
The solution of (95) includes the determination of the local equilibrium concentrations involving the following species: fuel, \(O_2\), \(CO_2\), \(CO\), \(H_2O\) and \(H_2\). For this purpose, the following equilibrium reactions are considered:

\[
2 \, CO + O_2 \leftrightarrow 2 \, CO_2 \tag{99}
\]

\[
2 \, H_2 + O_2 \leftrightarrow 2 \, H_2O \tag{100}
\]

The system of coupled differential-algebraic equations resulting from the correlated equilibrium conditions (44) is solved by means of an appropriate numerical technique [40]. Hereby, the equilibrium concentration of the fuel is assumed to be defined by the maximum possible consumption.

The transition from premixed to mixing-controlled combustion is modelled by means of the transition function \(\xi_{prog}\) in (96). This function is related to the local combustion progress \(\gamma\) as follows

\[
\xi_{prog} = \left(\frac{\min[\gamma, \gamma_{trans}]}{\gamma_{trans}}\right)^{C_{\xi}} , \tag{101}
\]

where \(\gamma\) in turn is specified as the portion of the local and instantaneous ignition progress variable exceeding the value at ignition:

\[
\gamma = C_{ig} - 1. \tag{102}
\]

The value of the local combustion progress variable, when transition to mixing-controlled combustion is completed, \(\gamma_{trans}\), and the exponent \(C_{\xi}\) are the parameters of this model. The former was selected such that the criterion for completed transition corresponds to an increase of the radical concentration represented by the ignition progress variable by two orders of magnitude (\(\gamma_{trans} = 99\)) and the latter was set to 0.5.

With this procedure, combustion starts as entirely premixed after ignition and then gradually, with increasing \(\gamma\), turns into mixing-controlled. As soon as the transition value \(\gamma_{trans}\) is reached, equation (101) evaluates to 1.0 and the characteristic time for combustion re-
sults from addition of the laminar and turbulent contributions, with the turbulent time scale dominating.

Note that, in order to allow for discretization or real fuel behaviour effects, in the implementation the two time scales, or rather their associated rates, are weighted with one additional model parameter, each. The values of these two parameters were determined in the model test phase and have subsequently not been altered.

5.4.2 Model Test

Testing of the model was again performed through simulation of the various operating conditions of the Sulzer A20S engine presented in 4.4.3.

The geometry employed in this context is shown in Figure 18. It makes use of the symmetry of the combustion chamber with a central injector in the flat cylinder head, where the small crevices besides the valves can be neglected. The simulations were hence performed on a 30 deg sector mesh, containing one of the twelve sprays. The injector is modelled in the top left corner and the grey symbols in its vicinity indicate the location and orientation of the spray.

![Figure 18: Geometry employed in the Sulzer A20S engine simulations (TDC position).](image-url)
Employing the same injection profiles as documented in Figure 6 yielded the pressure and rate of heat release patterns confronted to their experimental counterparts in Figure 19.

The predictions for the start of combustion are in very good agreement with the experimental results throughout the load range. The ignition model is hence performing equally well in real engine applications as in the previous validation under idealized conditions.

All computed rate of heat release histories are characterized by a premixed peak, eventually becoming more pronounced towards low loads, in accordance with the experimentally observed behaviour. Note that the excellent agreement of the pressure curves in the initial combustion phase is indicating an even better performance of the model than the direct comparison of the heat release rates (see discussion in section B.3 in the Appendix). Only at the very low part load, the transition function (101), controlling the shift of weights between the chemically- and the mixing-controlled burning modes in the course of combustion, apparently tends to lead to an underestimation of the extent of the premixed peak.

When considering the later phase of combustion, the agreement between experiment and simulation is clearly deteriorating and additionally varies with engine load. Note that the model was tuned to match the peak pressure of the 75% load case by adapting the aforementioned weighting parameters, mainly the one for the turbulent rate. In this particular case - and to a varying extent in the other cases as well - the general characteristic of the heat release pattern is in good agreement between experiment and simulation. However, the peak of the mixing-controlled phase in the simulations is generally reached at an earlier time (typically shortly after occurrence of the peak injection pressures). As a consequence, the peak cylinder pressures are also predicted at an earlier crank angle. Moreover, when comparing the various loads, a trend towards higher and earlier mixing-controlled peaks with decreasing load can be deduced that is much more pronounced in the simulations than in the experiments. For the full load operating condition, this leads to a considerable underprediction of the peak cylinder pressure.
Figure 19: Comparison of pressure and rate of heat release (ROHR) histories from measurement and 3-D simulation for four different loads at constant speed for the Sulzer A20S.
In the following subsections, some of the effects observed are analysed in more detail and the main features of the model will be reviewed by means of a validation against alternative modelling approaches.

5.4.2.a Transition from Premixed to Mixing-Controlled Combustion

The effect of the formulation of the transition function is highlighted in Figure 20.

![Figure 20: Comparison of rate of heat release rates from experiment and 3-D simulations employing the present transition function and the approach of Kong et al. top row: standard range diagrams, bottom row: focus on the initial combustion phase.](image)

It shows a comparison of the rate of heat release histories obtained by means of the transition function according to Kong et al. [104] and with the present model for the 75 and 50% load cases in the above series of tests. For comparison, the respective experimental rate of heat release patterns are shown in the same diagrams. Note
that both models were tuned in order to correctly predict the peak pressure at 75% load.

With both approaches, a fast initial rise of the burning rate after ignition is obtained. However, whereas with the present definition of the transition function a clearly discernible premixed peak is observed, the original approach of Kong et al. yields a very smooth transition to the apparently mixing-controlled combustion phase. With their model, the level reached after the initial rise is again increasing with decreasing load; however, it is generally lower than with the present approach.

In order to achieve the same peak pressures, the mixing-controlled part of combustion has to be slowed down with the Kong et al. model, when compared to the present approach. After the peak injection pressures have been achieved, the burning rates fall to the same levels (in fact even slightly below) as with the present model.

These effects can be explained by means of a more detailed analysis of the underlying concepts and their actual impact on the determination of the combustion time scale. In Figures 21 and 22 the dependence of the transition function on the local combustion progress and the probabilities of values in individual ranges are shown for the two approaches, respectively. The probabilities represent those of a fraction of the chemical energy being released in conjunction with a combustion time scale determined with a value of the transition function $\zeta_{\text{prog}}$ from the respective interval.

Figure 21 shows the situation for the Kong et al. approach, where the local combustion progress $\gamma$ is given as

$$\gamma = \frac{Y_{CO_2} + Y_{H_2O} + Y_{CO} + Y_{H_2}}{1 - Y_{N_2}}, \quad (103)$$

and the transition function $\zeta_{\text{prog}}$ is formulated as

$$\zeta_{\text{prog}} = \frac{1 - \exp[-\gamma]}{1 - \exp[-1]}, \quad (104)$$
as illustrated in the left-hand side diagram. The right-hand side dia-
gram gives an indication of the relevance of the resulting values of
\( \gamma \), in intervals of 0.1.

![Graph showing transition function and probability]

Figure 21: Dependence of the transition function on local
combustion progress and probability of the individual
values in the approach of Kong et al.

Obviously, as a consequence of the formulation of the combustion
progress variable, the probability of values of the transition function
exhibits a pronounced maximum at about 0.6 to 0.7. Starting from
moderate probabilities of close-to-zero values right after ignition,
probabilities are steadily increasing towards this maximum (Note
that for non-negligible EGR rates, the initial combustion progress
determined according to (103) already takes on values well above
zero).

Generally, as a consequence of the ongoing fuel consumption, the
values of the combustion progress variable are eventually shifted to
higher levels. During injection, however, the continuing evaporation
partly restores lower values and thus slows down this increase. Fi-
nally, when all the fuel has been injected and evaporated, the gradual
further increase of the combustion progress variable basically even
hampers the burnout of the fuel due to the increased weight of the
turbulent time scale.

These characteristics are particularly manifest in the predictions
for the initial combustion phase, where the model is incapable of
capturing the premixed peak observed in the experiments: Very
early, and moreover smoothly, the weight is shifted towards mixing-
controlled combustion, in contrast to the rather bimodal structure that would be required for the prediction of a dent after the premixed peak.

It is worthwhile noting that the (almost case-invariant) probability distribution function is clearly reflected in the heat release rate histories obtained with this model, superimposed with the injection rate histories.

Figure 22 represents the same relation between combustion progress and the transition function as well as the probability distribution of the latter with the present model ((102), (101)).

![Figure 22](image-url)

Figure 22: Dependence of the transition function on local combustion progress and probability of the individual values in the present model.

Here, the probability distribution is clearly bimodal: After a first peak at values close to zero, the probability degressively decreases down to a minimum at a value of the combustion progress variable just below 1.0 followed by a pronounced maximum at the highest value. Note that the shape of this distribution is again rather insensitive to the case investigated, except for the height of the maximum (indicated by the interruption line), which is dependent on the total amount of fuel.

The decrease after the first peak can easily be explained by consideration of the local combustion progress: After ignition, the dominance of the (already sufficiently low) chemical time scale results in high fuel consumption rates. However, in contrast to the above
model, these high fuel consumption rates are not associated with correspondingly high values of the combustion progress variable. Since the latter quantity is related to the local instantaneous value of the ignition progress variable computed from (92), it is continuously (and progressively) increased as the temperatures rise. This progressive increase is reflected in the eventually reduced probabilities in the intermediate range, as this range of values is transversed very fast by the individual cells.

All cells finally take on the maximum value, after their combustion progress variable exceeds the critical value. This concept prevents any inherent slow-down effects in the burnout phase as observed with the above model. Note that this approach does not impose any constraints on the initial composition of the cylinder charge, either.

5.4.2.a Combustion Chemistry

It was speculated in an earlier investigation [149], that the combustion chemistry model has a strong effect on the predictions of heat release rates. In the simulation of a large two-stroke engine, the consideration of a local equilibrium as in the present study yielded rate of heat release histories in much closer agreement with experimental data than an approach based on the assumption of complete combustion.

Figure 23 shows the corresponding comparison of rate of heat release histories for the 75 and 50% load cases in the above series of tests, plotted against the experimental data. The full lines represent the present approach, whereas the dashed curves relate to simulations, where only \( CO_2 \) and \( H_2O \) were considered as products.

Obviously, in the early burnout phase, the present model predicts higher heat release rates than the complete combustion approach and hence yields more realistic results. In the premixed and early mixing-controlled phases up to the peak values, the curves are differing but slightly: Note that the model parameters in the complete combustion approach were tuned for identical peak pressures, hence burning rates are slightly higher than with the present model. With identical
The effect of the local equilibrium assumption on the character of the heat release is highlighted in Figure 24, which, for the same cases as above, compares the rate of heat release with the rate of fuel consumption - in the complete combustion approach, the two are identical.

Whereas the heat release rates decay after the premixed peak, the fuel consumption rates are further increasing, indicating the produc-
tion of considerable amounts of intermediate species. Only in the burnout phase, the fuel consumption rates sink again below the heat release rates and the remaining chemical energy is released via oxidation of the intermediates.

When considering the fundamental equations of the model, the better performance of the local equilibrium approach can only be explained as a consequence of the partial oxidation of the intermediate species, in particular CO: When compared to unburnt fuel, a corresponding amount of chemical energy stored in intermediate species is associated with higher mass fractions of the latter. These in turn lead to higher gradients and hence enhance the mass transfer via turbulent diffusion. As a consequence, the spatial distribution of the yet unreleased chemical energy after the end of injection may be more uniform with intermediate species and thus allow faster release in the early burnout phase.

5.4.2.b Turbulence Effects

As a consequence of the predominantly mixing-controlled character of combustion in this type of engine, reflected in the formulation of the model ((95), (96)), the description of turbulence has a very strong effect on the predictions of the combustion model.

The left-hand side diagram in Figure 25 gives an indication of the temporal evolution of the turbulent time scale spectrum during injection and combustion for the 75% load case: It shows the minimum and maximum values as well as the volume-average and a weighted average of the turbulent time scales in the computational domain.

The maximum value experiences only slight modifications as a consequence of injection. The volume-average is more strongly affected by the injection process: It is reduced by a factor of four, reaching its lowest level near the end of injection. From then on, it is continuously increasing again. The minimum value is drastically decreased at start of injection, by almost one order of magnitude in total. At the end of injection, a similar sudden increase is observed, followed by a more smooth transition back to the initial level before injection.
In order to obtain some more detailed information on the turbulent time scales actually relevant to combustion, a weighted average of the turbulent time scale is considered, additionally. For this purpose, the locally yet unreleased chemical energy stored in either fuel or intermediate species was employed as the weighting factor for the local values of the turbulent time scale.

This weighted average is most sensitive to the start of injection, which leads to a decrease by more than one order of magnitude within a few degrees crank angle. Afterwards, it steadily increases again during the remainder of injection, which can be explained as a consequence of the propagation of the spray.

Figure 26 shows the spatial distributions of the turbulent time scale, the yet unreleased chemical energy and the heat release rate on a vertical cut through the spray at TDC. For the 75% load case, this corresponds approximately to the middle of the injection period.

The lowest values of the turbulent time scale are located in the region around the intact core of the spray as indicated by the large droplets present in the vicinity of the injector. Both in axial and radial direction (with respect to the spray axis) from this region, the values rapidly increase. This distribution is, apart from an increasing...
volume swept by values slightly higher than the background flow level, hardly affected by the propagation of the spray.

The maximum of the unreleased energy is located downstream of the intact core region and decreases rather smoothly towards the tip and the periphery of the spray. Here, the propagation of the spray clearly determines the distribution by means of transporting the fuel and intermediate species both in axial and radial direction from the spray axis.

These differences in the distribution of time scales and yet unreleased energy, in particular their different temporal evolution, are clearly reflected in the characteristic of the weighted average value of the turbulent time scale during injection: The increasing relevance of the higher time scale regions towards the tip and the periphery of the spray with the increasing local concentrations of fuel and intermediates leads to the abovementioned increase towards the end of injection.

After the end of injection, this effect is even more pronounced. The fast decay of turbulence in the earlier highly turbulent regions in combination with the decreasing fuel concentrations in this region enhances the relevance of the regions with higher turbulent time scales. This is valid both for the weighted average of the turbulent time scale, rapidly converging against the volume-averaged value, and the actual combustion, as can be seen in the fast decrease of the heat release rates after injection has stopped.
The right-hand side diagram of Figure 25 shows this strong effect of the end of injection as observed with all loads on the weighted average of the turbulent time scale.

5.5 Nitric Oxide Formation Model

Nitric oxide emissions are, as with the zero-dimensional model, determined from the cylinder-averaged \( NO \) plus \( NO_2 \) concentrations at the end of the closed cycle. The computation of the temporal evolution of these concentrations involves the solution of the associated conservation equations for \( NO \) and \( NO_2 \) as well as for the relevant intermediate species. In order to allow for the consideration of a more detailed mechanism than the commonly used extended Zeldovich, the species database was extended accordingly.

The computation of the chemistry source terms to the conservation equations is performed by means of equations (40) through (44), decoupling fast and slow reactions as outlined in 2.5. The local reaction rates and equilibrium constants pertaining to the individual reactions employed are determined on the basis of cell-mean quantities and the solution relies on the standard procedures offered by KIVA-3 as mentioned in 5.1.3.

The details of the mechanisms employed are given in Appendix A.2. Note that only equilibrium reactions 3 through 6 are allowed for in the determination of radical concentrations in the post-flame region, since equations 1 and 2 are already used in the local equilibrium calculations associated with the combustion model.
6 Results and Discussion

The predictive capability of the two models is demonstrated mainly by comparing the results of the simulations to the data obtained in an experimental investigation conducted in parallel at the authors lab [134]. For a wide range of operating conditions and various operating modes, the predictions are validated against the experimental results in terms of rate of heat release (ROHR) histories and nitric oxide emissions. In the following section, this experimental database is presented including notes on the determination of initial and boundary conditions of the simulations from these results.

6.1 The Experimental Database

In the investigation of Stebler [134], the effect of various operating parameters on the air and fuel systems side on the performance of a medium-size, medium-speed 4-stroke engine was studied. The variations included changes in valve timing, viz. the application of the Miller system, high-pressure exhaust gas recirculation (EGR), controlled turbocharging by means of a variable turbine geometry (VTG) turbocharger and Common-Rail fuel injection. It could be demonstrated that the high flexibility of such a system, where all the individual components can be controlled efficiently, allows substantial reductions of nitric oxide emissions without penalties in fuel consumption or soot emissions.

The experiments were performed on a Sulzer 9S20 engine operated in the co-generation mode, i.e. at constant speed. The specifications of this technology demonstrator engine are listed in Table 4. Considering the broad variety of results obtained with different initial conditions of the cylinder charge and variations of the injection patterns, this database has to be considered an excellent reference. However, we have to keep in mind that this study aimed at the explanation of the observed effects by means of global trends rather than at the generation of reference data (For a general discussion of requirements for the establishment of reference data for simulations see Appendix B).
Both fuel consumption and charge air volume flow are measured for the entire system; therefore, the distribution among the individual cylinders is unknown. The same applies to the engine’s power output and its pollutant emissions. Accordingly, the simulations are based on a representative cylinder fed with the proportional fractions of the total fuel and air masses and contributing proportionally to the engine power output and emissions. Note that monitoring of the peak pressures of the individual cylinders yielded partly non-negligible differences, thus indicating that this assumption may not be justified under all circumstances.

The actual charge air masses in the cylinder are determined from correlations of the cylinder charge initial state at IVC with the inlet manifold state. These correlations were derived from the results of cycle simulations for the representative cylinder, which reproduced the actual engine behaviour. The scavenging characteristics are also taken from these simulations.

The fuel injection rate pattern as well cannot be measured directly and has to be derived from time-resolved measurements in the injection systems. With the standard injection system, the fuel pressure in

### Table 4: Main data of the Sulzer 9S20 research engine.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>bore, m</td>
<td>0.2</td>
</tr>
<tr>
<td>stroke, m</td>
<td>0.3</td>
</tr>
<tr>
<td>compression ratio, -</td>
<td>13.6</td>
</tr>
<tr>
<td>number of cylinders, -</td>
<td>9</td>
</tr>
<tr>
<td>speed, rpm</td>
<td>1000</td>
</tr>
<tr>
<td>power output, kW</td>
<td>1420</td>
</tr>
<tr>
<td>injector number and location</td>
<td>one central</td>
</tr>
<tr>
<td>- orifice number, -</td>
<td>12</td>
</tr>
<tr>
<td>- orifice diameter, mm</td>
<td>0.285</td>
</tr>
<tr>
<td>- spray vertical angle, deg from horizontal plane</td>
<td>-10</td>
</tr>
</tbody>
</table>
the injector body and the valve needle lift were recorded for a single cylinder. With the Common-Rail injection system, the pressure in the fuel supply line at the injector entry of the same cylinder was monitored together with the signals to the solenoid. The actual injection patterns were again determined through correlations derived from detailed hydraulic simulations of the respective injection systems ([122], [123]).

Time-resolved measurements of the cylinder pressure were also performed for one cylinder only - in fact, all time-resolved measurements relate to the same cylinder. A pressure sensor mounted flush with the combustion chamber surface yielding a piezo-electrical, hence differential signal was applied. This signal was then adjusted by matching it to the absolute signal from the piezo-resistive pressure sensor in the inlet manifold. The best timing of this adjustment was determined by means of cycle simulation. However, the major problem with these signals results from the fact that the sensor for cylinder pressure was uncooled, mainly because of limited installation space. Due to the high sensitivity of these sensors to temperature (absolute) as well as temperature fluctuations, the resulting pressure histories are of rather poor quality in terms of quantitative relevance. This is even more the case for the rate of heat release histories obtained from the analysis of the pressure histories. However, for the investigation of trends with modified operational parameters these data were absolutely sufficient.

For this reason, the results of the simulations in terms of cylinder pressure histories are never compared directly to the corresponding experimental ones. Note that the simulation results were checked for consistency of the values of the indicated work between IVC and EVO with the values from reference cycle simulations under the same conditions.

For the same reason, the computed rate of heat release histories are never confronted directly to those derived from the measured pressure histories. In that case, however, another effect has to be considered as well: The analysis of the cylinder pressure data is typically based on the application of a single-zone model of the cylinder con-
tent. Consequently, all fluid properties are determined for cylinder averaged conditions, whereas in reality, as is reflected in 3-dimensional and to almost the same extent also in multiple-zone simulations, the local conditions govern the fluid properties, which are mostly strongly non-linear functions of temperature. This leads typically to an underestimation of heat release rates in the initial combustion phase and a corresponding overestimation in the late phase, as can be shown by comparing the results from single-zone and two-zone analysis (see e.g. [150]). These deviations can be avoided by analogous postprocessing of the simulation results for consistency. However, in view of the quantitative deficiencies of the experimental pressure data already, this was neglected in the present study.

As a consequence of all these considerations, all the validation test results presented below are based on comparisons of trends with respect to the qualitative variation of rate of heat release patterns instead of direct comparisons of the individual results.

6.2 The 0-Dimensional Model

In the first part, we assess the sensitivity of the model to its key parameters, including an investigations of the necessary detail of the reaction mechanism for the description of Thermal NO formation. After the establishment of an appropriate set of key parameters, which was applied in all subsequent simulations, the predictive capability of the model is demonstrated. This is done by confronting the simulation results for modifications of initial conditions of the charge air at IVC and for injection rate history modifications to the corresponding experimental data. Finally, the performance of the model with respect to geometry modifications will be addressed.

6.2.1 Sensitivity to Key Model Parameters

The key model parameters can be identified as the number of exhaust gas zones and the relative mixing velocity, i.e. the ratio of the mixing velocity (84) to the mixing-controlled burning velocity (79). Additional key parameters of the simulations can be seen in the de-
tail and accuracy of the reaction mechanism applied respectively the kinetic data of its main reactions.

6.2.1.a Zone Number and Relative Mixing Velocity

A large number of simulations covering a wide range of zone numbers and relative mixing velocities was performed in order to identify an appropriate choice of this pair of parameters.

Figure 27 shows the results of these simulations in terms of nitric oxide emissions computed as a function of exhaust gas zone number and relative mixing velocity for the full load operating condition of the engine in the reference state. For comparison, the range of measured emissions is superimposed through shading of the regions, where the computations yielded corresponding values.

![Figure 27: Computed NO + NO₂ emissions as a function of zone number and relative mixing velocity, engine operated at full load in the reference state, shaded regions indicate corresponding range of measured emissions.](image)

The resulting surface is characterized by two trends, associated with the effects of zone number and mixing velocity, respectively:

6.2 The 0-Dimensional Model
Firstly, with increasing zone number, the computed emissions increase until they reach an asymptotic value. The number of zones required for this purpose is, however, strongly dependent on the relative mixing velocity - for high values of this parameter, the asymptotic value is not entirely reached within the range of the above diagram. The general asymptotic behaviour of the iso-mixing-velocity curves is the obvious consequence of the improved spatial discretization with increasing zone numbers.

Secondly, when increasing the relative mixing velocity, starting from very low values, the computed emissions are first increasing to a high maximum level, from which they are decreasing again sharply down to extremely low values. In this trend, the influence of two competing effects becomes clearly visible:

The initial increase can be attributed to the fact that concentrations of oxygen, hence of oxygen radicals as well, rise significantly in the exhaust gas zones. This concentration increase of the reaction partner for molecular nitrogen in the initiating reaction of the Thermal NO mechanism (51) enhances NO production. At the same time, temperatures are not considerably affected yet by the still small amount of fresh gas added and residence times of the combustion products at high temperatures are still sufficiently long to prevent them from becoming the limiting factor.

With further increased mixing velocity, this is no longer the case: Now the temperatures of the exhaust gas zones are eventually decreasing, leading to lower reaction rates - the residence times at sufficiently high temperatures are reduced as well. This effect first compensates for the effect of increased oxygen supply to the combustion products, leading to the distinct maximum in computed emissions, and becomes predominant when further raising the mixing rate.

The range of measured emissions is touched twice by the curves of computed emissions for constant zone numbers: Firstly for practically no mixing at all, secondly for relative mixing velocities in the order one. The concurrence in the absence of mixing is rather surprising, particularly in view of the fact that corresponding investiga-
tions for other operating conditions confirmed this observation. The reasons for this coincidence are unclear; however, its existence helps understanding why approaches neglecting the mixing process can nevertheless yield reasonable results.

The agreement of computed and measured emissions with relative mixing velocities in the order one corresponds to the expectations based on theoretical considerations: Taking into account the strong relation of mixing-controlled combustion and mixing of fresh gas to the combustion products, both effects must be associated with the same time-scale. The mixing process of a modelled product zone, however, has to be more intensive: On the one hand, it has to provide for the amount of fresh gas required for the combustion process, which is, in reality, conveyed through the zone. On the other hand, the zone itself is progressing from the flame towards the fresh gas ambience. Consequently, it absorbs additional fresh gas by covering a range of the concentration gradient driving the mixing process, which is eventually increasing and shifted towards higher fresh gas concentration values. Therefore, the relative mixing velocity has to be higher than, but still on the scale of one, which is exactly where the computed emissions coincide with the experimental data, for a sufficiently high number of zones.

In order to find a good compromise between accuracy and computation time requirements, the asymptotic behaviour with increasing zone number was studied with a constant value of the relative mixing velocity for various test cases representing extrema of the spectrum of operating conditions investigated. The resulting trade-off between CPU time requirements - the computations were performed on a R8000 processor - and prediction quality in term of the relative deviation from the asymptotic value of the computed $NO + NO_2$ emissions is presented in Figure 28.

The individual curves refer to the full load case of the engine in its reference state, a part load case with a marked premixed peak, a full load case with high EGR and a full load case with Common-Rail injection. The numbers in the diagram indicate the zone numbers applied in the simulations.
Obviously, to reach the asymptotic value, very high zone numbers and correspondingly CPU-time-expensive simulations are required. However, considering the trends with the different cases we can state that these are in fact very consistent: Even with the extreme cases, the difference between individual relative deviations hardly ever exceeds a few percent.

Therefore, all subsequent simulations were performed with a rather low zone number of 15, which reduced the computation time to a few minutes. The relative mixing velocity was slightly reduced accordingly in order to achieve an approximate reproduction of the experimental data.

Figure 28: Trade-off between CPU time requirements on a R8000 processor and the relative deviation of $NO + NO_2$ predictions from the asymptotic value for various operating conditions.
6.2.1.b Mechanism Detail and Kinetic Data

In order to assess the requirements for the detail of the mechanism for Thermal NO formation, various strategies were employed:

In a first step, the basic mechanism was reduced systematically by means of sensitivity analysis data obtained in NO formation simulations under stationary homogeneous conditions. The individual conditions investigated in these simulations spanned the range of conditions typically encountered locally in diesel engines [151]. Atom-flow analysis [152] was employed for the detection of insignificant reaction paths and the elimination of negligible intermediate species.

The results of the simulations for the various degrees of reduction were then compared in terms of deviations in the NO formation (or reduction) rates from the results of the full mechanism. Appropriate cut-off values for both the absolute and relative deviations were introduced for the evaluation of the various reduced mechanisms. The results of this investigation can be summarized as follows:

- Deviations between the extended Zeldovich and the full mechanism are in the 10 to 20% range under relevant conditions. It is expected, therefore, that engine emission predictions with the two mechanisms yield similar differences.

- The additional consideration of nitrous oxide, $N_2O$, alone already allows to reduce the error by up to 50%.

- Neglecting nitrogen dioxide, $NO_2$, deteriorates mainly the predictions of reduction rates.

- The compounds NH and HNO act as non-negligible intermediates in both the formation and the reduction process.

- A reduced mechanism considering the species NH, HNO, $NO_2$ and $N_2O$ and the associated reactions in addition to those of the extended Zeldovich mechanism allows to maintain both the absolute and relative deviations at tolerable levels (below the cut-off values selected as 8000 ppm/sec and 5%). Reactions additionally involving other nitrogen-hydrogen compounds are
of minor relevance for $NO$ formation or reduction.

In the second step, the mechanisms representing the various degrees of reduction were applied to the simulation of the same engine test cases as above in order to assess the influence of mechanism detail on both prediction quality and CPU time requirements. The results of this investigation are shown in Figure 29:

![Figure 29: Predictions of $NO$ (plus $NO_2$, if applicable) emissions with reduced mechanisms for various operating conditions, normalized with full mechanism results and effect of degree of reduction on CPU time requirements.](image)

The bars denote the computed resulting $NO$ plus, if applicable, $NO_2$ values normalized with the respective values obtained with the full mechanism. The five degrees of reduction refer to the respective mechanisms listed in Table 5, characterized by the species considered in addition to the extended Zeldovich mechanism. The associated elementary reactions and their kinetic data are specified in Appendix A.1.
The engine simulation results reflect the findings from the investigation under stationary conditions listed above:

- With the extended Zeldovich mechanism alone, the deviations from the full mechanism results are on the scale of 10 to 20%. Trends with the various operating conditions differ by up to 10%. Note that the quality of the predictions scales with the global air-fuel ratio (decreasing between the cases considered as follows: part load > Common-Rail > reference > high EGR). CPU time, however, is reduced by almost 60%.

- The additional consideration of $NO_2$ yields almost the same results, however at the expense of 10% less reduction in CPU time requirement.

- Supplementing the extended Zeldovich mechanism with 5 additional reactions involving $N_2O$ as the single additional species improves the predictive quality considerably: Deviations are in the order 5% with differences between the individual trends of up to 3%. CPU time is slightly less than half of the value required with the full mechanism.

- Accounting for both, $N_2O$ and $NO_2$, further reduces the deviations in individual trends to 2.5%, while maintaining the average error at the same level. At the same time, CPU time requirements are slightly increased.

### Table 5: Characterization of reduced mechanisms for Thermal $NO$ formation.

<table>
<thead>
<tr>
<th>degree of reduction</th>
<th>detail</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>extended Zeldovich + $NH$, $HNO$, $N_2O$ and $NO_2$</td>
</tr>
<tr>
<td>2</td>
<td>extended Zeldovich + $N_2O$ and $NO_2$</td>
</tr>
<tr>
<td>3</td>
<td>extended Zeldovich + $N_2O$</td>
</tr>
<tr>
<td>4</td>
<td>extended Zeldovich + $NO_2$</td>
</tr>
<tr>
<td>5</td>
<td>extended Zeldovich</td>
</tr>
</tbody>
</table>
The mechanism including \( NH, HNO, N_2O \) and \( NO_2 \) yields the best agreement with the full mechanism. Deviations are below 2%; however, the difference between minimum and maximum deviations is at almost the same value. In comparison with the simulations applying the full mechanism, the CPU time requirements are still reduced by more than one third.

As a consequence from these results, it was decided to perform all subsequent simulations with a mechanism representing the second degree of reduction, since this one allowed to reduce the deviation between trends sufficiently in conjunction with considerable savings in computational resources.

Kinetic data of individual elementary reactions can vary substantially, depending on the source. On the one hand, this is the consequence of uncertainties associated with their experimental determination, which are typically in the order 2 in the high-temperature range. On the other hand, different mechanisms distribute weights differently among the elementary reactions, often as a consequence of differences in the intended field of application. Therefore, though the individual mechanisms may be validated comprehensively and may even yield almost identical global results, kinetic data of the individual reactions can still be different.

In order to assess the sensitivity of emission predictions to uncertainties with respect to the kinetic data of the individual reactions, these were varied covering a range of two orders of magnitude and the resulting \( NO + NO_2 \) values were compared to the results of the unmodified mechanism. Figure 30 shows the obtained trends of those four reactions that yielded noticeable variations.

As one would expect, the highest sensitivity is associated with the starting reaction of the extended Zeldovich mechanism (51): Specifically in the range about the specified value, even slight variations easily produce deviations in the emission predictions in the 10% range.

The results are considerably less susceptible to variations of the kinetic data of the further reactions from the extended Zeldovich
scheme ((52), (53)): In the entire range considered, relative changes in the emission predictions hardly ever exceed 10%.

The conversion of nitrous oxide, $N_2O$, to nitric oxide, respectively the inverse reaction (56), affects the emission predictions specifically, if enhanced. This is again a clear indication that nitrous oxide is an important intermediate, which controls in particular the reduction of nitric oxide.

The data presented are averages from simulations of the same engine test cases as above. Note that the results of the variations with respect to the last reaction exhibited a strong dependence on the operating conditions: The trend with increased pre-exponential constants was enhanced with decreasing air/fuel ratio, suggesting an increased relevance of the nitrous oxide reaction path under either locally or globally lean conditions.

Figure 30: Sensitivity of $NO + NO_2$ predictions to variations in the value of the pre-exponential constant in the Arrhenius formulation of the respective reaction rate.
6.2.2 Predictions for Variations of Engine Operating Parameters

The engine operating parameters investigated here include engine load, timing of inlet valve closing and start of injection, charge air composition, viz. EGR and water content, as well as injection rate modifications when changing from the standard to the Common-Rail injection system and applying various injection pressures with the latter system.

6.2.2.a Water content

The introduction of water into the combustion chamber by means of either fumigation, direct water injection or emulsification of the fuel is a well-known method to reduce nitric oxide emissions [81]. Though this effect has not been addressed directly in the experimental investigation, it had to be considered in the evaluation of the measured data due to considerable variations of the ambient conditions, in particular relative air humidity and ambient temperature, in the course of the experiments [134].

The simulation results are compared directly to the measured data and therefore, the humidity of the charge air has to be taken into account accordingly. In order to assess the model response to variations in water content, a parametric study was performed and the results were validated against data from literature ([81], [153], [154], see Figure 31).

The individual data originate from experiments on engines of different size employing various techniques of water introduction:

In the experiments of Heinrich et al. [154], the effect of water injection into a single-cylinder research engine operated at low load was investigated for two timings of the water injection: Early, viz. at TDC in the scavenging cycle and late in the cycle at about the timing of the fuel injection. Their data are therefore believed to mark the range of emission reductions achievable with direct water injection.

In a more recent publication, however, Velji et al. [153] report only minor deviations between emissions with water injection into
the inlet manifold and with direct water injection late in the cycle. Their experiments were performed on a single-cylinder engine of comparable dimensions and operating conditions as the Sulzer S20 engine that the presented computational results refer to. Therefore, their direct water injection results are considered as the more appropriate direct reference when compared to the data of Papadopoulos [81] that were obtained on a high-speed diesel engine.

The simulation results are in very good agreement with the experimental data: The computed trend with increasing water content lies right in the middle of the range marked by the data of Heinrich et al. Furthermore, the computed emission reductions are in general only slightly smaller than the ones observed by Velji et al., which appears reasonable in view of the abovementioned deviations between early

Figure 31: Comparison of computed reductions of nitric oxide emissions as a function of water content with experimental data from various sources (Papadopoulos [81], Velji et al. [153], Heinrich et al. [154]).
and late water injections. Note that, in the simulations, the increased water content was modelled by adaptation of the initial conditions.

6.2.2.2 Engine Load at Constant Speed

The ability of the model to reproduce modifications in the rate of heat release history as a consequence of load variation was already demonstrated in Figure 7 (Chapter 4). The following comparison is limited to the load range between 50 and 100%, the reasons being severe uncertainties in the experimental cylinder pressure histories pertaining to extensive cyclic variations at low part load. Also, as discussed previously, the quality of the heat release predictions is substantially reduced when premixed combustion becomes predominant and it is expected that this effect arises in the emission predictions accordingly.

Figure 32 shows the results of a comparison of rate of heat release histories and emissions from experiment and simulation for the engine operated in the Miller system (see 6.2.2.c). The experimental heat release rates show the well-known trends of increasing ignition delay with reduced load associated with an increase of the premixed combustion part. Also, the peak of the mixing-controlled phase is shifted towards the start of combustion and tends to increase.

These effects are reflected in the simulations: The ignition delay increases accordingly with decreasing load, as a consequence of the lower temperatures at start of injection. The larger fraction of fuel evaporating and mixing during this phase results in a higher and broader premixed peak. The peak of the mixing-controlled combustion phase, which is usually closely coupled to the end of injection, is shifted as in the experiments. However, the experimentally observed tendency of this peak to increase at lower loads is only present in the first load reduction step. At half load, the premixed peak is already too dominating in the simulations for allowing the identification of a peak in the mixing-controlled phase.

The trend of decreasing nitric oxide emissions with reduced load, which was observed in the experiments, is well reproduced in the simulations. In particular, the adversary effects of generally reduced
temperature levels and of the increased premixed parts on $NO_x$-emissions are clearly discernable. Whereas the former effect inhibits the formation of $NO$, the latter enhances it as a consequence of the associated steeper initial temperature rise. This results in the characteristic curvature of the emission-load diagram (see also Figure 33).

6.2.2.c Inlet Valve Timing - Miller System

On the test engine, the original camshaft was replaced with a design, where the period during which the inlet valve is fully open was reduced by 52 deg CA. IVO timing as well as opening and closing characteristics were kept unchanged. The resulting IVC timing before BDC in conjunction with increased charge air pressure allows the reduction of temperatures during the high-pressure cycle when compared to the standard layout. This leads to a reduction of $NO_x$-emissions without penalty in fuel consumption; in fact, the efficiency of the engine was even slightly increased.

With practically unchanged injection timing, the reduced overall temperatures with the Miller system result in an increase of the igni-
tion delay with the associated more pronounced premixed peak. Both the heat release rate histories from experiment and simulation (Figure 33), which represent the 75% load cases in the two operating modes, illustrate this behaviour. Obviously, the mixing-controlled phase is hardly affected.

The emissions with the standard layout exhibit an adverse trend to the one discussed above for the Miller system. Keeping in mind that, with the standard layout, premixed peaks are substantially smaller than with the Miller system, the associated effect on NO formation can be expected to be diminished accordingly. The less pronounced increase of emissions at high load, however, is not entirely understood. It is speculated that the further increase of overall temperatures is partly compensated for by the decreased amount of oxygen, hence lower availability of oxygen radicals for NO formation.

The general trend of NO\textsubscript{x}-emissions as a function of load for both operating modes as well as the emission reduction with the Miller system are well predicted. However, the degree of reduction of
NO\textsubscript{x}\textsuperscript{-}emissions with the Miller system is overestimated by up to 10% in the simulations.

6.2.2.2 Exhaust Gas Recirculation

The Miller system on the test engine was supplemented with exhaust gas recirculation as a means to additionally reduce NO\textsubscript{x}\textsuperscript{-}emissions. Figure 34 shows the effect of maximum EGR rate at full load achievable with the employed high-pressure EGR system (13.2%).

In the rate of heat release histories, slight but not substantial differences can be found. In particular, the low quality of the experimental data with high EGR does not allow to draw general conclusions apart from the fact that the maximum of the heat release rate appears to be slightly reduced. The same is observed in the simulations that also show a small increase of the ignition delay and hence the premixed peak, as one would expect as a consequence of the tendency towards lower temperatures at start of injection with EGR, provided efficient charge air and EGR cooling can be realized.
The EGR rate of 13.2% yielded a reduction of $NO_x$-emissions of 28% when compared to the level achieved with the Miller system alone. The prediction is in good agreement with the experimental data, suggesting only a slightly higher potential of EGR for emission reduction than observed on the engine.

6.2.2.e Injection System

The conventional Pump-Line-Nozzle (PLN) injection system of the test engine was replaced with a Common-Rail (CR) system. In order to assess the isolated effect of this transition from one system to the other, two cases at full load with comparable injection duration were selected. Note that the same injector specification was applied with both injection systems. The two cases thus correspond to equivalent average injection pressures.

The effect of the injection system on the rate of injection (ROI) profile is highlighted in the top diagram of Figure 35:

The opening characteristics is not altered substantially as a consequence of the similar internal structure of the injector tips. However, with Common-Rail injection, the injection rate rises directly to the maximum level, only exposed to the low-frequency pressure oscillations in the system resulting from the opening of the injector. At the end of injection, the injector closes within a few deg CA and the injection rate decays fast.

With the conventional system, after the injector is fully open, the injection rate is further increasing as a consequence of the pump’s continuing action until the peak pressure is reached. After that point, the system pressure decays slowly and the injector closes only after the injection pressure has fallen sufficiently below the injector opening pressure.

This injection characteristics has its effect on the rate of heat release as illustrated in the bottom diagrams of Figure 35. Note that, as a consequence of the non-identical start of injection, the effect of the injection system on ignition delay and the premixed peak cannot be addressed here.
As a consequence of the almost rectangular shape of the injection rate, the rate of heat release with Common-Rail increases faster initially and has a broader maximum. The more rapid closing of the injector is reflected in a correspondingly faster decay of heat release rates after the end of injection.

The heat release rate predictions show the same initial trend: As a result of the initially faster injection, the heat release rate rises more rapidly and its maximum is broadened. However, the absolute values are underpredicted and, as a consequence of the higher amount of yet unburnt fuel after closing of the injector, the heat release rate predicted with Common-Rail decays even slower than the one with the PLN system. This in turn affects the predictions for $NO_x$-emissions, as is illustrated in Figure 36:

Whereas, in the experiment, the emissions with Common-Rail are slightly reduced in comparison with those with the conventional injection system, the simulations suggest an increase. The analysis of the computed evolutions of the $NO + NO_2$ volume fractions with both injection systems (right-hand side diagram in Figure 36) clearly
reveals the effect of the overprediction of heat release rates in the late combustion phase: \( NO \) formation is extended further into the expansion phase.

The consideration of the mixing rate effect on emission predictions, which we discussed in 6.2.1.a, leads to another explanation of the overprediction of the emissions: Since the burning and mixing rates are directly coupled, an underprediction of the former can be expected to be associated with an underestimation of the latter as well. In view of the strong effect of such an underestimation (compare Figure 27), it can be speculated to result in an overprediction of the \( NO \) formation during the main combustion phase.

The underprediction of burning rates during injection is attributed to deficiencies of the present turbulence model. Since the similar effect was observed in the 3-dimensional simulations (see 6.3.3), the issue will be discussed in more detail in that context.

6.2.2.f Injection Pressure

Figure 37 shows a comparison of two Common-Rail test cases with similar operating conditions (full load, \( \sim 5\% \) EGR) and injection timing, but different injection pressures (1200 vs 1400 bar).
The experimental heat release rate patterns show the expected increase with injection pressure throughout the injection phase. The simulation results exhibit the same behaviour; however, the effect appears to be slightly overestimated, especially in the beginning. The faster combustion obviously enhances $NO$ formation. The simulations, in agreement with the experiments, yield an increase in $NO_x$-emissions with higher injection pressure. In the simulations, however, the effect is underpredicted, which can again be explained as a consequence of the mixing rate effect on emission predictions: An overprediction of mixing rates as a result of the abovementioned slight overestimation of burning rates with increased injection pressure may lead to a decrease in predicted emissions.

Figure 37: Comparison of results from experiment and 0-D simulation for the variation of injection pressure with the Common-Rail injection system, top: heat release rates, bottom left: injection rates, bottom right: emissions.
6.2.2.g Injection Timing

The effect of injection timing with otherwise similar conditions (full load, ~5% EGR, 1400 bar injection pressure) is demonstrated in Figure 38:

![Figure 38: Comparison of results from experiment and 0-D simulation for the variation of injection timing (Common-Rail system), top: heat release rates, left: emissions.](image)

The heat release rate histories from the experiment suggest a transition towards an almost triangular shape with retarded injection. In view of the wiggliness of the experimental data it is difficult, however, to draw final conclusions. Especially the trend of decreasing premixed peaks with later injection, present in the simulations, can hardly be discerned in the experimental curves.

In contrast to the experimental data, the simulation results show a decrease in the maximum of the heat release rate with injection retard. Since the injection pressures are identical in all three cases, this can only be explained by considering the predicted evolution of the turbulence intensity (compare Figure 5): The latter results from superposition of the contributions from the charge air flow and from injection. Since the simulations predict a steady decay of charge-air-
flow-induced turbulence close to TDC, after the superposition with the injection-generated turbulence, lower levels of overall turbulence intensity result with retarded injection.

The emission results show the well-known trend of decreasing emissions with injection retard; however, the simulations tend to underpredict the trend, which is again related to the underprediction of burning, hence mixing rates with later injection and the associated tendency towards an overestimation of emissions.

6.2.3 Predictions for Geometry Variations

As a consequence of the only quasi-dimensional character of the present model, the correct reproduction of geometrical effects can hardly be expected. Nevertheless, the ability to deal with specific geometry variations was addressed, in particular with respect to the injector configuration and the engine size.

6.2.3.a Injector Configuration

It is a well-known fact that there exists an optimum orifice number for engines with a single central injector with respect to engine efficiency. In order to investigate the effect of the number of orifices on emissions, Wärtsilä NSD performed experiments with various injector configurations on a Sulzer S20 engine [155]. In these configurations, the total orifice cross-section, hence injection duration when maintaining the same injection pressure level, was kept constant.

The results of the experiments served as a reference for a similar computational investigation: In [156], the present model was applied in conjunction with a cycle simulation tool for the prediction of, among others, the effect of injector configuration on engine efficiency in terms of the brake specific fuel consumption (bsfc) and emissions.

The results of both the experimental and computational investigations are shown in Figure 39 for the engine operated at half load:

In the experiments, the 12 orifice design yielded the best fuel consumption. With 10 and particularly with 16 orifices, fuel consump-

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Results and Discussion

Emission was higher. $NO_x$-emissions however decreased continuously between 10 and 16 orifices. It has to be mentioned, however, that the results from the 16 orifice injector experiments are not beyond dispute. With this injector, the engine load could not be raised above 50% and there are strong indications for another effect superimposing with and possibly even dominating the orifice geometry effect [155].

The computations were not able to reproduce this behaviour: Only the increase in bsfc with smaller orifice number was predicted in accordance with the experimental evidence. All the other simulations yielded trends opposite to the experimental ones. In particular, $NO_x$-emissions were predicted to increase with orifice number - mainly as a consequence of more pronounced premixed peaks with smaller orifices, resulting from faster evaporation.
However, as will be shown below, with increasing orifice numbers, interactions between the individual sprays gain more and more importance and the approach based on a representative isolated individual spray does no longer apply.

### 6.2.3.b Engine Size

The capability of the model to predict trends with engine size was assessed by applying it to the simulation of a large medium-speed engine. In view of the increasing importance of the premixed combustion phase with decreasing engine size, respectively increasing engine speed, an extension of the investigation to smaller engines was neglected.

The data presented below refer to a Sulzer ZA40S engine with the following main data:

<table>
<thead>
<tr>
<th>Table 6: Main data of the Sulzer ZA40S engine.</th>
</tr>
</thead>
<tbody>
<tr>
<td>bore, m</td>
</tr>
<tr>
<td>stroke, m</td>
</tr>
<tr>
<td>compression ratio, -</td>
</tr>
<tr>
<td>speed, rpm</td>
</tr>
<tr>
<td>rated power output, kW/cyl</td>
</tr>
</tbody>
</table>

The engine was equipped with a conventional injection system and a central injector with 10 orifices of diameter 0.7 mm. In its standard layout, inlet valve closing is several deg CA before BDC; therefore, the following comparison is based on the results of the Sulzer S20 engine operated in the Miller system.

Figure 40 shows the comparison of experimental [155] and computational results for the two engines operated at full load. The experimental heat release data for the larger engine are characterised by the complete absence of a premixed peak and, apart from the burnout phase, a close to symmetrical shape.

The simulation results reproduce this behaviour: A premixed peak is not observed and the general character of the curve is very similar
to that of the experimental data. However, when applying identical model constants, absolute values of rate of heat release are considerably underpredicted for the larger engine during the main combustion phase (dashed curve). After adaptation of the constant controlling the mixing-controlled combustion rate (79), the resulting rate of heat release history is in excellent agreement with the experimental results.

With respect to $NO_x$-emissions as well, the predicted trend with engine size reproduces the experimental data sufficiently well. Hence, we can state that for engines of comparable characteristics - in particular with respect to the charge air flow structure - the mere adaptation of the combustion model constant can already be sufficient for reasonable predictions of heat release and $NO_x$-emissions.
6.3 The 3-Dimensional Model

All the subsequently presented results were obtained for a selection of temporal and spatial discretization parameters based on the best practice approach derived from a sensitivity study to both temporal and spatial resolution and outlined in the Appendix C. For the S20 engine cases, the mesh depicted in Figure 18 and (in a detail view of the injector region) Figure A9 was employed.

In the first section, the performance of the model in terms of quantitative emission predictions will be addressed for one typical operating condition of the reference engine, followed by a brief discussion of sensitivity to key model parameters. The ability of the model to predict trends with respect to variations of initial and boundary conditions as well as geometry parameters is assessed in the next section through comparison with the same set of experimental data as above. Another part of the chapter is dedicated to investigations into interactions of individual sprays and their potential effect on global results. Finally, a few indications on potential future enhancements are given.

6.3.1 Quantitative Nitric Oxide Emission Predictions

Figure 41 shows the comparison of rate of heat release histories and emission results from experiment and simulation for the S20 engine operating at full load with the Miller system.

As already noted in the context of the validation tests with the A20S engine (5.4.2), the general characteristic of the heat release patterns is in good agreement between experiment and simulation. However, one major difference cannot be neglected: After very similar premixed peaks and transitions to the mixing-controlled combustion phase, the computed curve reaches its peak earlier than the one derived from the measured pressure trace and considerably underpredicts the burning rates in the later phase of combustion. Hence, the predicted peak pressure is both lower than the measured one and achieved earlier in the cycle. Moreover, the burnout phase is very long in the simulations as a consequence of the high remaining quan-
tities of yet unreleased chemical energy and the apparent low consumption rates due to the fast increase of the turbulent time scales after the end of injection (see discussion in 5.4.2.b).

The computed evolution of \( NO \) and \( NO + NO_2 \) volume fractions in the cylinder, obtained with the most detailed mechanism employed in the present study (see discussion below), is characterized by a maximum gradient in the phase after the peak of the heat release rate and reaches a practically constant value well before 45 deg after TDC. The absolute level of the associated resulting emissions is a factor four below the experimental data.

Note that the fraction of \( NO_2 \) obtained in the simulations was always in the order 1% of the total \( NO + NO_2 \).

### 6.3.2 Sensitivity to Key Model Parameters

The observation of maximum nitric oxide formation gradients in the late combustion phase, where the model obviously underpredicts the heat release rates, motivates the investigation of the effect of this underprediction on simulated emissions. Additionally, the sensitivity of the predicted emissions to detail and accuracy of the reaction
mechanism applied was tested for various degrees of simplification of the chemical scheme.

6.3.2.a Mechanism Detail and Kinetic Data

Starting from a baseline mechanism (22 kinetic and 6 equilibrium reactions involving 16 species - plus fuel), corresponding to the first reduction step of the detailed mechanism employed in the 0-dimensional simulations (compare 6.2.1.b), several degrees of reduction were tested. Additionally, the performance of the approach frequently used in previous investigations (simple extended Zeldovich reaction scheme with kinetic data according to Heywood [43]) was assessed.

The individual mechanisms were applied to the same variety of test cases as in the similar sensitivity studies with the 0-dimensional model. Figure 42 shows the effect on both predictive quality and CPU time requirements.

The bars denote the computed resulting NO plus, if applicable, NO\textsubscript{2} emissions normalized with the respective values obtained with the baseline chemical scheme. The five degrees of reduction refer to the respective mechanisms listed in Table 5, characterized by the species considered in addition to NO and N as in the extended Zeldovich mechanism (and the source of the kinetic data, if applicable). The associated elementary reactions and their kinetic data are specified in Appendix A.2.

In contrast to the findings from the similar investigation for the 0-dimensional model, the computed emissions are much more sensitive to reduction from the baseline mechanism: The emission results are lowered by a factor of two already with the first reduction step. Further reduction down to the extended Zeldovich mechanism, however, yields only slight modifications: Trendwise, the emission predictions are further reduced. Only the simulations with extended Zeldovich and rate constants from [43] gave substantially lower emissions, thus again supporting the accuracy requirements in terms of kinetic data.
The variation of sensitivities between individual cases is very similar for all reduction steps: Apparently, the deterioration of predictions with the high EGR test case is less pronounced than with the

![Graph](image)

**Figure 42:** Predictions of $NO$ (plus $NO_2$, if applicable) emissions with reduced mechanisms for various operating conditions, normalized with baseline mechanism results and effect of degree of reduction on CPU time requirements.

The variation of sensitivities between individual cases is very similar for all reduction steps: Apparently, the deterioration of predictions with the high EGR test case is less pronounced than with the

**Table 7:** Characterization of reduced mechanisms for Thermal $NO$ formation.

<table>
<thead>
<tr>
<th>degree of reduction</th>
<th>detail</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>extended Zeldovich + $N_2O$ and $NO_2$</td>
</tr>
<tr>
<td>2</td>
<td>extended Zeldovich + $N_2O$</td>
</tr>
<tr>
<td>3</td>
<td>extended Zeldovich + $NO_2$</td>
</tr>
<tr>
<td>4</td>
<td>extended Zeldovich</td>
</tr>
<tr>
<td>5</td>
<td>extended Zeldovich, kinetic data from [43]</td>
</tr>
</tbody>
</table>
other cases. It is speculated therefore, that for modifications of charge air composition the detail of the chemistry model is more relevant than for other changes of the initial conditions or for variations of the injection boundary conditions.

The additional expense associated with the consideration of more detailed chemistry is rather moderate: Employing the extended Zeldovich instead of the baseline mechanism decreases the CPU time requirements by no more than 11%, despite the reduction in the number of conservation equations to be solved from 24 to 19. In view of the associated substantial increase in predictive quality this small additional expense appears well justified and the baseline mechanism hence was applied in all subsequent investigations.

6.3.2.a Rate of Heat Release in the Late Combustion Phase

As observed above, the simulations yield a maximum of the overall nitric oxide formation gradient in the phase shortly after the peak heat release rate. It must be expected, therefore, that the underprediction of the burning rates in this phase has a strong negative effect on emission formation predictions. In order to verify this, a numerical experiment was performed, where the rate of heat release in the late combustion phase was increased artificially. This was done by introducing an additional term in the formulation of the transition function (101), active only for $t > t_{end, inj} - \Delta t_{ebo}$:

$$
\zeta_{prog} = \zeta_{prog} \exp \left[ \frac{t_{end, inj} - \Delta t_{ebo} - t}{t_{ebo}} \right]
$$

(105)

The parameters in this additional term, $\Delta t_{ebo}$ and $t_{ebo}$ were selected as 10 and 18 deg crank angle, respectively, in order to match the experimental heat release. Equation (105) hence suppresses the otherwise dominant turbulent time scale in the determination of the local burning rate during the late combustion phase and thus enforces burnout.

Figure 43 shows the effect of such a procedure on both heat release rate and the evolution of $NO + NO_2$ volume fraction for the same test case as above.
The experimental heat release rate is well modelled with this approach: Height and location of the peak value are very similar and, in the subsequent decay phase, the curves largely overlap. Obviously, the integral heat release must also be in good agreement.

The predicted evolution of NO and NO + NO$_2$ volume fractions shows the expected behaviour: With enforced burnout, the predicted emission level is increased by a factor of more than two. Still the curves with the standard model and with enforced burnout exhibit the same characteristic: With this case, the peak gradient is reached between 15 and 25 deg after TDC and the volume fraction then converges towards its final level before 35 deg after TDC.

The same approach was again applied to the set of test cases already subject to previous sensitivity studies. Figure 44 shows the comparison of the results obtained with the standard model and the enforced burnout approach, where the predicted emissions are normalized with their respective experimental values. Note that the same set of values for $\Delta t_{ebo}$ and $t_{ebo}$ was employed and no tuning to the individual cases was performed.

Figure 43: Key results for the full load case with the Miller system with standard combustion model and enforced burnout: Left: Comparison of rate of heat release histories from experiment and 3-D simulation. Right: Computed evolutions of the NO and NO + NO$_2$ volume fractions in comparison with the measured emission level.
For all cases, a similar improvement of the emission predictions is achieved. Moreover, the relative deviation between the individual results is decreased: Whereas, with the standard model, the difference between minimum and maximum value is 8% at an average level of 22%, this difference amounts to 12% at an average value of 50% with enforced burnout, percentages relating to measured values. The variation with enforced burnout is hence by approximately one quarter smaller in relative terms.

Nevertheless, even when increasing the burning rates during burn-out by this method, the measured emissions are still underpredicted. We also have to keep in mind that this procedure is highly artificial: In reality, the combustion in this phase is entirely determined by turbulent mixing and the underprediction of burning rates must hence rather be attributed to an underprediction of turbulent exchange processes in general. By local forcing of the combustion reactions,
the exchange is only indirectly enhanced via maintenance of high spatial gradients. At the same time, however, the weights between the oxygen-consuming reactions are also shifted: As the combustion reactions are favoured, the oxygen availability for nitric oxide formation is in turn reduced and hence formation rates tend to be decreased. A more accurate prediction of the turbulent exchange processes and the underlying turbulent flow field generated by the injection process can thus be expected to also yield better emission predictions.

As a conclusion from this numerical experiment we can state that the underprediction of burning rates in the late combustion phase constitutes the main source of the deficiencies of the model in terms of quantitatively correct prediction of nitric oxide emissions.

The subsequent validation against experimental data refers again to the standard model. Note that, in contrast to many other investigations, no enforcement of the emission formation rates was employed, as such a procedure is not considered suitable with the detailed chemistry model of nitric oxide formation used here. Therefore, all comparisons of emission results are based on normalization with the respective experimental and computed reference values.

**6.3.3 Predictions for Variations of Engine Operation Parameters**

As in the case of the 0-dimensional model, the effect of both initial and boundary condition variations was investigated. The former include engine load, exhaust valve timing and charge air composition (EGR) variations, the latter refer to the effect of injection rate pattern modifications with the various injection systems and various injection pressure levels with Common-Rail.

**6.3.3.a Engine Load at Constant Speed**

The comparison of rate of heat release histories from experiment and simulation for the engine operated in the Miller system at loads between 50 and 100% shown in Figure 45 supports the conclusions from the previous combustion model tests (5.4.2):
The predicted increasing ignition delay as well as the growing relevance of the premixed combustion phase with decreasing load are correctly reflecting the experimental evidence.

The advance and tendential increase of the peak of the main combustion phase towards part load is observed in a very similar manner in both the experimental and computational results. It is worthwhile noting that the effect is much less pronounced than with the earlier simulations in the context of the combustion model tests. In fact, the trend of the predictions with varying load is in considerably better agreement with the experimental data than during those tests (compare Figure 19).

The deficiencies of the model in predicting the late combustion phase, however, prevent a better agreement with the experimental data through their stronger relative effect with shorter injection duration and hence towards lower loads: The comparison of the evolution of turbulent time scales during injection (Figure 25) revealed a strong similarity between various loads. In combination with the similarity of the injection rate patterns (Figure 6) in their late phases
this suggests that the absolute amount of unreleased energy at the end of injection must be similar for all cases. Hence, the relative effect will be more pronounced for shorter injection durations.

The predicted emission values as well as their experimental counterparts are normalized with the respective full load values. The simulation results reflect the experimentally observed trend of decreasing emissions towards part load. The effect is, however, substantially overestimated. This can be traced back again to the increasing relevance of the underprediction of the late combustion phase with decreasing load. As was shown in the previous section, the nitric oxide formation is mainly determined by the heat release in this phase. Hence, the relatively stronger effect of the underprediction will, trendwise, result in correspondingly reduced predictions of the nitric oxide formation gradient.

6.3.3.b Inlet Valve Timing - Miller System

The effect of the IVC timing advance before BDC in combination with increased charge air pressure is shown in Figure 46. The comparison of rate of heat release histories refers to the 75% load operating condition. The measured and computed emissions are normalized with the respective values at full load in the standard mode.

The change in the overall characteristic of the heat release rate with the transition from the standard to the Miller operating mode is in excellent agreement between experiment and simulation: The increasing ignition delay, which is slightly overpredicted in the computations, results in a more pronounced premixed peak. In the earlier mixing-controlled phase before the peak, the overall burning rates with Miller are slightly below the ones of the standard mode. In the later phase, however, the curves are almost identical.

The comparison of emissions between experiment and simulation again suffers from the problems of the model already addressed in the previous sections and the resulting discrepancies in absolute values. Nevertheless, the general trend of decreasing emissions towards lower loads (except for the 50% load case in the standard
The emission-reducing effect of the Miller system is also obtained in the predictions, the degree however strongly varying between the various load cases: In the 75% load case, the relative reduction is in good agreement between experiment and simulation, whereas it is heavily overestimated at half load and clearly underpredicted at full load.

6.3.3.c Exhaust Gas Recirculation

Numerical predictions of the additional effect of high EGR rate (13.2%) at full load with the Miller system are compared to the respective experimental data in Figure 47. The measured and computed emissions are normalized with the values obtained in the absence of EGR.

In contrast to the 0-dimensional simulations (compare Figure 34), the 3-dimensional model yields a slight decrease of the ignition delay and a correspondingly reduced premixed peak with EGR, in accordance with the trend suggested by the experimental data.

Figure 46: Comparison of results from experiment and 3-D simulation for the variation of inlet valve timing, top: heat release rates at 75% load, left: emissions.
Apparently, the pure thermodynamic effect of reduced temperatures at start of injection as a consequence of EGR, which the 0-D model is only considering, is superimposed with local effects enhancing ignition, which the 3-D simulation is capable of capturing.

In the mixing-controlled combustion phase, the lower peak value discernible in the experimental heat release pattern is also obtained in the simulations.

The nitric oxide emissions are predicted to decrease substantially with high EGR rate. This is in accordance with the measured data; however, the effect is overestimated in the simulations.

6.3.3.d Injection System

The response of the model to the modification of the injection rate pattern associated with the transition from the Pump-Line-Nozzle (PLN) to the Common-Rail (CR) injection system is compared to the experimental results in Figure 48. The presented data refer to the full load operating condition with the Miller system without EGR. Emissions are normalized with the respective PLN values.
The change in general characteristic with accordingly modified injection rate boundary conditions is similar in experiment and simulation. After a less pronounced premixed peak as a consequence of the later start of injection, the heat release rate in the mixing-controlled phase initially follows closely the one obtained in the PLN case and then reaches an almost constant level, where it remains until the end of injection. However, in the simulation, this plateau is reached much earlier and is hence at a lower level. The fast decay of ROHR at the end of injection, which is observed in the experimental curve with Common-Rail, is therefore not present in the simulations. This is the clear consequence of the correspondingly higher amount of yet unreleased chemical energy in the simulation of the Common-Rail system when compared to the PLN case (see also Figure 49 below).

Figure 48: Comparison of results from experiment and 3-D simulation for the transition from the Pump-Line-Nozzle to the Common-Rail injection system, top: heat release rates, bottom left: injection rates, bottom right: emissions.

6.3 The 3-Dimensional Model
This underprediction of burning rates in the main combustion phase is clearly reflected in the emission predictions, which suggest a much higher emission reduction with the Common-Rail system than observed on the engine.

In order to better understand the reasons for this inability of the model to correctly predict the effect of a variation in the characteristic of the injection boundary condition, the predicted evolutions of weighted and volume-averaged turbulent time scales (compare 5.4.2.b) as well as the evolution of yet unreleased chemical energy with the two systems are compared in Figure 49.

![Figure 49: Comparison of temporal evolutions of volume- and weighted average values of the turbulent time scale (left) and yet unreleased chemical energy (right) with the Pump-Line-Nozzle (PLN) and the Common-Rail (CR) injection systems.](image)

The evolution of unreleased chemical energy is not very different between the PLN and CR cases: The curves increase steadily towards the respective end of injection timings, where they are at a similar level. Their slight variations in curvature during injection are obviously reflecting the differences in shape of the injection rate patterns. For a similar behaviour as in the experiment, the increase towards the end of injection with Common-Rail had to be much less pronounced and the level achieved considerably lower. This would basically require lower turbulent time scales to be predicted with Common-Rail during the late injection phase.
However, the values of the turbulent time scales actually obtained with the present model rather show the opposite behaviour: The volume-averaged values are generally higher with the CR case and the weighted average values, at the same level in the initial phase, increase much faster to even higher levels before the end of injection than with the PLN case.

These differences in both volume- and weighted average values must be associated with variations in spatial distribution or spray structure. Figure 50 compares the spatial distributions of yet unreleased chemical energy and turbulent time scale on a vertical cut through the sprays at 10 deg after TDC.

![Figure 50: Spatial distribution of the turbulent time scale (left, in ms) and the yet unreleased chemical energy (right, in J/m³) on a vertical cut through the spray at 10 deg after TDC for the Pump-Line-Nozzle (PLN, top row) and the Common-Rail (CR, bottom row) test cases.](image)

The general structure of the sprays, as manifest in the spatial distribution of unreleased chemical energy, is very similar between the two cases, the slight variations in penetration and radial expansion being mainly due to the different start of injection timings.

The distribution of turbulent time scales also exhibits strong similarity; however, the region of very low values around the spray core in the vicinity of the injector with the Pump-Line-Nozzle system is not present in the Common-Rail case.
We can thus conclude that the relative underprediction of burning rates in the main combustion phase with Common-Rail is the consequence of differences in the prediction of turbulence structure with the various injection profiles. This implies either the inability of the turbulence model in use here to correctly reproduce the effect or deficiencies of the combustion model, in particular the chemistry-turbulence interaction, where spatial distribution effects may have to be considered. Both aspects will be looked at in a more detailed manner in 6.3.6 below.

6.3.3.e Injection Pressure

The predictions for a variation of injection pressure with Common-Rail from 1200 to 1400 bar at full load (Miller) and ~5% EGR are compared to the corresponding experimental results in Figure 51. Emission values are presented with reference to the 1200 bar levels.

The experimentally observed trend with increased injection pressure towards higher level of ROHR in the main combustion phase at practically unaltered behaviour in the initial phase is well reproduced by the simulations: The ignition delay as well as the premixed peak are almost identical and the curve subsequently rises faster towards a higher and narrower peak. In the burnout phase, the rate of heat release is then accordingly reduced.

The effect of injection pressure on nitric oxide emissions is predicted correctly in terms of the trend towards higher values, the degree of modification is, however, again overestimated, possibly as a consequence of a relatively less pronounced underprediction of burning rate in the early burnout phase with increased injection pressure.

6.3.3.f Injection Timing

Figure 52 shows the comparison of experimental and computational results for a variation of injection timing (start of injection between 4 and 8 deg before TDC) with the engine operated in the Miller mode at full load at ~5% EGR and 1400 bar injection pressure. The measured and computed emissions are normalized with the respective values of the cases with SOI at 8 deg before TDC.
The computed heat release rates indicate (as did the results from 0-D simulation) a decrease of the premixed peak that is not obvious in the experimental data. Apart from that, the ROHR curve is merely shifted by two degrees with the first SOI retardation step. With further delay, however, the peak of the main combustion phase is also decreased, in contrast to the observations in the experiment, where the delay resulted in higher maximum ROHR values.

The reason for this deviation is unclear, the simplicity of the underlying combustion chamber geometry model may, however, contribute by means of the elimination of the parasitic volumes and the associated squish flows that can be expected to enhance exchange processes close to TDC. Note that the effect of this neglect must be expected to be even more pronounced in the 0-dimensional

Figure 51: Comparison of results from experiment and 3-D simulation for the variation of injection pressure with the Common-Rail injection system, top: heat release rates, bottom left: injection rates, bottom right: emissions.
simulations, where the large-scale squish flow induced by the shallow piston bowl is not accounted for either.

The predictions for nitric oxide emissions again yield the correct trend; however, they tend to overestimate the reduction potential of injection retard, presumably as a consequence of the increasing deviation in the ROHR predictions from the experimental data with increasing retard discussed above.

### 6.3.4 Predictions for Geometry Variations

The ability of the model to correctly predict trends with variations of geometric parameters was assessed by means of investigating the effect of injector configuration and engine size.

#### 6.3.4.a Injector Configuration

The effect of injector configuration was addressed performing the same study of various combinations of orifice number and diameter at constant total orifice cross-section as in the previously mentioned experiments at Wärtsilä NSD (see 6.2.3.a).
The simulations did again not include the scavenging phase. Identical initial conditions corresponding to typical values at 50% load of the respective engine and the same total fuel mass were prescribed in all the cases. The results thus provide only a first indication of the consequences on fuel consumption (bsfc) and emissions, which are, in the experiments, superimposed with the additional effects associated with the effective bsfc and initial condition variations.

The results of this study in terms of bsfc and emission variations from the standard 12-orifice design are shown in Figure 53, plotted against the experimental data. Note that the bsfc effect was estimated based on the consideration of the piston work during the closed cycle and assuming an invariant effect of the scavenging phase.

![Figure 53: Comparison of results from experiment and 3-D simulation for the variation of injector orifice number at constant total cross-section.](image)

The general trend of the bsfc predictions reflects the effective behaviour of the engine: Both the increase of the orifice number from
12 to 16 and the decrease to 10 deteriorate the efficiency, though the predicted effect is rather small.

The trend of increasing emissions with larger orifices at constant total cross-section is reproduced correctly, the absolute variation being again substantially overestimated. With the higher orifice number, however, the simulations predict an increase of the emissions, in contrast to the experiments, where a strong decrease was observed. However, as previously mentioned, the experimental data for the high orifice number case may not be considered very reliable and, therefore, this deviation must not be overemphasized.

In order to obtain deeper insight into the spray interaction phenomena governing injector configuration effects, an appropriate numerical experiment was defined, whose results are presented in 6.3.5 below.

6.3.4.b Engine Size

In order to assess the ability of the model to correctly predict variations in combustion characteristics and emission formation with engine size, the Sulzer ZA40S engine (for its main data see Table 6) was simulated additionally.

The grid employed in these simulations is shown in Figure 54. The number of computational cells at TDC is similar to the S20 ge-
ometry. Hence, the relative resolution per spray is similar, too. However, in view of the considerations in Appendix C, resolution effects cannot be excluded, in particular as a consequence of the large differences in detail of the representation of the injector. Note that this geometry also was not optimized in the spray core region and hence noticeable stability problems had to be faced.

The results from these simulations are compared to those of the S20 engine operated at full load in the Miller mode with the conventional injection system and without EGR (Figure 55). Computed and measured emissions are normalized with the respective S20 results.

![Figure 55: Comparison of results from experiment and 3-D simulation for different engine sizes, top: heat release rates, simulations with identical and adapted model constant, left: emissions.](image)

Applying the same set of model constants to both engines yields a substantial underprediction of burning rates during the main combustion phase with the larger engine. Note that the 3-D simulations, in contrast to the 0-D results, indicate the presence of a - though rather small - premixed peak for the larger engine as well. Such a premixed peak is not present in the data derived from the experimental pressure curve. However, as the heat release analysis was
not performed by means of the same tool for both engines (and rather adhoc for the ZA40S [155]), this deviation should not be overrated.

The underprediction of burning rates in the mixing-controlled combustion phase requires the adaptation of the corresponding model constant for recalibration, viz. the weighting parameter for the turbulent rate (see 5.4.1). After matching of this single parameter, the rate of heat release history is in good agreement with the experimental data and the change in characteristic with engine size reflects the engine behaviour.

The simulation with matched combustion model parameter yields a substantial relative increase of emissions from the S20 level. The general trend is hence again in qualitative agreement with the experimental evidence, however considerably overpredicted.

6.3.5 Investigation of the Interaction of Multiple Sprays from the same Nozzle

In order to study the effect of orifice size and number in more detail, an isolated investigation of spray interaction effects in a model geometry was performed, thus eliminating secondary effects due to piston motion and potential spray-wall interactions. This investigation basically reiterates upon an earlier study of the author ([157], [139]), applying the present, more advanced combustion model and the detailed chemistry for nitric oxide emission formation instead of the simpler approaches used previously.

In this study, the total injector orifice cross-section was selected according to the S20 specifications and test cases with 8, 12, 16 and 20 holes of correspondingly adapted diameter for identical total flow area were simulated. Injection boundary conditions were imposed according to the full load injection rate pattern of the S20 engine equipped with a conventional injection system.

The simulations were performed for a cylindrical constant-volume combustion chamber of diameter 20 cm, corresponding to the S20 dimension, and of 5 cm height in order to avoid interactions with the upper and lower boundaries. Central injection from the centre of the
geometry with horizontal orientation of the uniformly distributed sprays was assumed. Initial conditions were set to 900 K and 100 bar, assuming a quiescent charge of fresh air. Each simulation included one pair of sprays in order to enable the direct visualization of the interaction on a horizontal cut plane through the sprays. The geometries employed for this purpose are shown in Figure 56.

![Figure 56: Geometries employed with the constant-volume chamber test cases - separations indicating location of backward face with higher hole numbers, injection radially outward from the centre on the geometry mid-plane.](image)

The key results from these simulations are presented in Figure 57. The rate of heat release histories already show a strong sensitivity to the hole number: With the 8-hole case, the main combustion phase is considerably delayed when compared to the other cases. Between the 12- and 20-hole cases, the location of the peak is almost identical, however, its height is continuously decreasing towards larger hole numbers. Additionally, the premixed peak is eventually advanced.
and increased with increasing hole numbers, despite the fact that ignition delay is identical in all the cases.

Many of these effects can be explained taking into consideration the variations in evaporation history with the various cases: The delayed main combustion phase with the 8-hole case must, at least partly, be attributed to the slower evaporation of the initially larger droplets. The other three cases do not exhibit large differences in evaporation behaviour, apart from the initial phase before ignition, which can hence be regarded as responsible for the variations in the premixed phase of combustion. The variations in height of the ROHR peak during the main combustion phase with the lower orifice numbers can, however, no longer be explained as a consequence of evaporation behaviour but must rather be attributed to differences in the spatial distribution of the key quantities.

The variations in the evolution of the $NO + NO_2$ volume fractions are partly a direct consequence of these differences in combustion characteristic: The delayed combustion in the 8-hole case results in
a later onset of noticeable nitric oxide formation. However, also with the higher hole numbers, a clear trend towards an earlier increase of the $NO + NO_2$ level can be discerned, possibly as a consequence of the higher premixed peaks. During the later phase, the differences in the formation behaviour are not that clear any more. Only with the 8-hole case, the higher burning rate levels in the late combustion phase help to understand the continuous further increase. With the other cases, the comparison of heat release rates in the late combustion phase would rather suggest higher nitric oxide formation gradients with higher hole numbers, in contrast to the effective behaviour, where the late phase gradient clearly decreases with increasing hole number.

Finally, this leads to the lowest $NO + NO_2$ production with the 20-hole case. Note that this result is not relevant to the corresponding engine, as, on the engine, the superimposed effect of expansion freezes the emissions at a much earlier stage. In fact, the situation at about 7.5 ms is much more representative of the real engine situation, as (compare Figures 41, 43), the freezing of emissions is achieved approximately at that time after start of injection.

In order to understand both the effect of decreasing height of ROHR peaks and variations in the late phase nitric oxide formation gradient opposite to the expectations, the spatial distributions of key quantities for combustion and nitric oxide formation must be taken into consideration. Figure 58 shows the distributions of key data such as oxygen mass fraction, yet unreleased chemical energy, temperature, heat release rate and $NO + NO_2$ mass fraction on a horizontal cut through the sprays for the 12-hole case after 4 ms.

The yet unreleased chemical energy is clearly concentrated in a region close to the spray axis, with increasing level towards the injector. Accordingly, the heat release rate distribution has its maximum in the region with the highest level of available chemical energy. Close to the spray tip a local minimum is observed, the combustion is proceeding on sort of an envelope around the spray. This minimum is clearly due to the corresponding depression in the oxygen

6.3 The 3-Dimensional Model
The temperature maxima are observed in annular structures around the regions of low heat release rate. This can be understood as the consequence of the slowing down penetration towards the spray tip, while the high burning rate regions are continuously feeding combustion products at practically constant speed to those

distribution, as the maxima are related to the high oxygen availability in the vicinity of the spray core region.

The temperature maxima are observed in annular structures around the regions of low heat release rate. This can be understood as the consequence of the slowing down penetration towards the spray tip, while the high burning rate regions are continuously feeding combustion products at practically constant speed to those
regions downstream. The regions along the axis, however, are heated up less. This must be attributed to the cooling effect of evaporation that reduces already the temperature of the unburnt fractions and accordingly affects the temperature of the reaction products downstream. The distribution of $NO + NO_2$ mass fractions is very similar to the temperature distribution with corresponding location of the maxima on annular structures around the spray axis shortly behind the spray tip, trendwise in regions with higher oxygen availability.

We can thus conclude that the distributions of oxygen mass fractions and temperature promise to provide the additional information required for the explanation of the abovementioned differences in combustion characteristic and emission formation behaviour in the various phases. Figures 59 and 60 show the distributions of these two key quantities on the same horizontal cut through the sprays as above for all the four cases at 4 and 7 ms, respectively.

The overall spray propagation is clearly varying with orifice size due to the higher initial momentum of the sprays originating from a larger orifice. Hence, the tips of the sprays have already reached the combustion chamber wall in the 8-hole case at 4 ms, whereas they are just approaching it in the 12-hole case and are still some distance apart in the other cases.

Additionally, with increasing hole number, the sprays start interacting as a consequence of the increasingly close vicinity to each other: Whereas, in the 8-hole case, the sprays are still unaffected by their neighbours, the oxygen distribution in the 12-hole case already indicates the formation of an oxygen-poor region where the envelopes of the two spray overlap. With the higher hole numbers, this overlap already extends far upstream and the isolated depression regions observed in the 12-hole case have merged into a connected region, evolving into an extended structure with the 20-hole case, which propagates in a front-like manner behind the spray tips.

Such a behaviour cannot go without effect on heat release rates, as the oxygen availability in the regions of high heat release is eventually reduced. The abovementioned effect of decreasing peak values of heat release rates with increasing hole number is hence the result
Figure 59: Spatial distribution of key quantities for nitric oxide formation on a horizontal cut through the sprays at 4 ms, left: temperature, right: oxygen mass fraction.
Figure 60: Spatial distribution of key quantities for nitric oxide formation on a horizontal cut through the sprays at 7 ms, left: temperature, right: oxygen mass fraction.
of reduced oxygen availability as a consequence of spray interactions.

In accordance with the merging of the oxygen-poor regions with increasing hole numbers, the annular structures of the high temperature regions observed in the low hole number cases develop into connected regions in the periphery of the sprays. These are covering increasingly large regions at higher maximum levels of temperature at that time, reflected in the effect of higher nitric oxide formation rates with high hole numbers in the early phase.

In the later phase (see Figure 60), the differences in spray propagation are even more pronounced: In the 20-hole case, the individual sprays can hardly be discerned any more and the entire flow structure has rather evolved into an outward-propagating front with the high temperature and low-oxygen regions largely overlapping. With the 16-hole case, the formerly connected high-temperature regions have apparently been disrupted and developed into isolated regions close to the axis and near the wall, where, at the same time, oxygen availability is low. A similar statement applies to the 12-hole case, where these regions are spread over almost the entire wall region, across the before separating gap with accordingly less pronounced minima in oxygen mass fraction. With the 8-hole case, the former annular structures have connected and are now reflected back from the wall into the yet oxygen-rich gap between the sprays.

All these observations give evidence that the temporal gradient of nitric oxide formation in the late phase depends on the relative location of high-temperature regions to regions of high oxygen availability. Apparently, with increasing hole number, the transition from the reflection of high-temperature regions into the oxygen-rich region between the sprays to the formation of isolated high-temperature and low-oxygen regions and finally to practically coherent fronts, results in decreasing emission formation gradients.

The conclusions from this investigation can be drawn as follows: The optimum selection of orifice number for lowest nitric oxide emissions is the result of an optimum matching of two subsequent effects:
• Initial nitric oxide formation rates related to the evaporation behavior and hence rate of heat release in the main combustion phase in combination with the location and extension of the high-temperature regions.

• Late nitric oxide formation rates as a consequence of the oxygen availability in high-temperature regions.

Needless to say that this optimum match additionally depends on the timing of injection, respectively the time available before the ongoing expansion freezes the pollutant concentrations.

6.3.6 Options for Further Development

In 6.3.3.d, the partial inability of the model to correctly predict the effect of modifications in the injection boundary conditions associated with the transition from the conventional Pump-Line-Nozzle to the Common-Rail injection system was traced back to deficiencies of the representation of the turbulent flow field or the turbulence-chemistry interaction model. In the following section, we try to preliminarily assess the relevance of those deficiencies by means of simple numerical experiments.

6.3.6.a Turbulence Model

Since the predictions of the turbulent flow field mainly depend on the quality of the turbulence model, the effect of modifications in the representation of turbulence was tested by means of additional simulations of the PLN and CR test cases employing the standard $k – \varepsilon$ model instead of its RNG variant applied throughout the present investigation (see also discussion in 5.2.1).

Figure 61 shows an analysis of the spatial distribution of turbulent time scale and yet unreleased chemical energy obtained in these simulations for the same time in the cycle as Figure 50.

With the standard $k – \varepsilon$ model, the resulting spray structures are considerably different from the ones observed with the RNG model: The sprays are not propagating freely into the combustion chamber; they rather attach to the cylinder head already shortly after the injec-
The penetration is considerably reduced and the radial expansion from the regions of high chemical energy accordingly increased. In these simulations, the latter regions are forming close to the upper boundary instead of on the original spray axis.

The distribution of turbulent time scales is altered in a similar manner: The regions of low turbulent time scale are no longer concentrated on the spray axis but rather embracing the entire region between the spray core and the adjacent boundary. From these regions, the values are continuously increasing towards cylinder liner and piston bowl.

Such a behaviour cannot be considered realistic. It would result in very poor combustion - in fact, the heat release rate predictions obtained in these simulations indicated very slow combustion in the mixing-controlled phase, in contrast to the experimental data. Moreover, an engine with such a spray propagation characteristic would suffer from severe reliability problems due to burning off from the valve underside.

Figure 61: Spatial distribution of the turbulent time scale (left, in ms) and the yet unreleased chemical energy (right, in J/m³), obtained in simulations with the standard $k-\varepsilon$ model, on a vertical cut through the spray at 10 deg after TDC for the Pump-Line-Nozzle (PLN, top row) and the Common-Rail (CR, bottom row) test cases.
As a conclusion from this comparison we can state that the predictions for both spray and turbulent flow field structure as well as for the resulting rate of heat release and emission characteristic are extremely sensitive to the quality of the turbulence model. Though the RNG $k-\varepsilon$ model yields sensible results in terms of spray structure, the predictive quality with respect to the turbulent flow field remains unclear and may be subject to adaptation of the model parameters. A thorough experimental validation of the prediction of turbulent flow fields induced by injection is therefore highly desirable.

6.3.6.b Turbulence-Chemistry Interaction Model

Assuming an adequate representation of the turbulent flow field with the RNG $k-\varepsilon$ model, the variations in the spatial distribution of the turbulent time scale between the PLN and CR test cases (see Figure 50) suggest an alternative approach for understanding the observed differences: With the PLN case, the minima of the turbulent time scale in the spray core region are lower than with the CR case, thus implying the existence of higher strain rates. It is a known fact that diffusion flames can only exist up to a certain local strain rate level, when the excessive straining leads to quenching of the flame [105]. This behaviour is typically described by means of a critical value of the scalar dissipation rate, which is a function of the fuel type, gas composition and thermodynamic state (see e.g. [23]). The scalar dissipation rate in turn is usually modelled as proportional to the inverse of the turbulent time scale [105].

Hence, in order to simulate this effect, a lower cutoff value for the turbulent time scale was introduced, corresponding to a local maximum rate constraint. Beyond this limit, the reactions were assumed to be quenched and the heat release was suppressed. This approach is not capable of modelling the complex extinction and re-ignition phenomena manifesting in the well-known S-shaped curve of the maximum temperature plotted over the inverse of the scalar dissipation rate (see e.g. [115]). It was hoped, nevertheless, to obtain an indication of the potential of a more detailed description of these effects.
Figure 62 shows the results obtained with this simplistic approach with respect to heat release rate histories and emissions.

Though the effect is rather small (compare Figure 48), the relative underprediction of the mixing-controlled peak with Common-Rail in fact decreased. Note that the hump in the PLN rate of heat release before the final decay due to the end of injection is the result of the local increase in turbulent time scale. As soon as the constraint value is exceeded, the chemical energy available is consumed at the still high local rates, resulting in a recovery of overall burning rate. The need for a more detailed consideration of the transient behaviour in terms of the abovementioned extinction and re-ignition phenomena in order to avoid such unphysical effects is obvious.

The improved quality of the emission predictions can be taken as an additional indication of the potential of a more fundamental approach for modelling the complex interaction of chemistry and turbulence, including transient effects.
7 Conclusions

In the present study, we explored the potential of zero- and three-dimensional models for combustion and nitric oxide formation in medium-speed diesel engines. Both types of model include a large variety of sub-models in order to account for the physical and chemical processes relevant to mixture formation, combustion and the actual pollutant formation. Many of these sub-models were developed in the course of the present work and each of them contributes to the overall performance of the respective full models. Therefore, before starting with the comparative evaluation of the two models, it is worthwhile reviewing the performance of the individual sub-models as well as the respective effects on the global predictive quality of the zero- and three-dimensional simulation methods.

7.1 Sub-Model Performance

Both types of model are based on very similar approaches in terms of modelling of combustion and emission formation:

Ignition is simulated by solving for an ignition progress variable on the basis of the instantaneous (and local, if applicable) chemical time scale for ignition. In the three-dimensional model, this time scale is determined from an approximation of the detailed ignition chemistry of a representative model fuel.

Combustion is modelled by means of approaches based on characteristic time scales of chemistry and turbulent mixing. The premixed phase of combustion directly after ignition is represented as controlled by chemistry and the corresponding time scale, the later phase is considered mixing-controlled and hence associated with the action of the turbulent time scale. The transition from the premixed to the mixing-controlled phase is modelled appropriately on the basis of phenomenological considerations.

The turbulent time scale is derived from the instantaneous (and local, in the three-dimensional model) values of representative turbulence parameters. These parameters are determined from the

7.1 Sub-Model Performance
solution of their evolution equations, based on variants or derivatives of the $k-\varepsilon$ turbulence model.

For the simulation of nitric oxide emission formation, substantially more detailed models of the chemistry in the post-flame region are used than commonly applied in this context. However, the contributions from reactions in the flame, in the form of Prompt- and Fuel-NO, are still neglected, as their inclusion would require yet considerably more comprehensive models of the chemistry of the actual combustion process.

With regard to the performance of these sub-models, the results documented in the previous chapters can be interpreted as follows:

The predictions for ignition, viz. the ignition delay, are always in good agreement with the experimental data. In the case of the three-dimensional model, the model has additionally proven its ability to correctly predict ignition locations in a constant-pressure spray combustion chamber. It has to be emphasized that the simulations for the considerable larger range of conditions encountered in the diesel engine applications, especially with respect to pressure, produced quantitatively correct results in terms of the ignition delays without re-tuning of the model parameters. This confirms the validity of the approach and its wide applicability.

The combustion characteristics obtained in the simulations are, in general, well reflecting the experimentally observed behaviour. In particular, the predictions for the premixed combustion phase as well as the transition to the mixing-controlled phase are in good agreement with the experimental results. In the later combustion phase, however, several limitations were identified:

- The model has not been able to reproduce the effect of the modification of the shape of the injection profile with the transition from the conventional Pump-Line-Nozzle to the Common-Rail system. In contrast to the experiment, where faster combustion with Common-Rail is observed, the simulations predict lower maximum heat release rates in the mixing-controlled phase. These predictions are the consequence of the
higher turbulent time scales (or higher minima in the spatial distribution, in the case of the three-dimensional simulations) yielded by the turbulence models.

- After the end of injection, the turbulent time scales steadily increase. Additionally, in the three-dimensional simulations, the before pronounced spatial distribution is rapidly smoothed. This results in a fast decay of overall burning rates directly after the end of injection, whereas the experimental heat release is only approaching its maximum in this phase. Moreover, the burnout of remaining quantities of unreleased chemical energy is considerably delayed into the expansion phase and the combustion duration is hence severely overpredicted.

These obvious deficiencies of the turbulence models employed here clearly act as a limitation to the performance of the presented simulation approaches. As most combustion models, even the most advanced ones, rely on correct predictions of the turbulent flow field and partly also use the turbulent time scale as an input parameter, the potential of these models for providing better results remains uncertain. Even though we saw in a preliminary test that the consideration of transient flame phenomena may offer a potential to improve the situation. Nevertheless, in view of the present results, further improvements are rather expected from either comprehensive validation studies on the basis of experimental investigations of the structure of the turbulent flow field in transient sprays or more advanced turbulence models.

With respect to the simulation of nitric oxide emission formation, the present study demonstrated, by various means, the relevance of reaction paths in addition to the commonly employed extended Zeldovich mechanism. The resulting more detailed chemistry model involves additional intermediates such as $HO_2$, $NH$, $HNO$, $NO_2$ and $N_2O$. The simulations performed with this model yielded the correct trends in almost all the cases considered. However, one should be aware of the fact that the chemistry model is not the single decisive factor determining the quality of nitric oxide emission predictions.

7.1 Sub-Model Performance
Apart from the detail of the chemistry model, the performance of predictive tools for nitric oxide emission formation in diesel engines depends to leading order on the quality of the predictions of heat release rate histories and hence the combustion model. As a consequence of the high sensitivity of NO formation to temperature, any misprediction of the heat release characteristic results in erroneous evolutions of average temperatures and associated temperature distributions that tend to amplify mispredicted trends.

The third phenomenon of decisive importance for the predictive quality of diesel engine emission formation models is the turbulent mixing between the hot combustion products and the surrounding fresh air. This process controls both the temperature and oxygen distributions and hence the oxygen availability in regions of high temperature. The rate of mixing is thus affecting the predictions of NO formation by means of determining the residence time of combustion products at high temperature and sufficiently high oxygen mass fractions. Note that, in the three-dimensional simulations, this process is represented by the transport processes associated with the turbulent flow field and can hence not be controlled separately. In contrast, in the zero-dimensional model, this mixing process is modelled explicitly, though again uniquely related to the turbulence level via the consideration of the turbulent time scale. Therefore, through appropriate selection of the model constants, the model could be tuned to produce quantitatively correct nitric oxide emission levels in spite of the deficiencies of the combustion model.

7.2 Comparative Evaluation of the Models

In order to assess the potential of the two models for the application in an engine development context, two main factors have to be taken into consideration: On the one hand, the predictive capabilities of the tools in terms of combustion characteristics and nitric oxide emissions. On the other hand, the associated computational effort, which varies considerably between the two methods. Additionally, limitations of the range of applicability have to be taken into account, which are the consequence of the validity of the underlying
assumptions being restricted to particular configurations (e.g. the assumption of a single representative spray in the case of the zero-dimensional model).

When considering a single operating condition as a reference, the performance of the two models in terms of the prediction of combustion characteristics is very similar: With the zero-dimensional model, only the peak level of the heat release rate in the main combustion phase is slightly higher, then followed by a correspondingly faster decay of burning rates than observed in the three-dimensional simulation. As already mentioned, both methods tend to underpredict burning rates in the phase directly after the end of injection, which has a strong impact on emissions predictions: In this phase, the temporal gradient of $NO$ formation takes on the highest values. As we noted above, this effect can be compensated with the zero-dimensional model by adapting the model parameter controlling the mixing of the combustion products and the remaining fresh gas. In the case of the three-dimensional model, however, such a tuning option is not available and the computed nitric oxide emission is considerably below the experimental data.

With respect to trends with variations of operating conditions, with the exception of modifications of the injection system, similar considerations apply: Both models are able to predict variations of the heat release rate pattern in a qualitatively correct manner and the trends in $NO$ emissions are, in general, also reproduced correctly. However, with the three-dimensional model, the emission trends are considerably overpredicted, whereas the zero-dimensional model yields even quantitatively correct predictions in most cases.

Both methods proved unable to predict the effect of the strong variations in the injection boundary conditions associated with the transition from the conventional Pump-Line-Nozzle to the Common-Rail injection system in a satisfactory manner. Whereas the computed variations of the shape of the rate of heat release history are still in accordance with the experimental observations, the variation in the height of the peak of the experimental heat release pattern is not reproduced. In this particular case, the zero-dimen-
sional model even suggests a wrong trend of the nitric oxide emissions, in contrast to the three-dimensional simulation.

Scaling effects between similar engines of different size cannot be quantitatively reproduced with either type of model. It is interesting to note, however, that the mere adaptation of one single model parameter, the weighting factor for the turbulent time scale in the determination of the instantaneous (and local, if applicable) burning rates, yields the correct prediction of the trends both with respect to heat release histories and nitric oxide emissions.

The zero-dimensional model fails to predict the effect of injector geometry variation, whereas the three-dimensional simulations suggest the correct trends, both in terms of engine efficiency and nitric oxide formation, though the latter effect is again overestimated.

The predictive qualities of the two models have to be set against the associated effort, in particular the time required for one simulation: Under the conditions applied in the present work in terms of number of zones used in the zero-dimensional simulations and spatial resolution employed with the three-dimensional model, the response times associated with the two models were as follows: For identical hardware (R8000 processor), simulation times with the zero-dimensional model were in the 10 to 20 minutes range, whereas the three-dimensional simulations typically lasted between 16 and 24 hours.

Hence, when considering the achievable accuracy in combination with the short response time, a well-tuned zero-dimensional model is the method of choice for fast potential estimating investigations, in particular for variations in global initial conditions such as charge air composition and thermodynamic state at the start of compression. Even for investigations of effects of (minor) modifications of the injection boundary conditions, it may already yield sufficient insight in order to allow the elimination of less promising concepts. By nature, zero-dimensional models are less suitable for the investigation of effects associated with more complex, geometry-related phenomena such as interactions of individual sprays and the interaction of
sprays with combustion chamber walls, which has not been addressed here.

It has to be mentioned that the above figures are obviously subject to changes as a result of the continuous further expansion of computational resources. The use of today’s hardware capacities easily allows to reduce these numbers by a factor of four when compared to the hardware available at that time. Therefore, the effort for three-dimensional simulations is considerably reduced in the meantime, allowing either the simulation of a larger number of variants or the use of further refined grids or more complex sub-models.

The strong point of three-dimensional models is their ability to deal with more complex systems involving interactions of multiple sprays such as observed in the investigation of the injector geometry effect or as encountered in large two-stroke diesel engines. In fact, a recent study demonstrated the potential of such a tool in the development process of those engines [158]. Moreover, they allow to study other, more complex configurations, e.g. multiple sprays associated with different initial or boundary conditions or even non-identical composition ([159], [160]). Even if the predicted trends may again be overestimated, these simulations nevertheless help to identify the most promising concepts and thus to narrow the range of variants to be investigated experimentally. Their application may hence result in considerable savings of testbed time and cost as well as overall development time.

Another important field of application of three-dimensional simulations of combustion and emission formation is the isolated study of complex spray-spray and spray-wall interaction effects under idealized conditions. As the investigation of the effect of number and size of injector orifices at constant total cross-section in a constant-volume combustion chamber showed, the elimination of superimposing effects allows to obtain important additional insight into the basic mechanisms and the relevance of local effects. This insight may then be used either as a starting point for further simulations for more realistic configurations or directly for the derivation of corresponding design rules.

7.2 Comparative Evaluation of the Models
Generally, both models require to some extent tuning in order to be able to reproduce the particularities in the behaviour of an individual engine. However, with the three-dimensional model, the number of tuning parameters and options is considerably lower than with the zero-dimensional model, where, additionally, the effort required for tuning the model to one particular engine configuration must not be underestimated.
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Appendices
A Reaction Mechanisms for Thermal NO Formation

The basic reaction mechanisms applied in the zero- and three-dimensional simulations together with the individual reduction steps are presented below.

A.1 Zero-Dimensional Simulation

The following table lists the fundamental reactions in the $H-N-O$ system as well as the reactions governing the combustion of $CO$ considered in the simulations as proposed by Miller and Bowman [64].

The first five columns serve for the indication of reactions employed in the various reduced mechanisms studied in 6.2.1.b. The kinetic data refer to the standard Arrhenius rate constant formulation, employing the activation energy $E_A$

$$k_{Arr} = A \cdot T^b \exp\left(\frac{-E_A}{RT}\right).$$

$A$ units are in mole/cm$^3$/sec/K$^b$, $E_A$ units in cal/mole, all data referring to the forward reaction.

In third-body reactions, the enhancement factors of the individual species are supplied, if applicable and different from unity.

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### Reaction Mechanisms for Thermal NO Formation

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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N$_2$H$_2$+O=NNH+OH</td>
<td>2.00E+13</td>
<td>0.0</td>
<td>1000.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N$_2$H$_2$+OH=NNH+H$_2$O</td>
<td>1.00E+13</td>
<td>0.0</td>
<td>1000.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N$_2$H$_2$+NO=N$_2$O+NH$_2$</td>
<td>3.00E+12</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N$_2$H$_2$+NH=NNH+NH$_2$</td>
<td>1.00E+13</td>
<td>0.0</td>
<td>1000.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N$_2$H$_2$+NH$_2$=NH$_3$+NNH</td>
<td>1.00E+13</td>
<td>0.0</td>
<td>1000.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A.1 Zero-Dimensional Simulation

A 3
A.2 Three-Dimensional Simulation

The following tables list equilibrium and kinetic reaction data as employed in the 3-D simulations.

### A.2.1 Equilibrium Reactions

In order to allow for species associated with incomplete combustion and dissociation, the following set of equilibrium reactions was curated:

<table>
<thead>
<tr>
<th>Reaction</th>
<th>A</th>
<th>b</th>
<th>$E_A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HNO+M=H+NO+M</td>
<td>1.50E+16</td>
<td>0.0</td>
<td>48680.0</td>
</tr>
<tr>
<td>HNO+OH=NO+H2O</td>
<td>3.60E+13</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>HNO+H=NO+H2</td>
<td>5.00E+12</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>HNO+NH2=NO+NH3</td>
<td>2.00E+13</td>
<td>0.0</td>
<td>1000.0</td>
</tr>
<tr>
<td>HNO+HNO=N2O+H2O</td>
<td>4.00E+12</td>
<td>0.0</td>
<td>5000.0</td>
</tr>
<tr>
<td>HNO+NO=N2O+OH</td>
<td>2.00E+12</td>
<td>0.0</td>
<td>26000.0</td>
</tr>
<tr>
<td>N+NO=N2+O</td>
<td>3.30E+12</td>
<td>0.3</td>
<td>0.0</td>
</tr>
<tr>
<td>N+O2=NO+O</td>
<td>6.40E+09</td>
<td>1.0</td>
<td>6280.0</td>
</tr>
<tr>
<td>N+OH=NO+H</td>
<td>3.80E+13</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>NO+HO2=NO2+OH</td>
<td>2.10E+12</td>
<td>0.0</td>
<td>-479.0</td>
</tr>
<tr>
<td>NO2+H=NO+OH</td>
<td>3.50E+14</td>
<td>0.0</td>
<td>1500.0</td>
</tr>
<tr>
<td>N2O+H=N2+OH</td>
<td>7.60E+13</td>
<td>0.0</td>
<td>15200.0</td>
</tr>
<tr>
<td>N2O+M=N2+O+M</td>
<td>1.60E+14</td>
<td>0.0</td>
<td>51600.0</td>
</tr>
<tr>
<td>N2O+O=N2+O2</td>
<td>1.00E+14</td>
<td>0.0</td>
<td>28200.0</td>
</tr>
<tr>
<td>N2O+O=NO+NO</td>
<td>1.00E+14</td>
<td>0.0</td>
<td>28200.0</td>
</tr>
<tr>
<td>N2O+OH=N2+HO2</td>
<td>2.00E+12</td>
<td>0.0</td>
<td>10000.0</td>
</tr>
</tbody>
</table>

Note that the backward reaction rates are determined from the forward reaction rates and the equilibrium constants of the individual reactions.
applied. The equilibrium data refer to the formulation of the concentration equilibrium constant $K_c$ as a function of temperature as employed in KIVA-3

$$\ln K_c = C_1 \ln T_n + \frac{C_2}{T_n} + C_3 + C_4 T_n + C_5 T_n^2,$$

where $T_n = T/1000$.

The individual constants were determined from the polynomial fits to the thermodynamic properties of the involved species as documented in [161], based on the JANAF tables [162] data.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
<th>$C_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>O2+2CO=2CO2</td>
<td>0.159512</td>
<td>68.16329</td>
<td>-10.7052</td>
<td>1.056709</td>
<td>-0.077514</td>
</tr>
<tr>
<td>O2+2H2=2H2O</td>
<td>-3.336134</td>
<td>56.8944</td>
<td>-0.787086</td>
<td>1.711533</td>
<td>-0.113220</td>
</tr>
<tr>
<td>O2+H2=2OH</td>
<td>-0.923541</td>
<td>-9.84274</td>
<td>3.944509</td>
<td>0.301089</td>
<td>-0.023534</td>
</tr>
<tr>
<td>O2+H2O=OH+HO2</td>
<td>0.585198</td>
<td>-34.8621</td>
<td>2.426098</td>
<td>-0.193372</td>
<td>0.010851</td>
</tr>
<tr>
<td>O2=2O</td>
<td>0.38654</td>
<td>-59.6955</td>
<td>3.502861</td>
<td>-0.319386</td>
<td>0.014215</td>
</tr>
<tr>
<td>H2=2H</td>
<td>1.008577</td>
<td>-51.7783</td>
<td>0.973202</td>
<td>-0.352458</td>
<td>0.011756</td>
</tr>
</tbody>
</table>

### A.2.2 Finite Rate Reactions

The reactions listed below correspond to the part of the kinetic scheme related to NO formation with the first reduction step employed in the zero-dimensional simulation.

In contrast to the formulation above, the kinetic constants used in KIVA-3 relate to the modified form of the Arrhenius rate constant formulation

$$k_{Arr} = A \ T^b \exp\left[\frac{T_A}{T}\right],$$

with the activation temperature $T_A$ in K.

Moreover, the kinetic data of the reverse reactions have to be specified explicitly. These were determined from the kinetic data of the forward reactions and their equilibrium constants applying Mechmod [163], fitting to temperatures 1000, 1750 and 2500 K.
<p>| | | | | | |</p>
<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>NH+O2=&gt;HNO+O</td>
<td>1.00E+13</td>
<td>0</td>
<td>6039.26</td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>HNO+O=&gt;NH+O2</td>
<td>1.86E+14</td>
<td>-0.31</td>
<td>7187.61</td>
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</tr>
<tr>
<td>V</td>
<td>NH+O2=&gt;NO+OH</td>
<td>7.60E+10</td>
<td>0</td>
<td>770.01</td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>NO+OH=&gt;NH+O2</td>
<td>5.93E+09</td>
<td>0.21</td>
<td>27942</td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>NH+NO=&gt;N2O+H</td>
<td>2.40E+15</td>
<td>-0.8</td>
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<tr>
<td>V</td>
<td>N2O+H=&gt;NH+NO</td>
<td>5.73E+21</td>
<td>-1.92</td>
<td>18071.55</td>
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<tr>
<td>V</td>
<td>NH+OH=&gt;HNO+H</td>
<td>2.00E+13</td>
<td>0</td>
<td>0</td>
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<tr>
<td>V</td>
<td>HNO+H=&gt;NH+OH</td>
<td>1.43E+17</td>
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<tr>
<td>V</td>
<td>NH+OH=&gt;N+H2O</td>
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<tr>
<td>V</td>
<td>N+H2O=&gt;NH+OH</td>
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<tr>
<td>V</td>
<td>NH+H=&gt;N+H2</td>
<td>1.00E+14</td>
<td>0</td>
<td>0</td>
<td></td>
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<tr>
<td>V</td>
<td>N+H2=&gt;NH+H</td>
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<tr>
<td>V</td>
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<td>0</td>
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</tr>
<tr>
<td>V</td>
<td>NO+H=&gt;NH+O</td>
<td>6.02E+14</td>
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</tr>
<tr>
<td>V</td>
<td>HNO+M=&gt;H+NO+M</td>
<td>1.50E+16</td>
<td>0</td>
<td>24499.25</td>
<td></td>
</tr>
</tbody>
</table>

| H2O Enhanced by 1.000E+01 |
| O2  Enhanced by 2.000E+00 |
| N2  Enhanced by 2.000E+00 |
| H2  Enhanced by 2.000E+00 |

|   | H+NO+M=>HNO+M | 2.73E+13 | 0.54 | -1100.43 |

| H2O Enhanced by 1.000E+01 |
| O2  Enhanced by 2.000E+00 |
| N2  Enhanced by 2.000E+00 |
| H2  Enhanced by 2.000E+00 |

<p>|   | HNO+OH=&gt;NO+H2O | 3.60E+13 | 0 | 0 |
|   | NO+H2O=&gt;HNO+OH | 1.49E+13 | 0.24 | 34940.88 |
|   | HNO+H=&gt;NO+OH | 5.00E+12 | 0 | 0 |
|   | NO+H2=&gt;HNO+H | 3.05E+10 | 0.57 | 26903.91 |
|   | HNO+NO=&gt;N2O+OH | 2.00E+12 | 0 | 13085.05 |
|   | N2O+OH=&gt;HNO+NO | 6.67E+14 | -0.4 | 21359.55 |
|   | N+NO=&gt;N2+O | 3.30E+12 | 0.3 | 0 |
|   | N2+O=&gt;N+NO | 6.68E+12 | 0.4 | 37707.29 |</p>
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<td>✓</td>
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<td>NO+H→N+OH</td>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>NO+HO₂→NO₂+OH</td>
<td>2.10E+12</td>
<td>0</td>
</tr>
<tr>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>NO₂+OH→NO+HO₂</td>
<td>8.45E+12</td>
<td>0.02</td>
</tr>
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<td>✓</td>
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<td>✓</td>
<td>NO₂+H→NO+OH</td>
<td>3.50E+14</td>
<td>0</td>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
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<td>NO+OH→NO₂+H</td>
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<td>✓</td>
<td>N₂O+H→N₂+OH</td>
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<td>N₂O+M→N₂+O+M</td>
<td>1.60E+14</td>
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<td>✓</td>
<td>N₂O+O→N₂+O₂</td>
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<td>0</td>
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<td>✓</td>
<td>✓</td>
<td>N₂O+O→2NO</td>
<td>1.00E+14</td>
<td>0</td>
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<td>✓</td>
<td>✓</td>
<td>2NO→N₂O+O</td>
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<td>0.92</td>
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<td>✓</td>
<td>✓</td>
<td>N₂O+OH→N₂+HO₂</td>
<td>2.00E+12</td>
<td>0</td>
</tr>
<tr>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>N₂+HO₂→N₂O+OH</td>
<td>1.39E+10</td>
<td>0.48</td>
</tr>
</tbody>
</table>

A.2 Three-Dimensional Simulation
B Notes on the Quality Requirements for Experimental Data for the Validation of Engine Simulation Results

The establishment of quantitative reference data for the validation of simulation results is substantially more demanding than the common determination of engine performance data, which relies on standard measurement procedures and often yields a rather qualitative instead of quantitative evaluation of engine behaviour. One has to be aware that quantitative reference data are not only needed for comparison with the simulation results, but also for the assessment of initial and boundary conditions. Potential uncertainties can result both from an inadequate global setup of the experiment and from the application of measurement techniques or evaluation methods that do not yield sufficiently exact and reliable data.

B.1 Setup of the Experiment

In general, single-cylinder experiments yield the better reference data than experiments on multi-cylinder engines, since the measured mass fluxes of both fuel and air as well as the power output and potential heat balance measurement data can be associated uniquely with this single cylinder. However, this requires a stable running condition of the engine at operating conditions representative of the operation of a corresponding multi-cylinder engine, and measurement techniques apt to handle the high temporal fluctuations of multiple system parameters. Since these latter conditions are often very difficult to fulfil, most experiments are, in spite of the serious drawbacks, performed on multi-cylinder engines.

Nevertheless, reliable reference data can be obtained on multiple-cylinder setups as well. However, this requires a substantially higher effort:

The assessment of the distribution of the individual mass fluxes among the cylinders actually requires measurements in the inlet and exhaust pipes as well as in the fuel systems of the individual cylin-
ders. However, such a procedure is associated with a major drawback: Especially in the air system, it can hardly be realized without affecting the system behaviour. Additionally, these flows are highly instationary and therefore, the actual fluxes cannot be determined by means of conventional methods well-proven for stationary flows.

Another difficulty is the determination of the contributions of the individual cylinders to the engine output in terms of power, emissions and heat rejection. Whereas the latter is not expected to vary significantly from cylinder to cylinder, both power output and emissions can exhibit substantial variations.

The contributions of the individual cylinders to the total power output can basically be estimated from their cylinder pressure analysis; however, this requires a full instrumentation of all the cylinders.

The emissions would have to be measured again in the exhaust pipes of the individual cylinders, which is very expensive on the one hand and difficult to realize on the other hand. These difficulties arise both from the limited access due to spatial restrictions and from the nature of the flow in those pipes, which is highly instationary (and spatially inhomogeneous). Especially for nitric oxides, to date no experimental technique exists that allows the fast, time- and space-resolved concentration measurements that would be required for sufficiently exact reference data.

If an external exhaust gas recirculation (EGR) is applied, the task is even more difficult, because the distribution of the recirculated gas among the cylinders has to be determined additionally, with the same problems as mentioned above for the cylinder-resolved emission measurements.

**B.2 Measurement Techniques**

A high quality standard of the instrumentation as well as of the experimental procedures is another prerequisite for the generation of reference data. Obviously, neglecting this rule, even if only in a single aspect, puts the quality of the entire experiment into jeopardy. The determination of mass fluxes both in the air and fuel systems, the
measurement of charge air component and emission concentrations as well as the establishment of the cylinder pressure history can be identified as the major sources of inaccuracies.

As already noted previously, the measurement of instationary mass flows is rather difficult. In most cases, the problem is tackled by introducing additional, adequately sized reservoirs into the system in order to damp out the oscillations. In the air system, this allows to transform instationary flows close to the cylinders into practically stationary ones at the side of the reservoir facing the ambience. In the fuel system, the reservoir is typically connected to a balance and fed discontinuously, thus allowing the gravimetrical determination of the fuel consumption. Inherently, both methods are only applicable for the investigation of stationary operating conditions and additionally require a stable running condition of the engine for representativity. A second aspect of these methods is the fact that the size and complexity of the system are increased considerably, with the consequence of a correspondingly higher risk of leakage.

Most experimental techniques for the measurement of concentrations require controlled conditions in a probe volume, which is fed discontinuously with small quantities of the gas to be examined. One of the problems of these techniques is their high sensitivity: The instruments have to be re-calibrated frequently. Another difficulty is again associated with the instationary character of the flows they are applied to: Either the probes are taken from a reservoir that can be assumed in a homogeneous state or they have to be taken from a part of the system that can neither be considered stationary nor homogeneous. In that latter case, the representativity of the results has to be secured through comprehensive validation experiments. It goes without further explanation that the placement of the sensors does greatly affect the quality of the results. Remember that time- and space-resolved measurements are virtually impossible.

Though time-resolved cylinder pressure measurements have been performed for decades, they still constitute a major source of uncertainty. Medium-sized to large engines are usually equipped with an
indicator cock, i.e. an external tube of small diameter, which is directly connected to the combustion chamber. This allows to place the pressure gauge at the closed, cold end of this tube and hence to measure at sufficiently low temperatures. However, apart from the possible superposition of tube-internal pressure fluctuations due to acoustic waves, this method exhibits another drawback: As a consequence of the non-negligible distance between the combustion chamber and the pressure sensor, the unique association of the crank angle and pressure signals is not possible any more. If the pressure sensor is mounted flush with the combustion chamber surface, this problem is circumvented. However, at this position, the sensors are exhibited to very high temperature fluctuations and, depending on their location, possibly also to high absolute values. Both hamper the sensor behaviour considerably; only through frequent re-calibration and efficient sensor cooling an adequate quality of the signals can be granted.

B.3 Evaluation Methods for Experimental Data

Numerous measured quantities require additional processing in order to obtain the data of interest. These processing steps often rely on simplifying assumptions and partly even involve a considerable modelling expense.

As an example, the composition of the cylinder charge during compression can neither be measured directly in a non-intrusive manner nor is it uniquely defined through the charge air composition, even if the latter can be measured in the inlet channel. It either requires the assumption of a scavenging efficiency and of a purity of the charge or the simulation of the scavenging process (or even better of the entire cycle) in order to determine the amount of residual gas in the cylinder. The same applies to the cylinder charge conditions at IVC in general, which typically serve as initial conditions for the simulations: They have to be determined either from empiric correlations with the state in the inlet manifold or by means of scavenging process, respectively full cycle simulations.
The uncertainty in terms of cylinder charge composition is even increased with EGR. As mentioned previously, the measurement of flow rates commonly involves the introduction of reservoirs in order to homogenize the flow. In EGR systems, both the spatial limitations and the associated pressure drops are virtually prohibitive for this approach. Therefore, the EGR rate is determined indirectly from the \( CO_2 \) concentrations in the inlet and exhaust manifolds. This procedure implicitly includes the assumption of negligible changes in the composition of the recirculated gas in the EGR system. In reality, however, especially in systems with EGR cooling, the water is removed to a considerable extent from the recirculated exhaust gas flow. Hence, the composition of the recirculated gas varies in a non-negligible manner between the inlet and the exhaust manifolds.

The fuel injection rate as well cannot be measured directly. In most experiments, the pressure history in one or several locations in the injection system is monitored together with the lift of the injector needle. From these data the effective injection rates have to be determined again either through empiric correlations or through detailed hydraulic simulations of the injection system. These in turn require the knowledge of the cylinder pressure evolution.

The problems of cylinder pressure measurements, which originate from the temperature sensitivity of the sensors, have already been addressed in the previous section. In the evaluation process, several additional complications arise:

Firstly, the signal from the pressure transducers is differential and therefore requires referencing in order to obtain absolute values. The pressure in the inlet manifold, which can be measured quantitatively and exhibits comparatively small fluctuations (in multi-cylinder engines!) is commonly employed as the reference value. However, the timing in the cycle, when the pressures in the manifold and in the cylinder can be set equal, remains to be identified. This again requires assumptions with respect to the flow through the inlet valve or again simulations of the scavenging process or of the entire engine cycle.
Secondly, strong oscillations may superimpose on the cylinder pressure signal. These originate from combustion-generated pressure oscillations on the one hand and component stress variations acting on the sensor on the other hand. Additionally, the general noise from the measurement system and structural vibrations resulting from the moving parts of the engine, e.g. the closing of the valves, hamper the signal quality. Since the frequency spectra of the signal of interest and of the jamming signals partly overlap, a complete and reliable separation of the two is not always feasible.

Finally, in order to determine the rate of heat release from the processed pressure signal, a simulation of the engine cycle has to be performed. Here again, initial and boundary conditions have to be assumed appropriately, preferably in conjunction with an iterative procedure. For simplicity, the simulation is usually based on a single-zone model, which strongly affects the comparability to results from spatially resolved simulations, as noted in 6.1.
C Notes on Resolution Effects on the Results of the Three-Dimensional Model

As a consequence of the formulation of various models and of the numerical techniques employed in KIVA-3, the solutions obtained with the present three-dimensional model cannot be expected to be resolution-independent.

C.1 Limiting Aspects

In particular, the following procedures and modelling aspects act as limitations with regard to the achievable accuracy (compare 5.1):

The strict overall prescriptions with respect to block structure do not always allow to use the grid best suited to the problem under consideration. Especially, as full connectivity is required and hence local refinement in regions with high spatial gradients can hardly ever be realized. In combination with the additional restrictions associated with the procedures for cell activation and deactivation, these prescriptions additionally act as strong limitations in terms of the complexity of model geometries that can be handled at all by the code.

The stepwise procedure employed by the ALE solution method inherently precludes implicitness in time. Also, the source terms due to spray and chemistry are determined explicitly and, to some extent, related to the rather arbitrary sequence of droplets and reactions. Moreover, the orders of the spatial discretization schemes available are rather low, which, to some extent, additionally limits the achievable accuracy.

The neglect of the volume of the droplets (see 2.4.1) in the solution of the gas phase already introduces some error, particularly for the dense spray regions. The procedures employed in coupling the solution of the two phases, where a unique association of the individual droplets and a single computational cell is assumed, are adding onto that. In particular, the consideration of the evaporation-model-related source terms in the cell, where the individual droplet resides,
imposes some limitations to the spatial discretization in regions with high amounts of liquid: If these regions are too well-resolved, the overall solution becomes unstable, as the automatic adaptation of the time step (see C.2 below) is no longer able to prevent divergence of the solution in individual cells as a result of sudden, substantial changes in spray source terms. These changes typically originate from discontinuous effects related to the droplet distribution function in combination with the high values of the source terms relative to the cell’s energy and mass content. Note that, for high spatial resolution, the movement of a vaporizing droplet into a cell, which was not exposed to evaporation in the previous timestep (and vice versa), also represents such a discontinuous effect.

In fact, most spray sub-models are inherently grid-dependent. This is specifically true for the collision model, where the collision probability is clearly related to the grid dimensions: First, the overall probability is dependent on the resolution, as collisions are only allowed for droplets residing in the same computational cell. Though this effect is partly compensated by the second, local resolution dependence, present in the formulation of the local collision probability as a function of the cell dimensions (38), we can hardly expect these two effects to cancel out each other on a global scale.

In the following sections, both the sensitivity to temporal and spatial resolution are discussed, including the identification of the major sources to those sensitivities. Potential improvements and a best-practice approach for simulations with the present status are proposed.

C.2 Temporal Resolution

KIVA-3 uses an adaptive time-stepping scheme, where the timestep for each successive computational cycle is computed considering the solution of the previous cycle in view of various accuracy-related constraints. These include maximum allowed local values of the strain rate, the chemistry and evaporation source terms as well as some kind of convective stability criterion. Furthermore, the timestep is adapted in order to exactly match the timing of par-
ticular events, e.g. the start of injection. An user-prescribed maximum value of the timestep serves as the upper limit and the growth of the timestep from cycle to cycle is additionally restricted.

This method is supposed to limit the effect of the largely explicit formulation of the solution procedure and has proven to be very computationally efficient. However, some sensitivity to the temporal resolution must be assumed. This has been investigated by varying the maximum allowed timestep with the S20 full load Miller operating condition case. The values tested range from 3.0E-7 to 1.0E-4 seconds.

Figure A1 shows the comparison of the most important simulation results obtained with the various values of the maximum allowed timestep: Whereas the pressure curves and rate of heat release histories are predominantly sensitive to reduction of the upper limit timestep to 1.0E-6 s and below, the emission formation predictions apparently exhibit a strong sensitivity to the maximum timestep throughout the range of values investigated. Particularly striking is the non-monotonous behaviour.

Figure A1: Comparison of key results for the S20 full load Miller case with various maximum timesteps, in stop left: pressure, bottom left: ROHR, top right: $NO + NO_2$. 

C.2 Temporal Resolution
The pressure curves with maximum timesteps above 1.0E-6 s show only minor variations in the initial phase, they all achieve the same peak pressure. With 1.0E-6 s, the peak pressure is underpredicted by almost 10 bar, further reduction of the maximum timestep increases the deviation.

The comparison of the rate of heat release histories gives a clearer picture of the effect: Decreasing the maximum timestep mainly affects the premixed peak - with the higher values, the initial increase of the burning rate is first slowed down until, eventually, lower peaks result. The main combustion phase is only affected with the very small timestep.

Hence, the underprediction of the peak pressure is, with 1.0E-6 s, only due to the underestimation of the premixed peak, whereas, in the 3.0E-7 s case, it is the result of an overall underprediction of burning rates.

With the lower maximum timesteps, the underprediction of the peak pressure is associated with clearly reduced $NO + NO_2$ emission predictions. Also, the relatively small deviation of the resulting values with 5.0E-6 and 1.0E-5 s may be attributed to the already noticeable difference in the premixed peak and its effect on temperature. The considerably lower value with the largest timestep, however, can no longer be explained by means of thermodynamic effects. It must rather be attributed to deficiencies of the numerical scheme, e.g. the explicit determination of source terms due to spray and chemistry.

In order to better understand the underlying phenomena, the actual timesteps used during the simulation have to be considered (left diagram in Figure A2): Four phases can be distinguished:

- Before start of injection (ca 12.5 deg CA before TDC), the timestep is at the maximum level.
- Between start of injection and ignition (occurring at ca 7.5 deg CA before TDC), the actual timestep takes on values slightly below 1.0E-5 s with maximum timesteps of 1.0E-5 s and above. It is only at a lower level when the upper limit is
From ignition to the end of injection (ca 16.5 deg CA after TDC), the timestep oscillates around 1.0E-6 s with high maximum timesteps. With lower values, the prescribed maximum acts as an upper limit to the oscillations, however, at the same time, the range of the oscillations is extended to lower values.

After the end of injection, the timestep returns to the maximum level and remains there throughout the expansion stroke.

The phase between start of injection and ignition must be considered essential for the establishment of the initial spray structure. Differences between the individual cases can, therefore, be expected to manifest themselves in variations of the spatial distribution of droplets and fuel vapour as well as the evaporation behaviour. Note that the abovementioned modifications of the premixed phase with reduced maximum timesteps already indicate the existence of such differences.

The right-hand side diagram in Figure A2 shows the evaporation behaviour observed with the various cases by representing the respective evolutions of the liquid fraction of the total instantaneous fuel mass (liquid, gaseous and burnt) inside the computational domain.
As expected, the evaporation behaviour with the two very large timesteps is practically identical. With 5.0E-6 s, the evaporation is already slightly slowed down and considerably further impaired when decreasing the maximum timestep even more. With those timesteps, even in the later injection phase, higher liquid mass fractions are observed.

Figure A3 shows a comparison of the spatial distribution of the yet unreleased chemical energy (compare 5.4.2.b) and the droplets at TDC obtained with the four smaller values of the maximum timestep. The size of the droplet symbols represents the radius of the spherical volume containing all droplets of the respective representative particles, enlarged by a factor of ten for better visualization.

With decreasing maximum timestep, two effects are apparent: On the one hand, the spray is becoming slimmer, in combination with a slight increase in penetration. On the other hand, the penetration of the liquid phase in the injector region is growing as well, shifting the location of high chemical energy, respectively fuel concentration, further downstream into the combustion chamber. Moreover, with very low maximum timesteps, the droplets are not completely evaporated in the near-nozzle region, but an aggregate of large, slowly evaporating droplets is travelling behind the tip of the spray.

All these effects point to the collision model, respectively its interaction with the breakup model, as the source of the problem:

Large droplets can only survive if they do not meet the breakup condition, i.e. if their relative velocity to the surrounding gas phase is sufficiently small. Such droplets can, however, only form through coalescence of smaller droplets already largely relaxed to the velocity of the induced flow. With smaller timesteps, the (overall) collision, hence coalescence probability is increased as the condition for the evaluation of collision probability, viz. the residence of pairs of representative droplet in the same computational cell, is met much more frequently. Therefore, despite the fact that the local and instantaneous collision probability is formulated timestep-dependent (38), the overall probability is increased.
Figure A3: Spatial distribution at TDC of droplets and yet unreleased chemical energy (in J/m$^3$) on a vertical cut through the spray, with various selections of the maximum timestep (in s).
As a consequence, the smaller timesteps promote the formation of large droplets travelling at the velocity of the surrounding fluid and hence poorly evaporating. This is particularly true during ignition, when the evaporation is not yet dominating in the breakup region. The large droplets close to the spray tip, observed in the 1.0E-6 and 3.0E-7 s cases, must therefore be considered residuals from that phase. Afterwards, the high temperatures due to combustion enhance the evaporation of product droplets from breakup, such that they do no longer have enough time to aggregate. The absence of any droplets between the breakup region and the drops at the spray tip supports this consideration.

The increasing length of the column of liquid droplets in the near-nozzle region together with the corresponding shift of the region of highest chemical energy indicate a decay in the performance of the spray breakup model with decreasing maximum timestep. This decay must, however, again be considered in the context of the collision model, respectively its interaction with the breakup model:

Recall that the spray breakup is modelled via delaying the first breakup of the injected drops (see 5.2.2). Since the deviation of the initial velocity between subsequently injected droplets is only moderate, the relative velocity for pairs of droplets is correspondingly small in the near-nozzle region. This relative velocity is decisive in the determination of the collision probability (38), the low values thus reduce the frequency of collisions, in particular in combination with a monomodal dropsize distribution at injection, as used in the first version of the breakup model [50]. In the further enhanced version employed in the present investigation, an initial dropsize distribution allowing also for droplets smaller than the injector orifice was introduced, which enabled better predictions of evaporating and reacting spray behaviour [90].

The departure from the monomodal distribution, however, also eliminates the ‘automatic’ prevention of collisions between droplets before the breakup region, as the smaller droplets are more rapidly relaxed and relative velocities hence increase. Therefore, droplets not yet having reached their breakup time may coalesce and hence
loose their deformation properties, which define their breakup time and the product droplets’ perpendicular velocity after breakup. Remember that the latter controls the overall spray angle (c.f. 5.2.2).

This may not have a strong effect with usual selections of the maximum timestep, since only a few droplets may be concerned. However, if collisions are again promoted, both the breakup length and the spray angle predictions will be affected. At first sight, it may be surprising that the breakup length is apparently increased instead of decreased. However, again we have to consider the effect of enhanced coalescence of small, largely relaxated droplets: Before ignition, coalescence is dominating the evaporation and hence shifting the region of ignition further away from the injector. This shift cannot be reversed in the later phase, as the location of the ignition sites also determines the regions of subsequent combustion - the high-temperature regions cannot propagate sufficiently far upstream the spray in order to overcome the dominance of coalescence in the near-nozzle region.

As a conclusion from these considerations, we can state that a sufficiently large maximum timestep should be selected in order to minimize the potential negative effects of the collision model. A more fundamental approach would require detailed investigations into the behaviour of the collision model. As an intermediate solution, the collision of droplets not yet having reached their initial breakup time could be excluded. This already promises to largely eliminate the abovementioned effects of the maximum timestep on breakup length and spray angle.

C.3 Spatial Resolution

The sensitivity of the results of the three-dimensional model to spatial resolution was assessed through individually varying the resolution in the radial, vertical and azimuthal directions. For this purpose, the number of cells in the standard geometry was decreased and increased by a factor of two, respectively. The resolution of the standard geometry was selected as: 24 cell layers in radial, 10 (head) plus 4 (bowl) plus minimum 2 (squish region) in vertical and 9 in azi-
muthal direction. All the simulations refer to the full load case of the S20 engine operated with the Miller system, however neglecting the effect of the compression stroke, employing appropriately adapted initial conditions shortly before start of injection.

**C.3.1 Resolution in Radial Direction**

Figure A4 shows the comparison of key results obtained with the variation of radial resolution, viz. pressure, rate of heat release and nitric oxide concentration histories. A strong sensitivity of both peak pressure and nitric oxide emission predictions is obvious. Whereas the timing of ignition and the height and extent of the premixed peak are almost insensitive, the mixing-controlled phase of combustion is strongly reacting to variations in radial resolution.

![Figure A4: Comparison of key results for the S20 full load Miller case with various degrees of radial resolution, top left: pressure, bottom left: ROHR, top right: $NO + NO_2$.](image)

In order to analyse this effect in more detail, the distributions of yet unreleased chemical energy and turbulent time on a vertical cut plane through the spray at 2 deg after TDC with the various cases are compared in Figure A5.
Obviously, the predicted spray structure varies with radial resolution: Whereas, in the low-resolution case, the spray is penetrating almost linearly along the axis prescribed by the injector orifice orientation, a slight deflection towards the cylinder head is already observed with the standard resolution. In the high-resolution case, the intermediate part of the spray is almost attached to the upper boundary, only the tip remaining on the original axis.

The range of turbulent time scales is practically unaltered, their spatial distribution, however, reflects the modified spray propagation with increased radial resolution: The turbulent time scale isolines, still resembling spray contours with the low-resolution case, open towards the cylinder head and are eventually flattening in this direction with increasing resolution. As a consequence, the gradient along the (theoretical) spray axis is getting steeper with increasing resolution and the burning out of the yet unreleased chemical energy closer to the spray tip is hence slowed down.

Figure A5: Spatial distributions of turbulent time scale (in ms, left column) and yet unreleased chemical energy (in J/m$^3$, right column) on a vertical cut through the spray at 2 deg after TDC for halved (top row), standard (middle row) and doubled (bottom row) cell numbers in radial direction.
In the low-resolution case, the extent of the region with high turbulent time scale close to the injector is larger when compared to the other cases. The associated higher burning rates help explaining the smaller volume of the region with high chemical energy, which constitutes the major difference between the energy distributions with the low- and standard resolution cases. With the high-resolution case, two isolated regions of high chemical energy exist: The one closer to the injector is considerably shifted downstream when compared to the other cases and the second one is located in the spray tip region, on the original axis. Both these observations indicate a similar effect of hampered evaporation as already observed in the context of the temporal resolution sensitivity study above. In fact, considering the actual simulation timesteps in the initial injection phase (right-hand side diagram in Figure A6), the average timestep before ignition is only slightly reduced between the low- and standard resolution cases.

With the high-resolution case, however, the timestep is by a factor of approximately four lower than with the standard resolution. This is the clear consequence of the timestep adaptation constraint based on the evaporation source terms. Since this constraint relates to a maximum allowable relative change of species density (or cell-integrated energy), the volume of the cell indirectly affects the maximum

Figure A6: Left: Evolution of the ratio of maximum local to average temperature during combustion. Right: Actual timesteps during injection and combustion with the various degrees of radial discretization.
timestep. Since increasing the radial resolution by a factor of two splits the cells in a ratio three to one instead of one to one as in the other directions, a corresponding reduction of the timestep has to be expected. The overall probability of collisions and coalescence is hence again increased and the formation of aggregates of large, slowly evaporating drops near the spray tip promoted.

The shift of the other region of high chemical energy must rather be attributed to the general modification of the spray structure. As a consequence of the attachment to the upper boundary, the availability of oxygen in this region is reduced. Moreover, as the turbulent time is higher there, and hence, turbulent transport is reduced in general.

The global change in predicted spray structure with radial resolution gives rise to the following speculations:

On the one hand, the vertical resolution above the spray must also be considered rather coarse. Increasing the radial resolution while maintaining the same number of layers in vertical direction may thus result in different qualities of the prediction of vertical and radial gradients. Particularly in combination with the known limitations of the spatial discretization schemes employed in KIVA-3, this may result in an amplification of numerical effects, leading to rather unphysical solutions.

On the other hand, recent investigations [164] showed that the predictions of spray propagation are strongly dependent on the selection of gas phase properties, in particular velocity, in the determination of the droplet/gas interaction source terms. A procedure employing interpolation depending on the droplet’s position inside a computational cell was demonstrated to yield better predictions than the one used by KIVA-3, which is based on the cell-average quantities. Such a procedure is hence also expected to reduce sensitivity to resolution in radial direction.

The decreasing nitric oxide emission predictions with increasing resolution are clearly the consequence of the reduced heat release rates in the main combustion phase. However, the better spatial resolution...
resolution is normally expected to yield more exact predictions of emissions as a consequence of the better resolution of gradients and local peaks. In order to verify this, the left-hand-side diagram in Figure A6 compares the evolutions of local maximum to average temperature during combustion (in order to eliminate the effect of differences in the absolute average values).

The characteristic of the curve with the two peaks can be explained as the result of the two combustion phases: The first peak is associated with the location of premixed combustion close to the ignition region, i.e. rather at the spray periphery, with a peak temperature subsequently decaying as a consequence of the eventual quenching due to mixing of fresh gas. The second peak results from the accumulation of hot combustion products from the main combustion region during the mixing-controlled phase in a region closer to the spray axis (see also Figures 58 - 60).

The differences between the individual curves are, however, rather small: The general level is the same, only the timing of the second peak is advanced with increasing resolution, which could be expected as a consequence of the modified spray structure.

**C.3.2 Resolution in Vertical Direction**

The effect of the variation of resolution in vertical direction is highlighted in Figure A7, showing the response of the most sensitive quantities.

With the low-resolution case, severe underprediction of heat release rates during the mixing-controlled combustion phase is observed, leading to considerably lower peak pressure and nitric oxide emissions. Only the premixed phase is apparently unaffected.

Between the standard and the high-resolution cases, only minor differences between the rate of heat release and pressure histories were obtained. The ignition delay with the high-resolution case is very slightly increased, the premixed peak being accordingly shifted and extended. Apart from this small variation, the curves are practically identical.
The more surprising is the difference in predictions of nitric oxide formation: Whereas the lower resulting $NO + NO_2$ level obtained with the low-resolution case has to be expected due to the underprediction of combustion rates and pressure, the decrease from the standard to the high-resolution case is not easily understood at first sight. Here, the comparison of the evolutions of the local maximum to mean temperature ratio provides additional information: In contrast to the abovementioned assumption, the increasing resolution does not favour the identification of peaks, but rather smooths them out. With the high-resolution case, the ratio of maximum to mean temperatures generally tends to a lower level throughout the main combustion phase. Additionally, the second peak is practically elim-
inated, the abovementioned accumulation of hot combustion products presumably being less pronounced.

### C.3.3 Resolution in Azimuthal Direction

The sensitivity to resolution in azimuthal direction could only be studied for a reduction from the standard case, as for an increased number of cell layers in azimuthal direction numerical instabilities prevented the obtention of a solution. Figure A8 shows the comparison of the key results with the two resolutions.

![Figure A8: Comparison of key results for the S20 full load Miller case with two degrees of azimuthal resolution, top left: pressure, bottom left: ROHR, top right: \( NO + NO_2 \).](image)

As in the case of vertical resolution, the low-resolution case yields slower combustion and hence lower peak pressure and emissions. Here, also the premixed peak exhibits some sensitivity to resolution. However, the overall effect of decreased azimuthal resolution on combustion is considerably less pronounced than with the vertical resolution case. Therefore, a less severe sensitivity can be assumed.

The stability problems noted above are already partly present with the standard azimuthal resolution and have to be attributed to the...
two-phase flow modelling approach employed by KIVA-3 in combination with its restriction of applicable grid structures: Since the solver is formulated for all-hexahedral, block-structured meshes with one-to-one connectivity and non-arbitrary block-patching options, a sector mesh as employed in the present study has to be modelled with a degenerated block face on the axis. This invariably leads to very small cells in the centre, which, in the case of central injection, automatically results in high spatial resolution of the spray close to the injector. Though this basically has to be considered advantageous, it is associated with severe stability problems related to the high values of the source terms in relation to the cell’s energy and mass content. Moreover, the basic assumption of negligible liquid volume when compared to the cell volumes is possibly no longer valid in these regions.

C.3.4 Conclusion: Best Practice Approach

Based on the above considerations, a best practice approach for the present study was derived, where the requirements for spatial resolution are defined for two main directions: along the spray axis and along both directions perpendicular to it.

Since an increase of resolution in vertical direction did not yield further improved predictions of rate of heat release and cylinder pressure histories, the standard resolution is considered sufficient. With respect to azimuthal resolution, equally perpendicular to the spray axis, the less pronounced sensitivity with reduced resolution than in vertical direction is taken as a clear indication for adequacy of the standard resolution, though no direct validation could be performed.

In radial direction, the further increase of resolution yielded rather questionable results for the predicted spray structure, which can, at least partly, be attributed to a non-adequate resolution in vertical direction. Since the separate study of vertical resolution did not support the need for better resolution in this direction and the substantially higher expense does not justify the (uncertain) benefit, the standard resolution was adopted. The study of radial resolution,
however, underlines the general need of critical assessment of the spray structure predictions for sensibility.

In order to reduce the stability problems associated with injection into very small cells, the equidistant vertex distribution was abandoned in the region close to the injector. Here, in the centre of the sector, larger cells were employed, with the azimuthal distance eventually decreasing towards the periodic boundaries. Figure A9 shows a detail view of this region, including a representation of the droplet volumes proportional to the grid dimensions.

Figure A9: Detail view of the near-injector region of the computational grid employed in the investigations relating to the Sulzer S20 engine. Cut plane parallel to the direction of the spray, size of the droplet symbols indicating effective liquid volume proportional to grid dimensions.
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