3D-Combustion Simulation: Potentials, Modeling and Application Issues

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Motivation for 3D-CFD ICE Simulation
Demands on an Industrial CFD Code
General Modeling Aspects
Combustion Modeling Concepts at DC
  - Spray Modeling
  - Combustion Modeling
  - Validation
Conclusion
Motivation for 3D-CFD ICE Simulation

**Improvements required by**
- Legislation
- Customer
- Environment

**TODAY Diesel Engines**
- Consumption
- Emissions (NO\textsubscript{x}, PM)

**Key-Technologies**
- Injection system
- Combustion design
- Turbocharging
- Exhaust gas aftertr.

**TARGET Diesel Engines**
- Consumption
- Emissions
- Costs

**Task:** Cost and time effective development of engine with low emissions and high fuel economy

**Challenge:** Large number of design parameters and complex variable interactions
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Demands on an Industrial CFD Code

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Demands on an industrial CFD Code

Package must be featured by

- High degree of predictability
- Low computational costs

Compromise solution!

What means prediction?

- It is sufficient to predict
  - trends (e.g. determine the most qualified bowl geometry)
  - relative results (e.g. NO\textsubscript{x}-Soot Trade-Off)
- Reduced tuning efforts; calibration of only physical parameters (e.g. droplet size, not mesh configuration)
Issues in CFD Modeling

Complex shaped moving geometry

Fuel jet: 2-phase flow

Turbulent flow

Combustion & Emissions complex chemistry

Predictability of CFD Code is determined by weakest sub-model

→ All sub-models should have about the same level of detail!
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Modeling Aspects

- Reduced mesh dependency:
  → Resolving of relevant length-scales
- Definition of realistic boundary conditions:
  → Coupling between cavitating nozzle flow and spray calculation
- Convergent droplet statistics:
  → Eulerian spray model near nozzle orifice
- Validated physical sub-models
  → for breakup and evaporation

Eulerian models in combination with orifice resolving meshes and boundary conditions from 3D simulation of nozzle flow!
Modeling Aspects

- **Conventional Diesel ignition:**
  - Consideration of detailed chemistry
- **Advanced combustion ignition, e.g. HCCI ignition:**
  - Consideration of detailed chemistry in low temperature range
  - Description of multi-stage ignition (Cool Flame)
- **Premixed combustion:**
  - Accounting for complex chemistry schemes
- **Turbulence-chemistry interaction:**
  - Consideration of heterogeneous mixture fields
  - Consideration of turbulent transport processes

Incorporation of validated detailed kinetics and accounting for turbulence interaction!
Emissions

Prediction of NOx, Soot, HC, CO:
→ Consideration of detailed chemistry

Miscellaneous:

• Accounting for real gas effects
• Accounting for elasticity effects
• Chemical schemes for alternative fuels
• Intelligent meshing strategies
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DC Approach for Spray

Crucial for predictive spray simulations are:

1. Resolution of relevant scales (hole diameter!) → spray adaptive mesh
2. Capture of droplet statistics → Eulerian spray model in near nozzle region
3. Boundary settings → Coupling between models for nozzle flow and spray
4. Suitable models for spray breakup and droplet evaporation

Influence of mesh refinement on statistics:

- Coarse mesh: 5 “parcels” per cell
- Fine mesh: 3 “parcels” per cell

⇒ decrease of “parcels” per cell

- Coarse mesh: 6 droplet classes
- Fine mesh: 7 droplet classes

⇒ Number of droplet classes independent of cell size
Comparison: Experiment and Simulation

Spray structure (angle and penetration) shows good agreement.
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DC Approach for Combustion

Requirements:

- High degree of predictability:
  - Consideration of Turbulence effects
    - Complex Interaction
    - Complex chemistry
- Low CPU-costs: Reasonable level of detail

Idea of Progress Variable Approach:

*Description of complex chemical phenomena with a *limited* number of representative progress variables*

Spatial-temporal information of the progress variable:

Solving of a general convective-diffusive transport equation

\[
\frac{\partial (\rho \psi_i)}{\partial t} + \nabla \cdot (\rho \tilde{u} \psi_i) = \nabla \cdot [D \nabla \tilde{\psi}_i] + \tilde{\psi}_i^s + \tilde{\psi}_i^c
\]

Issues:

1. Identification of characteristic progress variables
2. Determination of mean chemical source terms
Progress Variable Approach: Definition of Progress variables
Zoning of the overall Diesel combustion on the basis of the heat release rate:

- Premixed combustion (chemistry-controlled)
- Diffusion combustion (mixing-controlled)

Heat release rate [J/°CA] vs. crank angle [°]

- Ignition delay (chemistry-controlled)
- Detailed kinetics
- Reduced kinetics
**Progress-Approach:** Determination of mean chemical sources terms

**PDF-Type Model:**
- Numerical separation
- PDF-Integration of “laminar” reaction rates

**Turbulent flow**
- Ensemble-averaging: mean and variance
- Probability density function (PDF)

**Chemical reactions (detailed kinetics)**
- \( C_2H_6 + O_2 = C_2H_5 + HO_2 \)
- \( C_2H_6 + OH = C_2H_5 + H_2O \)
- \( C_2H_6 + O = C_2H_5 + OH \)
- ...
### DC Approach for Combustion

<table>
<thead>
<tr>
<th>Turbulent mixture: (reality)</th>
<th>Standard-Models</th>
<th>PDF-Progress-Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fuel</strong></td>
<td>Mean values</td>
<td>Probability density function (PDF)</td>
</tr>
</tbody>
</table>

#### Mixture fraction $Z$

- **0** Mixture fraction $Z$
- **1**

#### Detailed kinetics:

- **Not applicable**, since too many species need to be transported!
- **Applicable**, since the transport of only a limited amount of well-defined progress-variables is needed!
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CFD-Setup:
- KIVA3v
- 1D-Eulerian Spray Model with spray adapted sector meshes
- 7-Species PDF-Timescale Model
- Model for component elasticity effects
- Model for real gas effects

Model parameter:
- Pre-exponential factor of the empirical chemical time-scale of the combustion model
Validation

Major features of combustion are captured accurately:
- Ignition delays
- Occurrence and order of peak pressure
- Expansion pressure

Premixed combustion is slightly over-predicted
⇒ empirical single chemical time-scale approach
Validation

Comparison between combustion photographs and numerical results

Left: combustion photographs from optical engine; Right: calculated temperature iso-surfaces T=1400K (mirrored view)
Validation

Example of a local flow analysis for a marine engine

- Temperatur [K]
- NO [-]
- Mischungsbruch [-]
- Russ [-]

CA -3.19
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I. Challenges in Diesel engine development requires intensive use of 3D Combustion Simulation

- in early conception phase by pre-selection of design parameters
- in testing phase as analysis tool

II. Demands on CFD models for industrial purposes are high degree of predictability and low computational costs

III. Modelling issues for advanced combustion concepts are

- validated detailed and chemical mechanism for all fuels
- correct description of turbulence chemistry interactions
- integrated simulation of nozzle flow, mixture formation, combustion emissions, coolant-flow and FE-structure dynamics