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

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Coronado, California

# Outline

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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

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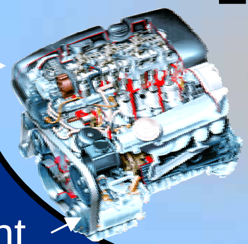
## Improvements required by

Legislation

Customer

Environment

**TODAY Diesel Engines**



☺ Consumption

☹ Emissions ($NO_x$, 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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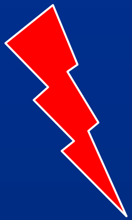
# Demands on an industrial CFD Code

## Package must be featured by

High degree of predictability



**Compromise solution!**

Low computational costs

plus

- Extensibility
- Ease-of use
- Best Practice
- …

## What means prediction?

☞ It is sufficient to predict

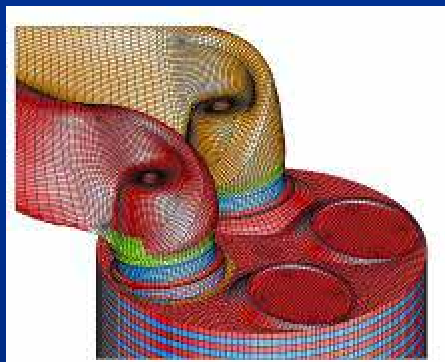
- trends (e.g. determine the most qualified bowl geometry)
- relative results (e.g. $NO_x$-Soot Trade-Off)

☞ Reduced tuning efforts; calibration of only physical parameters (e.g. droplet size, not mesh configuration)

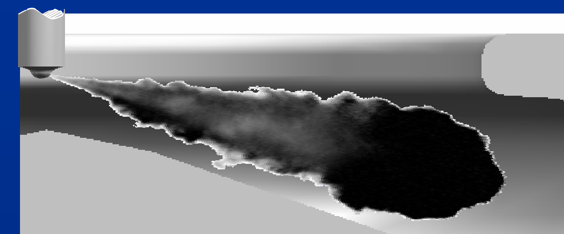
# Issues in CFD Modeling

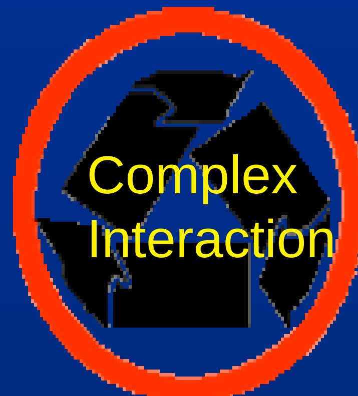


Complex shaped moving geometry



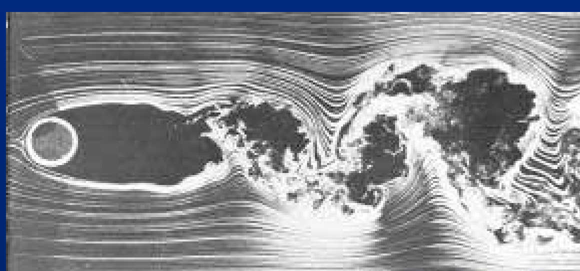
Fuel jet: 2-phase flow






Combustion & Emissions
complex chemistry

Turbulent flow



**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

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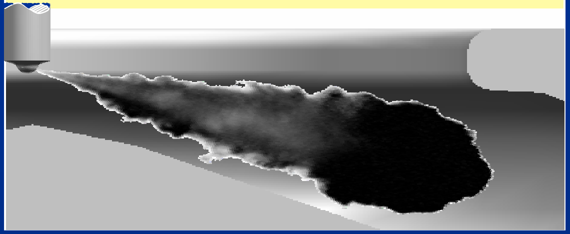
**Mixture formation:**



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

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

# Modeling Aspects

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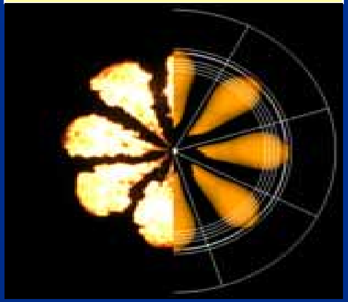
**Combustion**



- 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!**

# Modeling Aspects

**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

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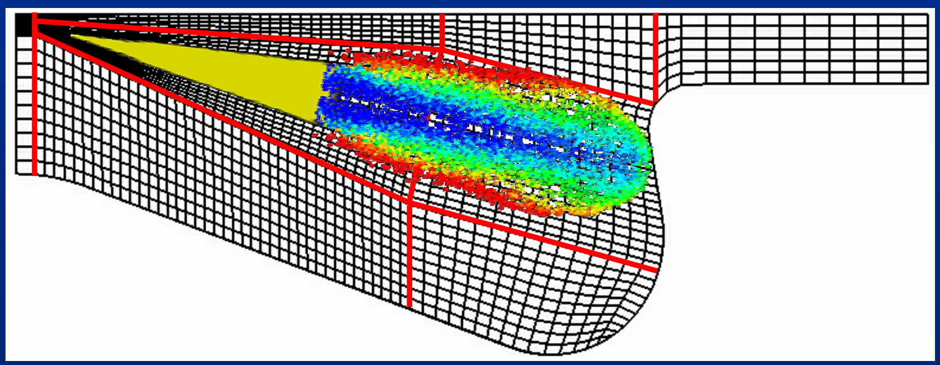
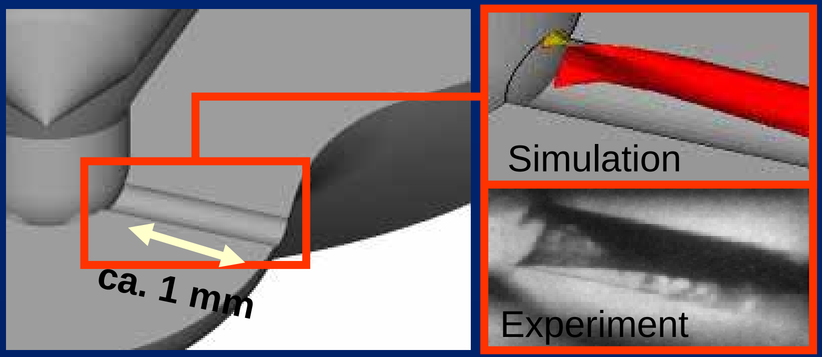
## Crucial for predictive spray simulations are:

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

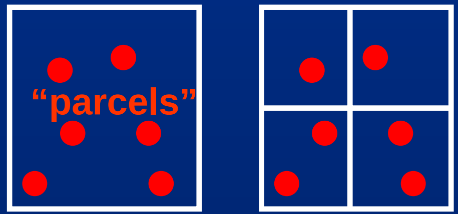





Influence of mesh refinement on statisti

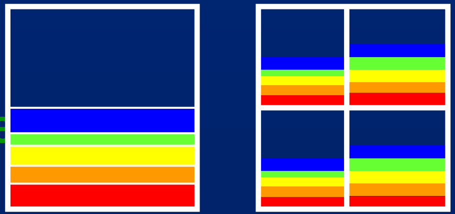
Coarse mesh Fine mesh

Stochastic spray model




⇒ decrease of “parcels” per ce

Eulerian-spray Mode



Coarse mesh Fine mesh

⇒ Number of droplet classes independent of cell size

# DC Approach for Spray

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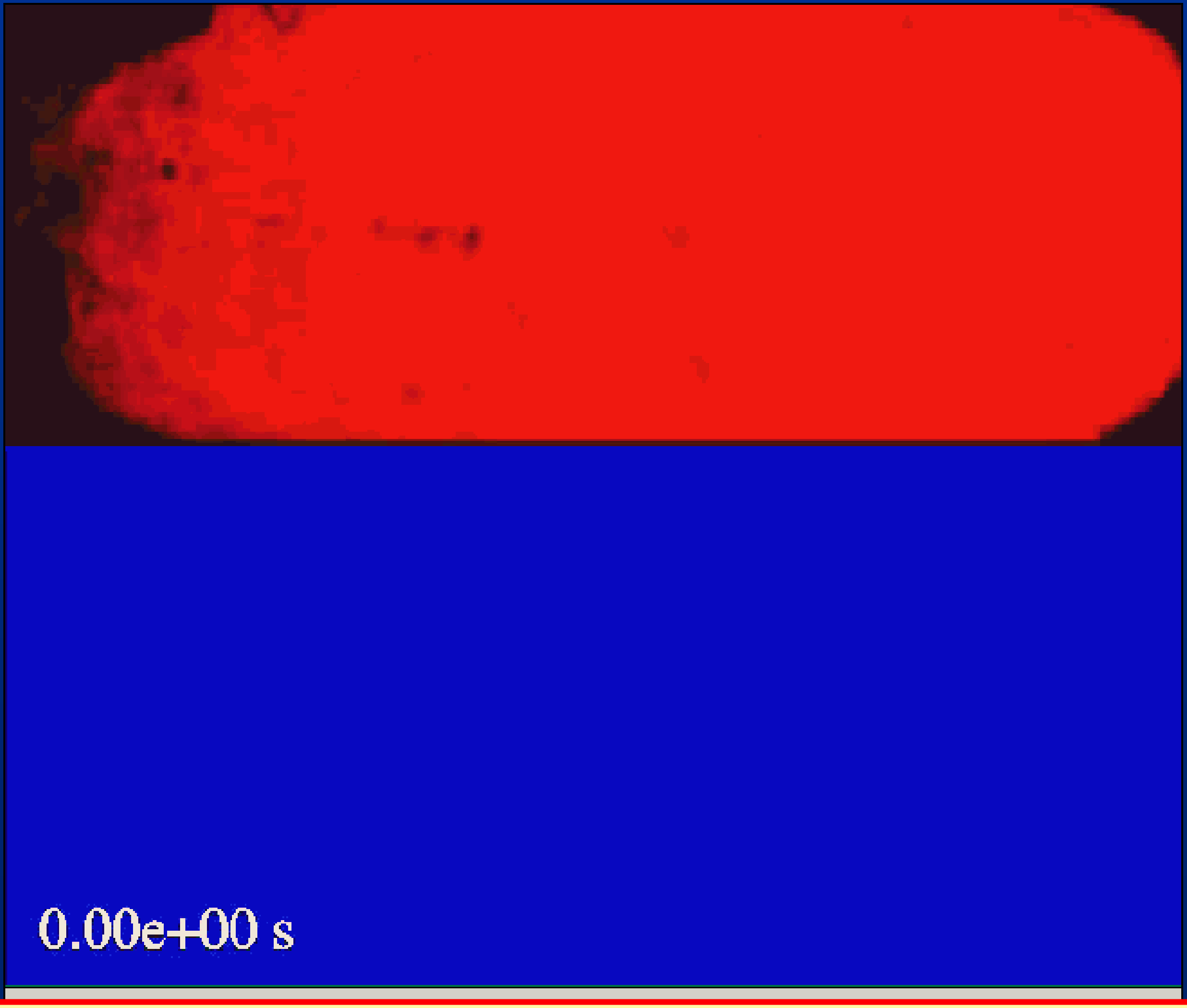
## Comparison: Experiment and Simulation




High temperature chamber

Simulated air-fuel ratio

- 10 < λ
- 2 < λ <
- 1 < λ <
- 0.7 < λ < 1
- λ < 0.7

**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 chemistry } — Complex Interaction

- 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

$$\frac{\partial(\bar{\rho}\tilde{\psi}_i)}{\partial t} + \nabla \cdot \left(\bar{\rho}\tilde{\vec{u}}\,\tilde{\psi}_i\right) = \nabla \cdot \left[D\nabla\,\tilde{\psi}_i\right] + \tilde{\dot{\psi}}_i^{s} + \tilde{\dot{\psi}}_i^{c}$$

**Issues:**

1.) Identification of characteristic progress variables

2.) Determination of mean chemical source terms

# DC Approach for Combustion

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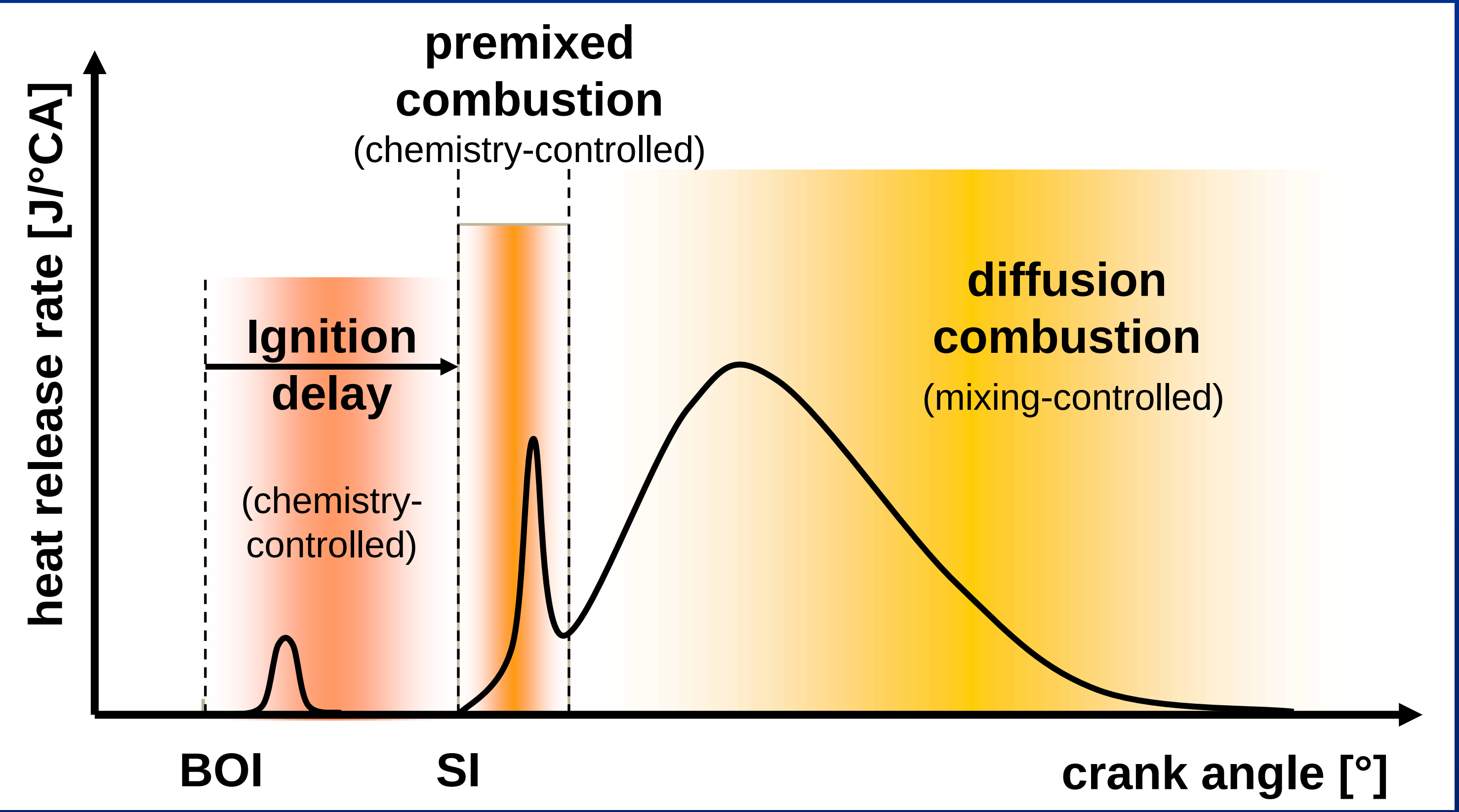
Progress Variable Approach: Definition of Progress variables

Zoning of the overall Diesel combustion on the basis of the heat release rate:




detailled kinetics

reduced kinetics

# DC Approach for Combustion

**Progress-Approach:** Determination of mean chemical sources terms

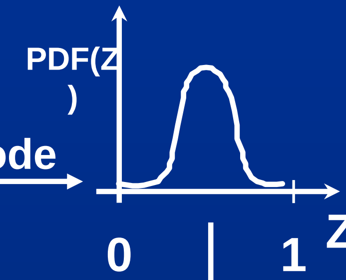
**Engine Combustion**


**Turbulent flow**

Ensemble-averaging: mean and variance

Probabilty density function (PDF)

CFD-Code



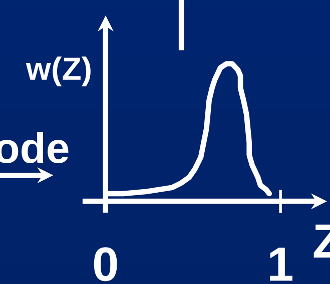

**Mean source terms:**

$$\overline{\omega_i} = \int_Z \dot{\omega}_i(Z) \cdot PDF(Z) dZ$$

**Chemical reactions (detailed kinetics)**

$C_2H_6 + O_2 = C_2H_5 + HO_2$
$C_2H_6 + OH = C_2H_5 + H_2O$
$C_2H_6 + O = C_2H_5 + OH$
. . .

Flamelet-Code




## PDF-Type Model:

- Numerical separation
- PDF-Integration of “laminar” reaction rates

# DC Approach for Combustion

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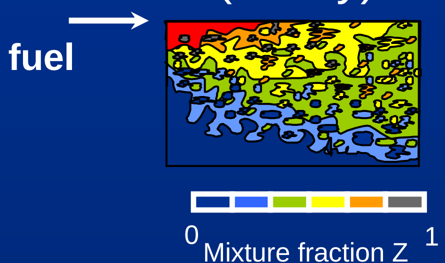
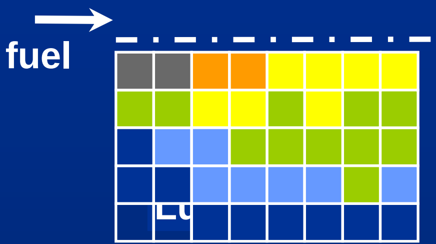
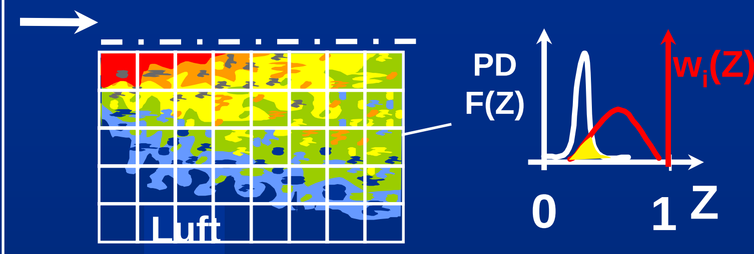
| | Standard-Models | PDF-Progress-Approach |
|---|---|---|
| **Turbulent mixture:** (reality)   | Mean values   | Probability density function (**PDF**)   |
| **Detailed kinetics:** | **Not applicable**, since too many species need to be transported! | **Applicable,** since the transport of only a limited amount of well-defined progress-variables is needed! |

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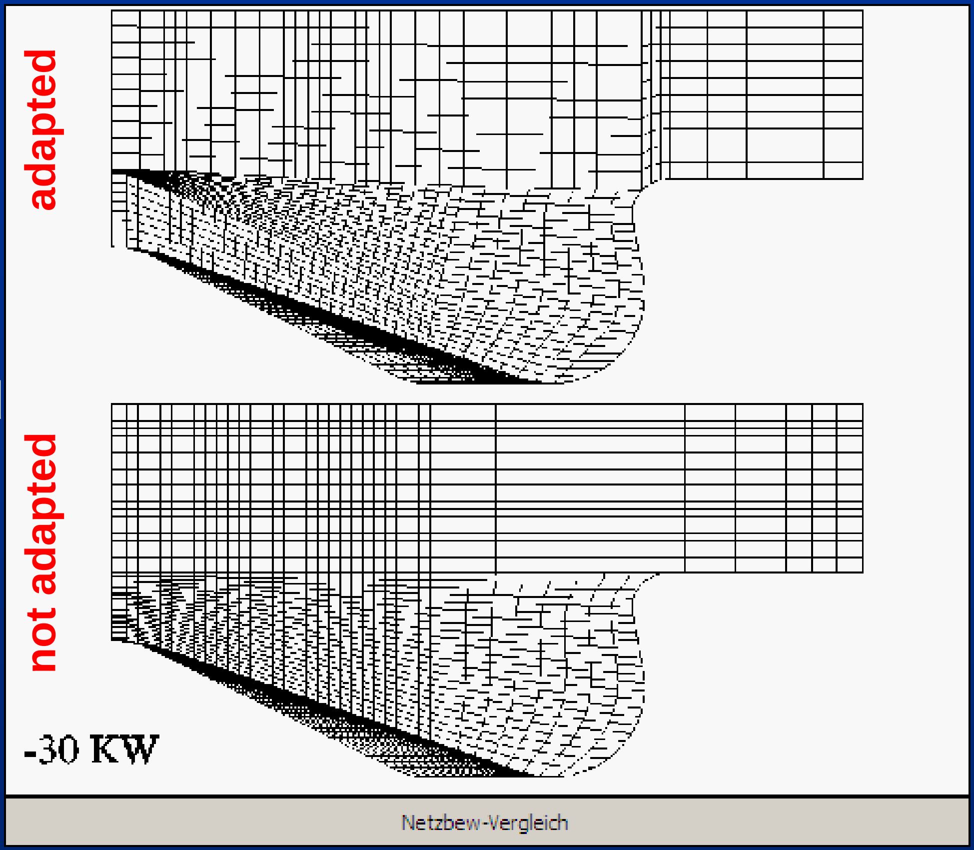
## CFD-Setup:

- KIVA3v
- 1D-Eulerian Spray Model with spray adapted sector meshes
- 7-Species PDF-Timescale Mod
- 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

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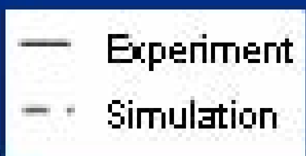
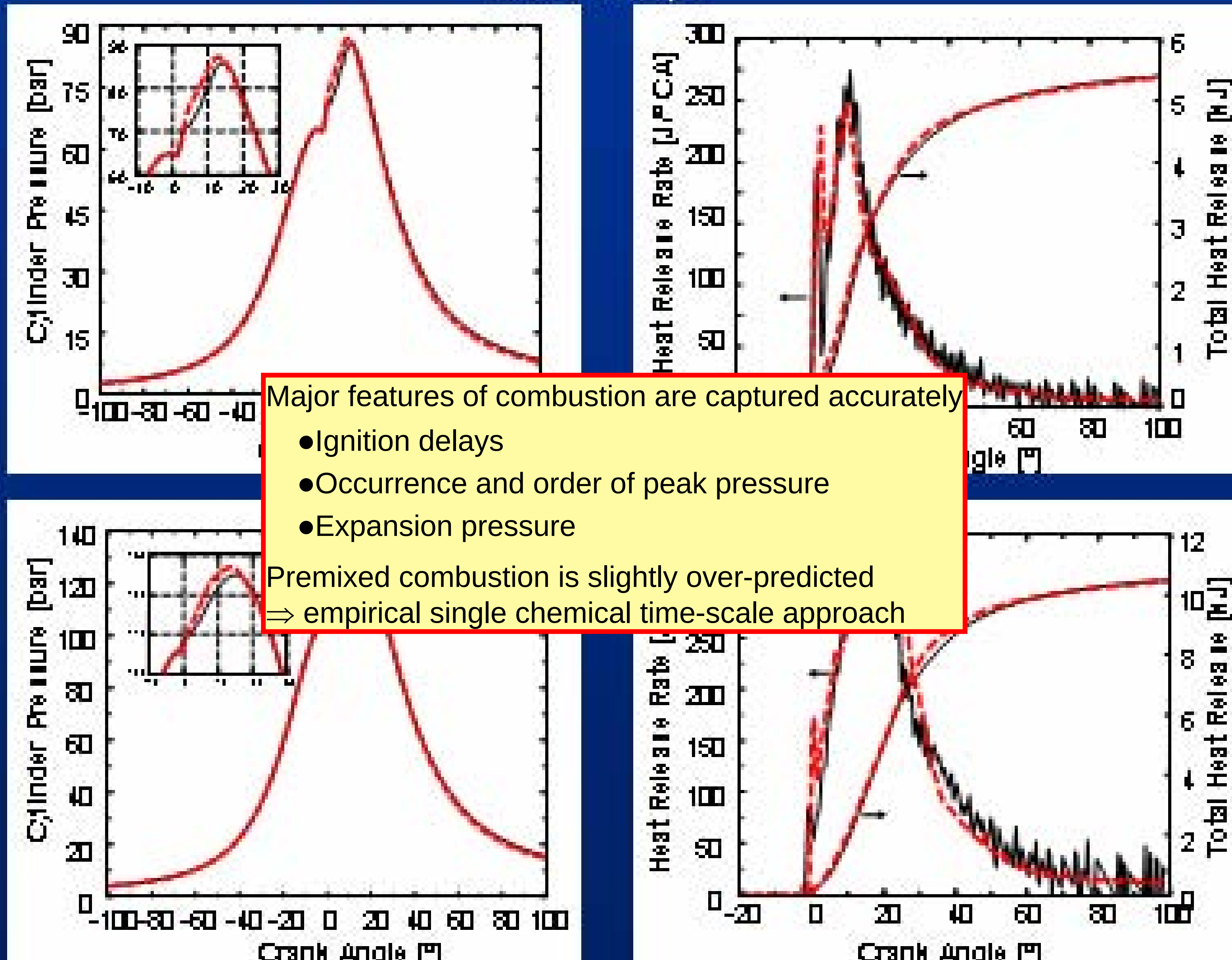
**Heavy duty truck engine:**

Part load




**Heavy duty truck engine:**

Full load




Major features of combustion are captured accurately

- Ignition delays
- Occurrence and order of peak pressure
- Expansion pressure

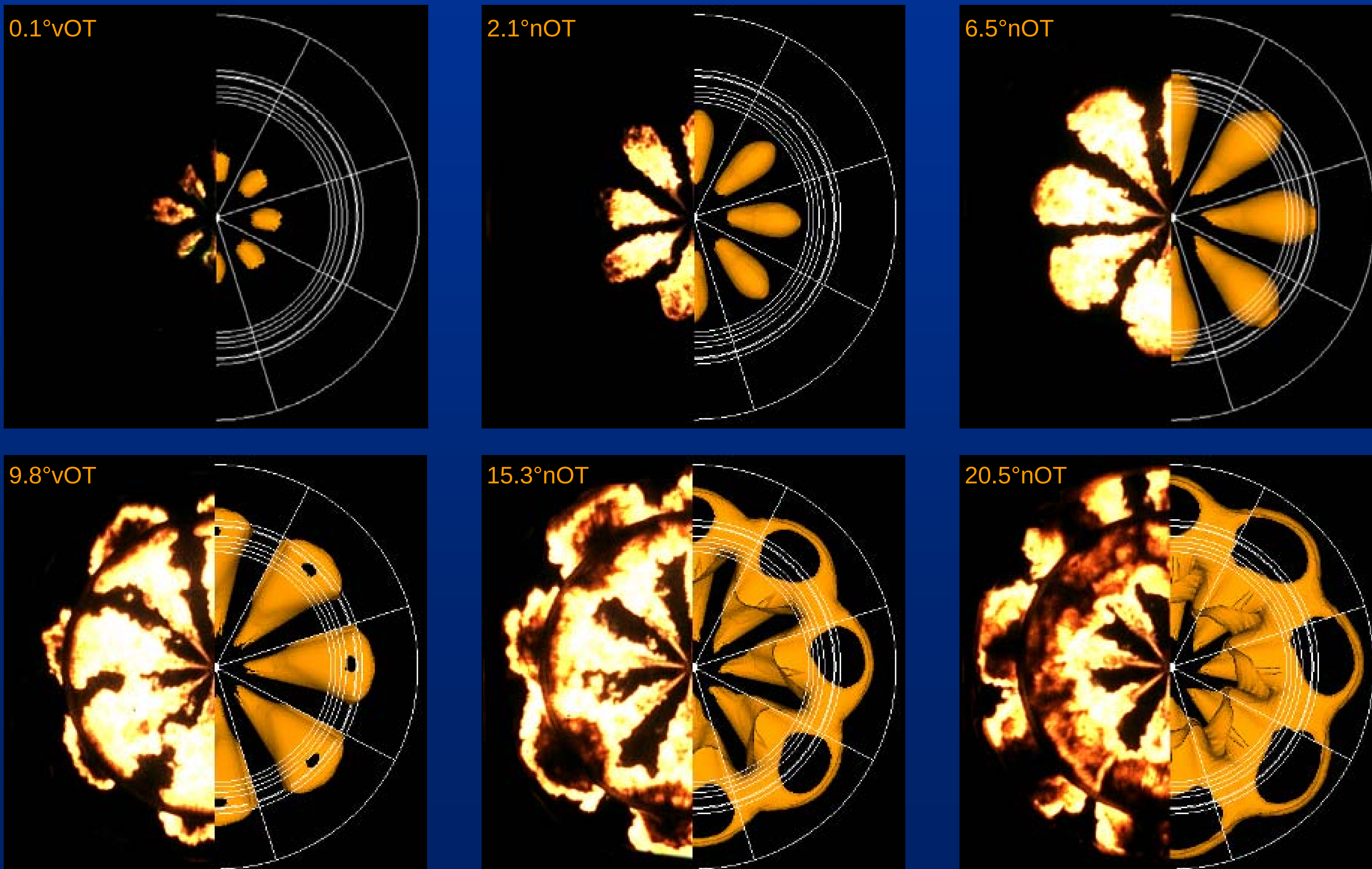
Premixed combustion is slightly over-predicted

⇒ 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

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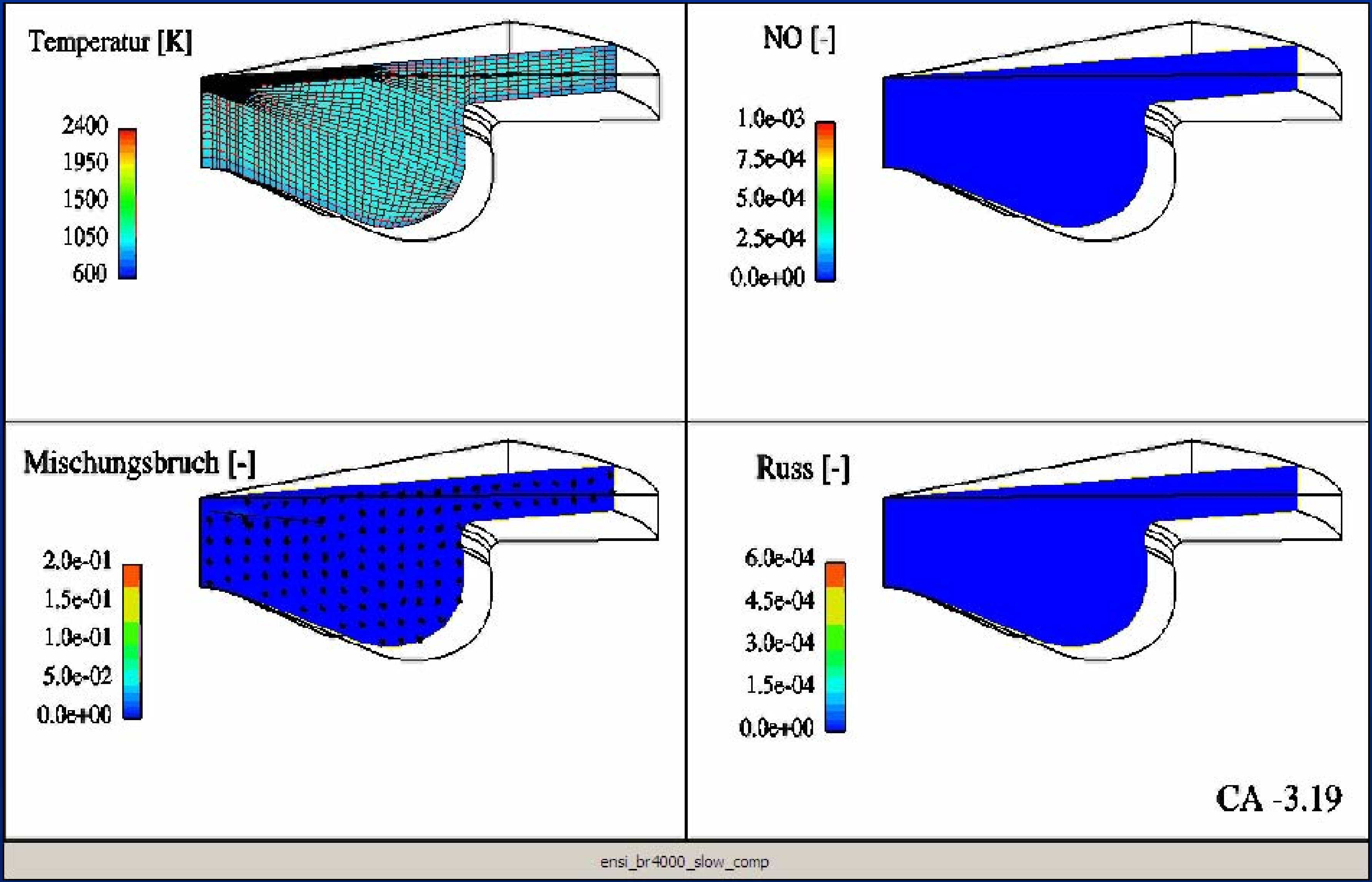
## Example of a local flow analysis for a marine engine



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# Conclusion

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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

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

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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