Further Application of the Fast Tabulated CPV Approach

Adina Werner[1] , Corinna Netzer[1], Harry Lehtiniemi[2], Anders Borg[2,4], Andrea Matrisciano[2,4], Lars Seidel[3], Fabian Mauss[1]

[1]Brandenburg University of Technology, Cottbus, Germany

[2]LOGE AB, Lund, Sweden

[3]LOGE Deutschland GmbH, Cottbus, Germany

[4]Chalmers University of Technology, Gothenburg, Sweden

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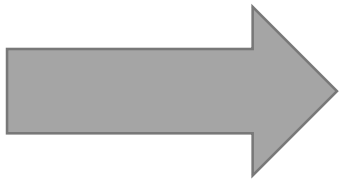
LOGE LUND COMBUSTION ENGINEERING

Objective

- The main target within internal combustion engine simulation is to get predictive simulations.
- Availability of detailed chemistry schemes and their complexity are increasing.

Dilemma in 3D

More species lead to more accurate results, but also to a high demand of computational costs

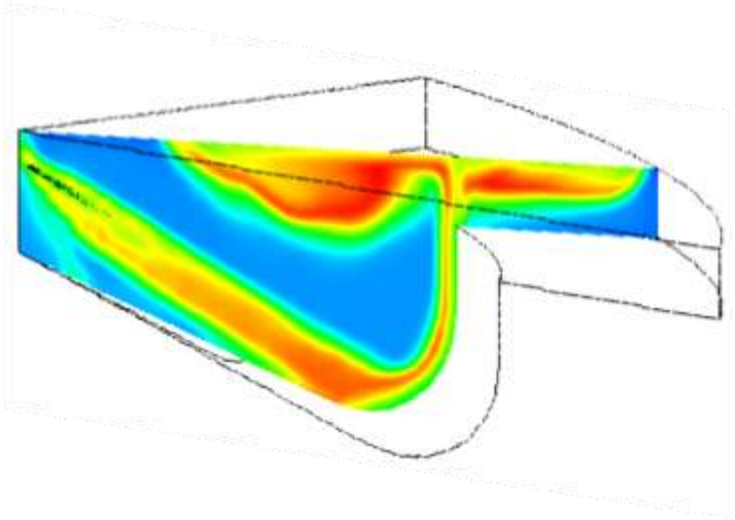


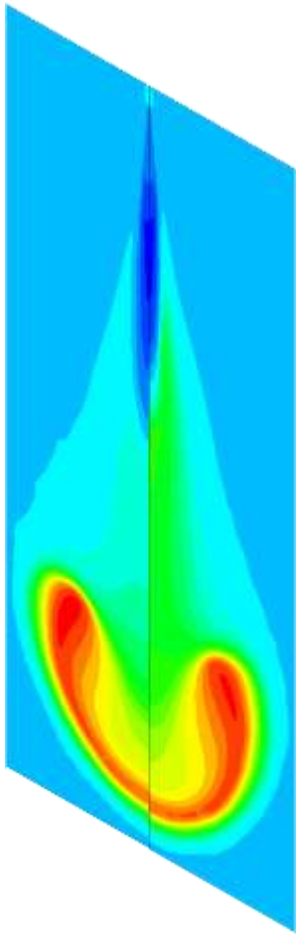
Solution

Tabulated chemistry approaches where CPU time is independent of the number of species in the reaction mechanism.

Outline

1. Objective
2. The Combustion Progress Variable (CPV) model
3. Applications
   1. Spray A
   2. Diesel Engine
   3. CPU Times
4. Conclusions





The Combustion Progress Variable (CPV) Model

General Idea of the CPV (Combustion Progress Variable) Model

- The larger the mechanism, the more species are transported and the more CPU time is required for solving combustion chemistry
- **Idea:**
  - Use h_{298} as progress variable as we have before for transient flamelet models and cell local CMC for combustion, and apply to the WSR combustion model
- **Benefit:**
  - Mechanism size will not affect CFD run-time, since all combustion chemistry is pretabulated and the number of scalars to transport will be the same regardless of chemical mechanism

The Progress Variable

- **Idea:** A progress variable C can be used for reconstruction of the thermo-chemical state on the whole reaction trajectory.

  C = 0: unreacted mixture

  C = 1: fully burned mixture

  Track both low and high temperature reactions

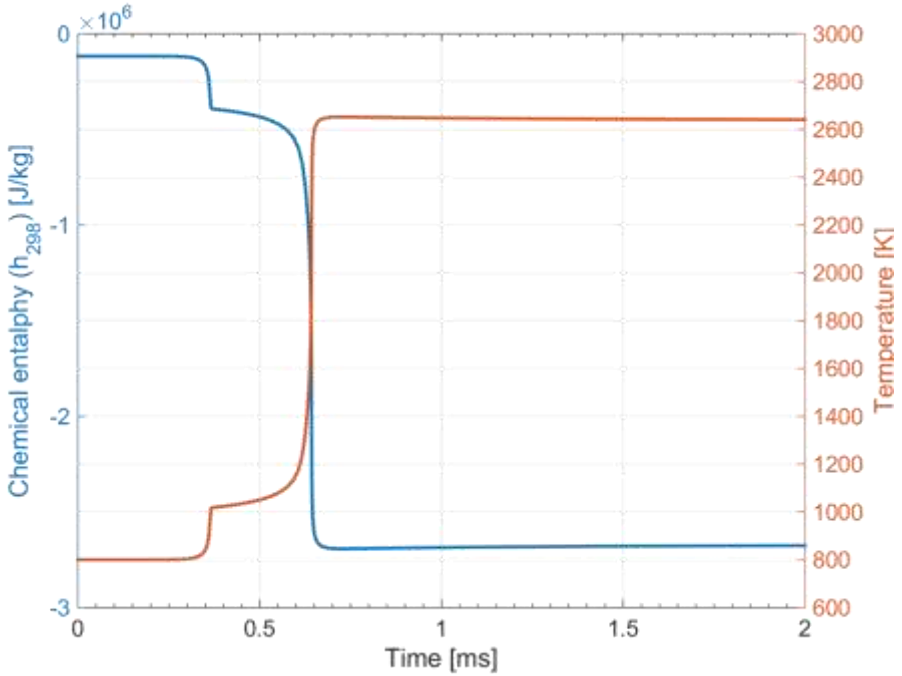
- The fuel oxidation is parametrized using chemical enthalpy h_{298}

$$C = \frac{h_{298} - h_{298,0}}{h_{298,eq} - h_{298,0}}$$

h_{298} current chemical enthalpy in the cell
$h_{298,0}$ enthalpy of formation at standard state (maximum)
$h_{298,eq}$ chemical enthalpy at maximum total heat release (minimum)

Lehtiniemi et al., Combust Sci Technol 178, 2006

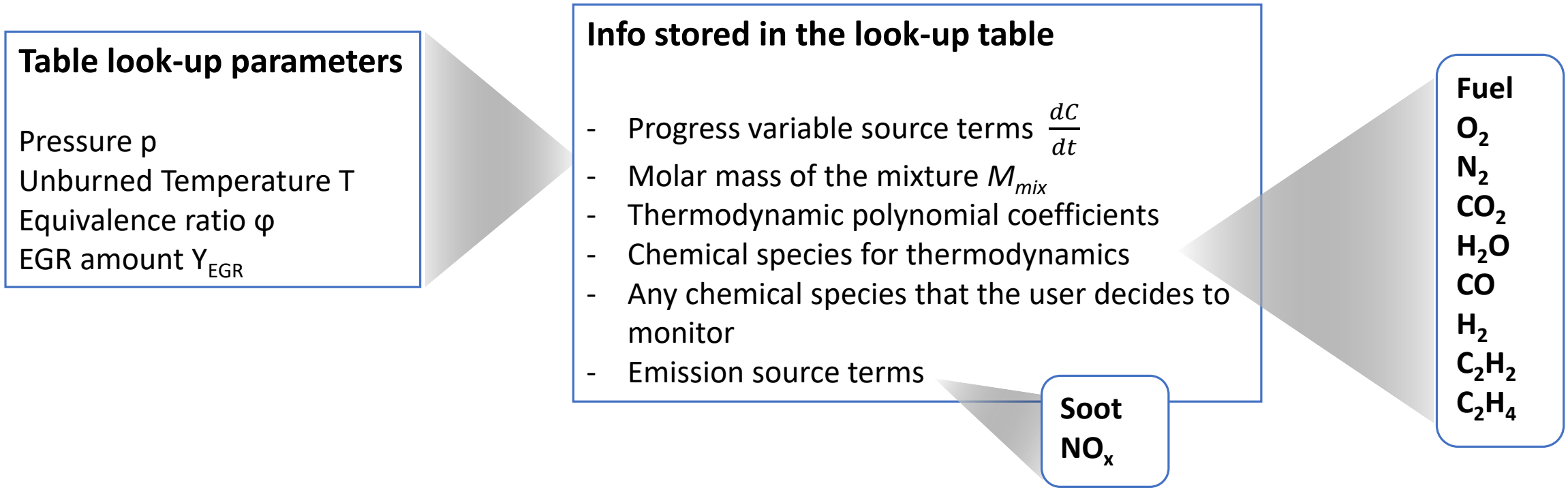
Matrisciano et al., SAE Technical Paper 2017-01-05



Chemical enthalpy and temperature as a function of time for a constant pressure calculation at 10 bar and 750 K for an n-heptane/ air mixture at ϕ=1.

Combustion Progress Variable Model

- Detailed chemistry scheme is solved using adiabatic constant pressure reactors
- The created table is surrogate sensitive, but independent of operating conditions as speed, engine geometry, EGR amount, load, ….
- A fully automated tool for the table generation is available: LOGEtable



Additional Transport Equations

- Mixture fraction

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t} + \nabla \cdot \left(\bar{\rho}\tilde{\boldsymbol{v}}\tilde{Z}\right) - \nabla \cdot \left(\bar{\rho} D_{\mathrm{t}} \nabla \tilde{Z}\right) = \overline{\rho \dot{\omega}_S}$$

Solved by CONVERGE — Solved by CPV

- Progress variable

$$\frac{\partial \bar{\rho}\tilde{h}_{298}}{\partial t} + \nabla \cdot \left(\bar{\rho}\tilde{\boldsymbol{v}}\tilde{h}_{298}\right) - \nabla \cdot \left(\bar{\rho} D_{\mathrm{t}} \nabla \tilde{h}_{298}\right) = \overline{\rho \dot{\omega}_{S,h298}} + \overline{\rho \dot{\omega}_{chem,h298}}$$

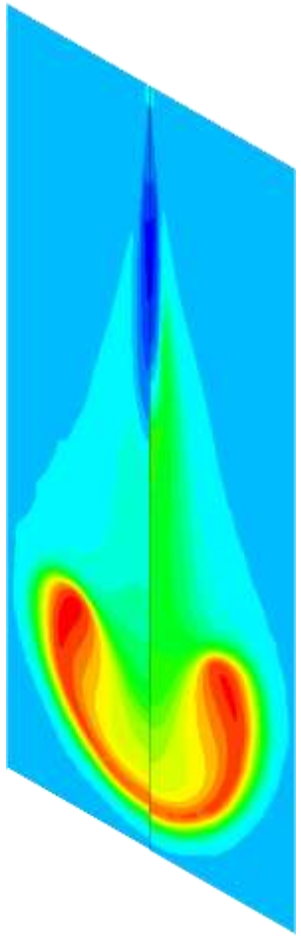
Solved by CONVERGE — Solved by CPV

- CPV thermo-species (9 species)

$$\frac{\partial \bar{\rho}\tilde{Y}_\alpha}{\partial t} + \nabla \cdot \left(\bar{\rho}\tilde{\boldsymbol{v}}\tilde{Y}_\alpha\right) - \nabla \cdot \left(\bar{\rho} D_{\mathrm{t}} \nabla \tilde{Y}_\alpha\right) = \overline{\rho \dot{\omega}_S}\delta_{\alpha\beta} + \overline{\rho \dot{\omega}_\alpha}$$

Solved by CONVERGE — Solved by CPV

Application: Spray A



Application: Spray A – Simulation Background

- Reaction scheme
  - n-dodecane reaction scheme with 487 species and 2331 reactions

Modified Seidel et al. 2015

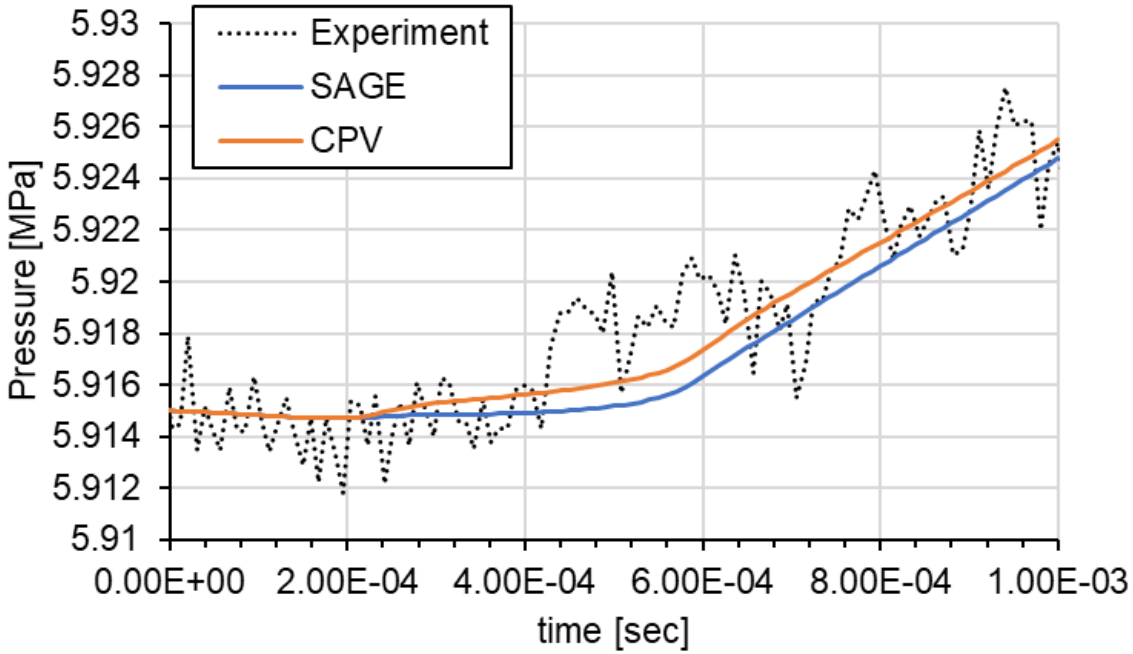
- CPV table

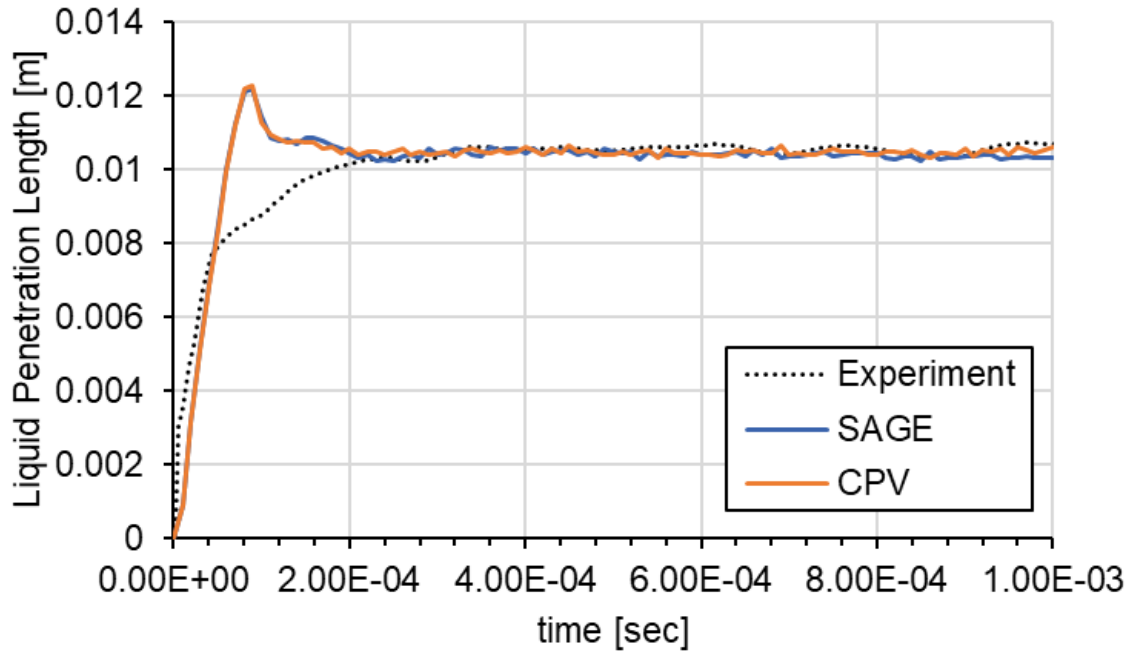
Property	Range	Grid points
EGR [%]	0.0 - 40.0	5
Equivalence ratio [-]	0.2 - 10.0	25
Pressure [bar]	1e+05 - 2e+07	18
Unburnt temperature [K]	250.0 - 1400.0	101

- Setup
  - Geometry: cube with a edge length of 108 mm
  - base grid: 2 mm
  - AMR (adaptive mesh refinement) and fixed embedding cone
  - Kelvin-Helmholtz (KH) model
  - Turbulence prediction: Reynolds Averaged Navier-Stokes (RANS) model and standard k-ε-model
  - Combustion prediction:
    - SAGE detailed chemistry solver
    - CPV combustion model
  - Species: N_2, O_2, CO_2, H_2O and NO

Application: Spray A – Combustion Prediction

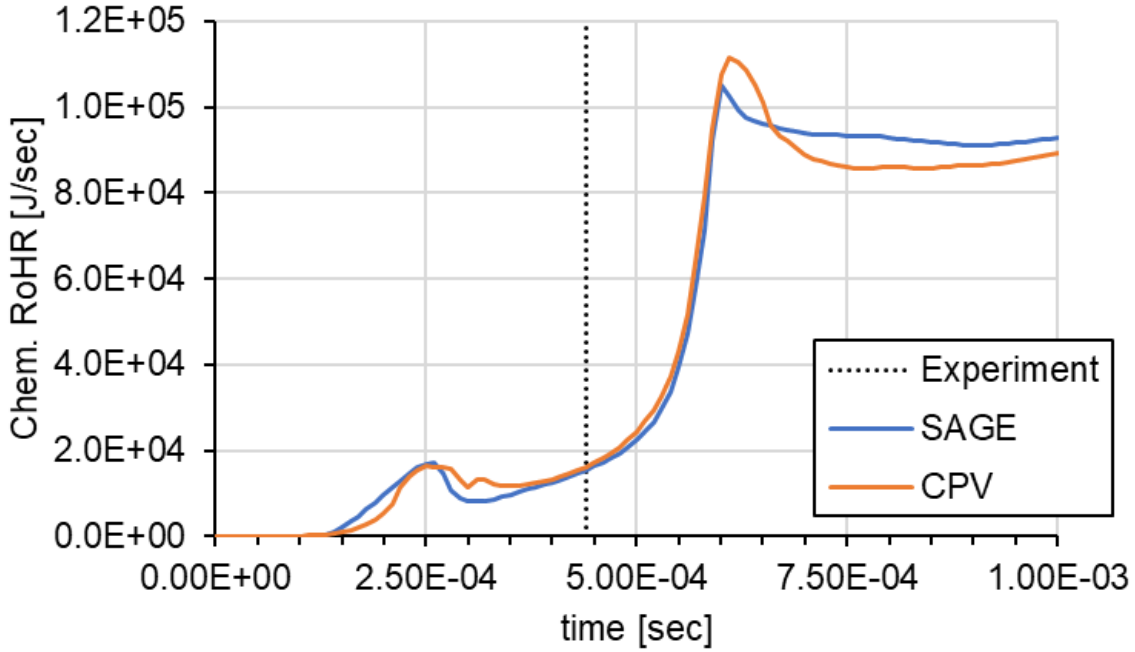
- Validation against experiment and SAGE

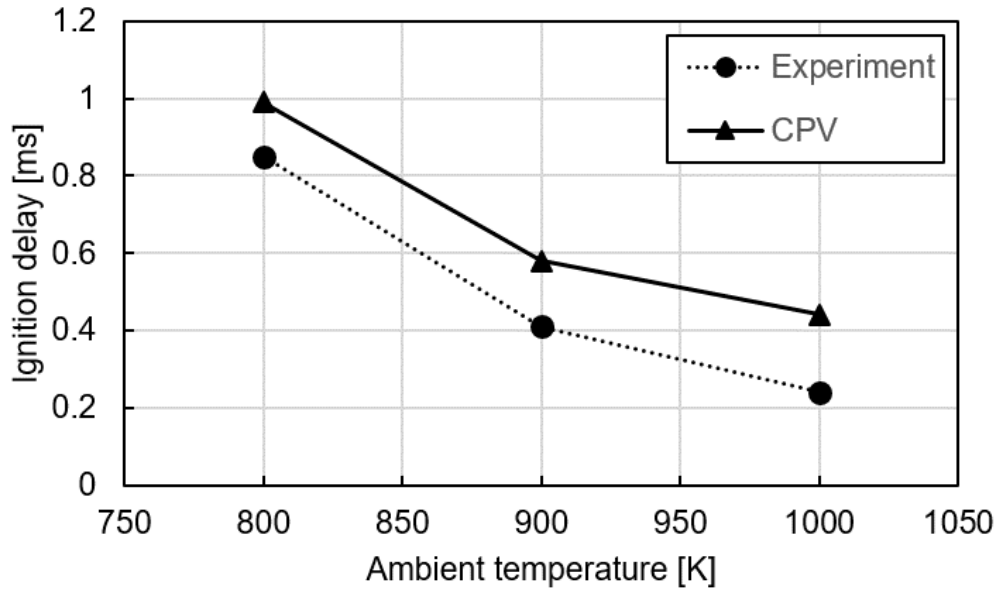




Application: Spray A – Combustion Prediction

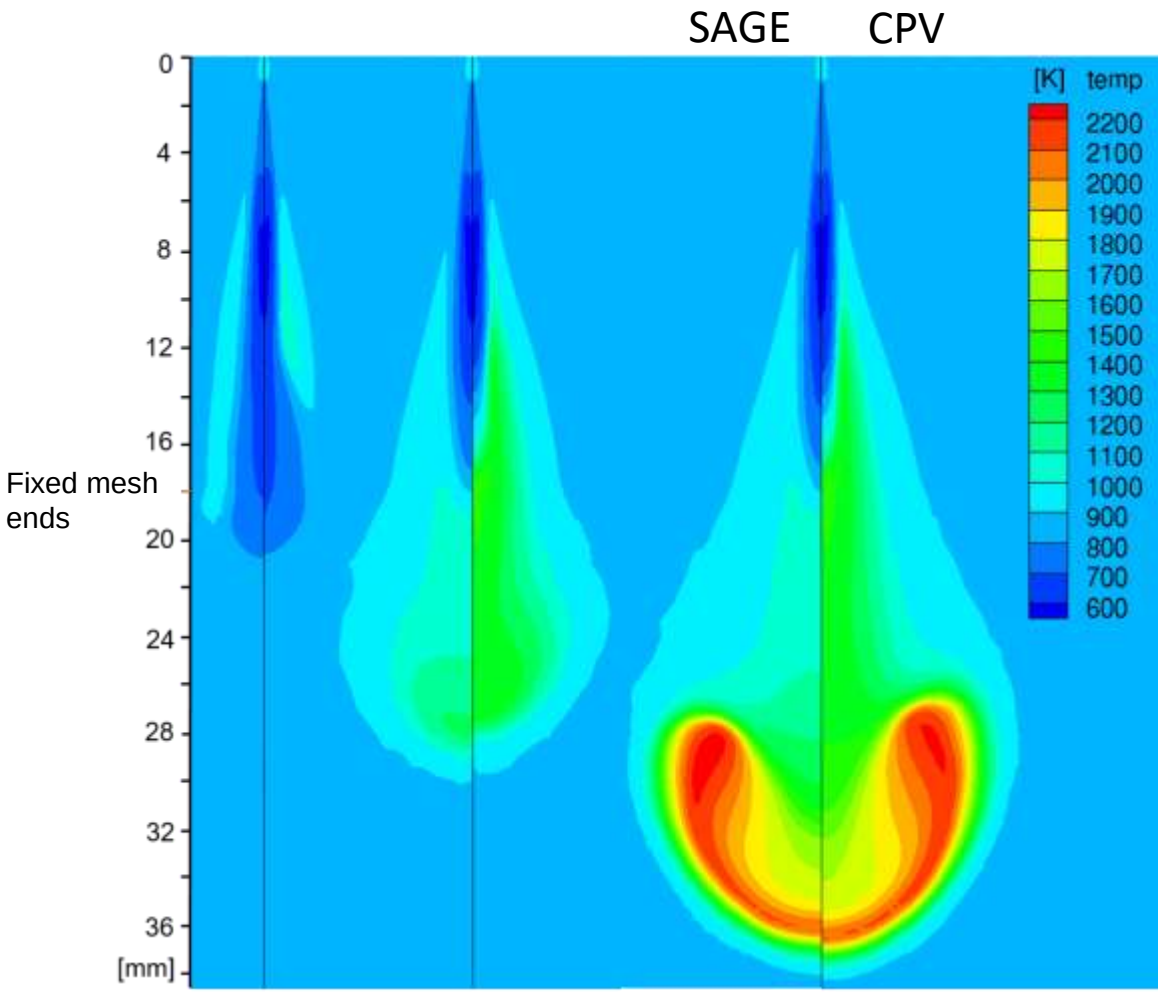
- Combustion duration comparison against experiment

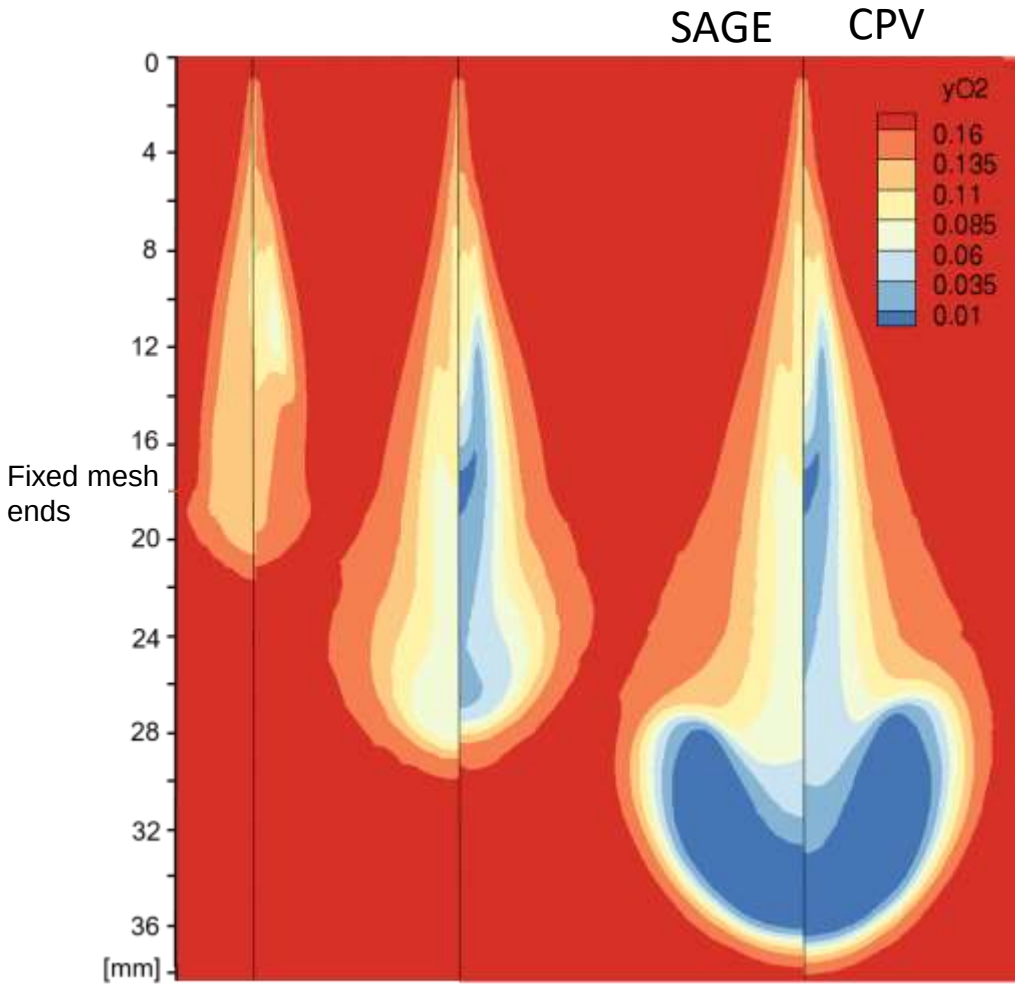


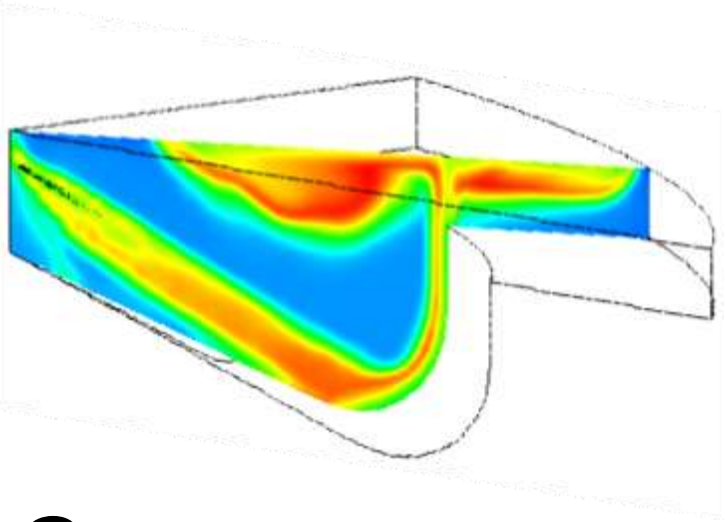


Application: Spray A

- Post processing plots at 0.2 ms, 0.425 ms, and 0.725 ms







Application: Diesel Engine

Diesel Engine Application

- Reaction scheme
  - n-heptane reaction scheme with 121 species and 594 reactions

Zeuch et al. 2008

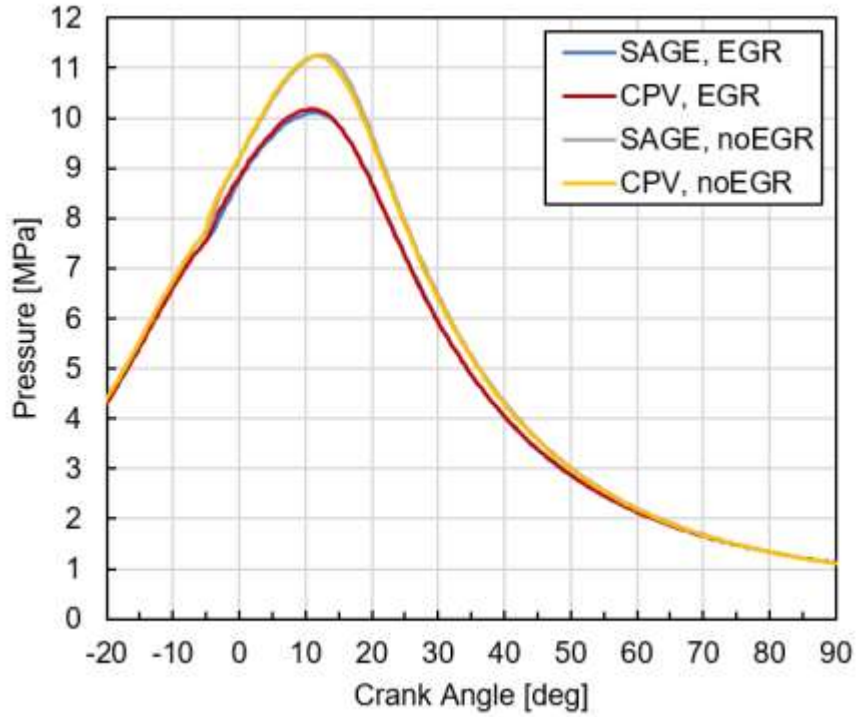
- CPV table

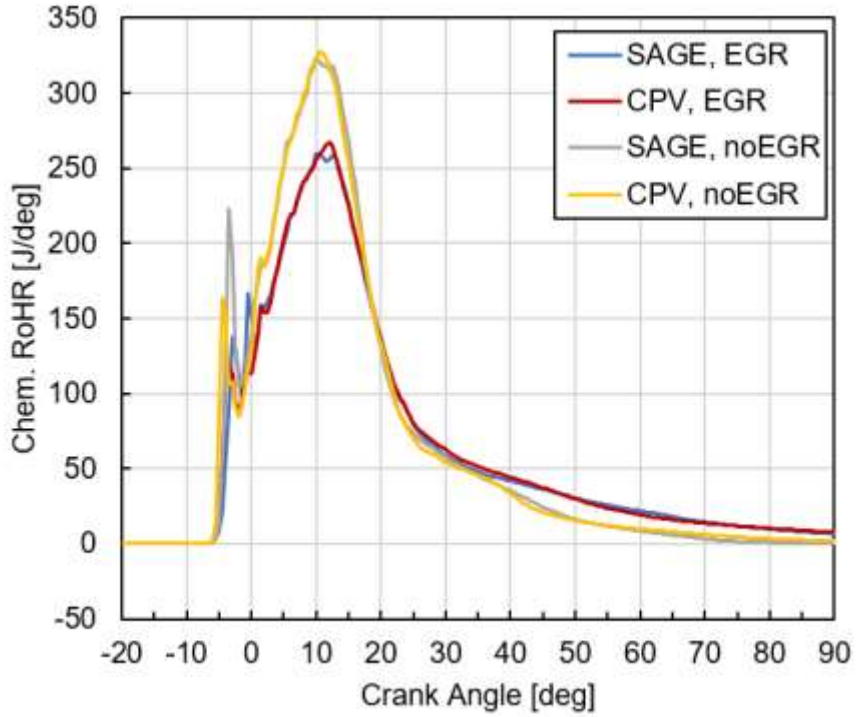
Property	Range	Grid points
EGR [%]	0.0 - 40.0	5
Equivalence ratio [-]	0.2 - 10.0	25
Pressure [bar]	1 – 200	24
Unburnt temperature [K]	300 - 1500	89

- Engine case
  - 1600 rpm
  - Single injection at 9°CA bTDC
  - EGR amount 4% and 30%
  - Bore 137.16 mm
  - Stroke 165.1 mm
  - Connecting rod 263 mm

Diesel Engine Application – Combustion Prediction

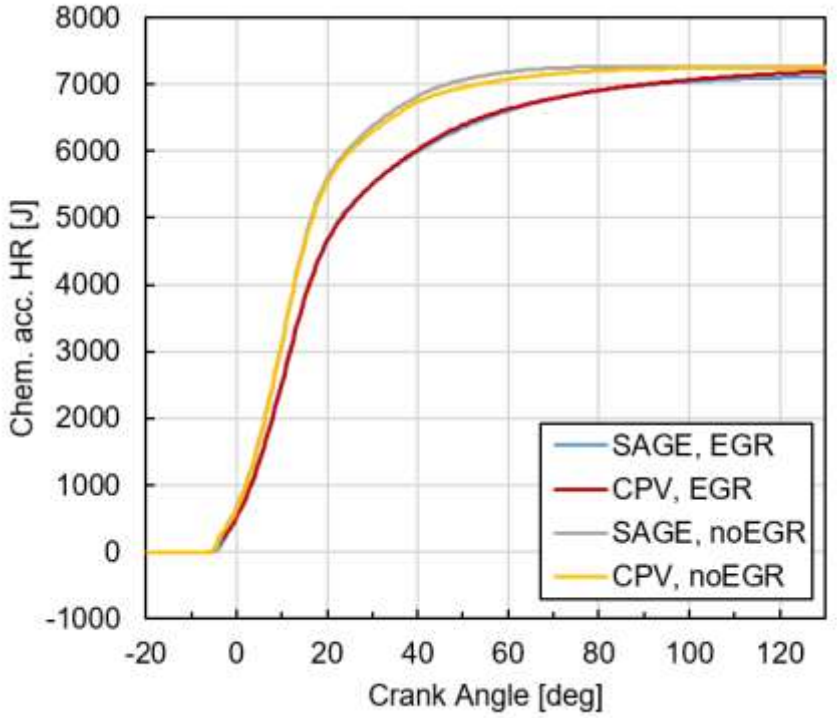
- Validation against SAGE
- No EGR and 30% EGR

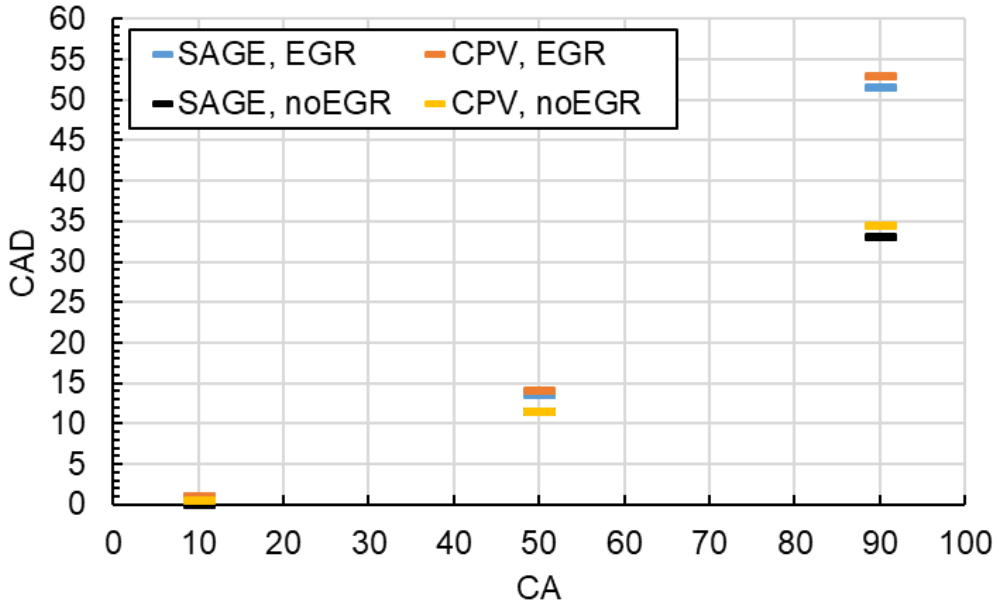




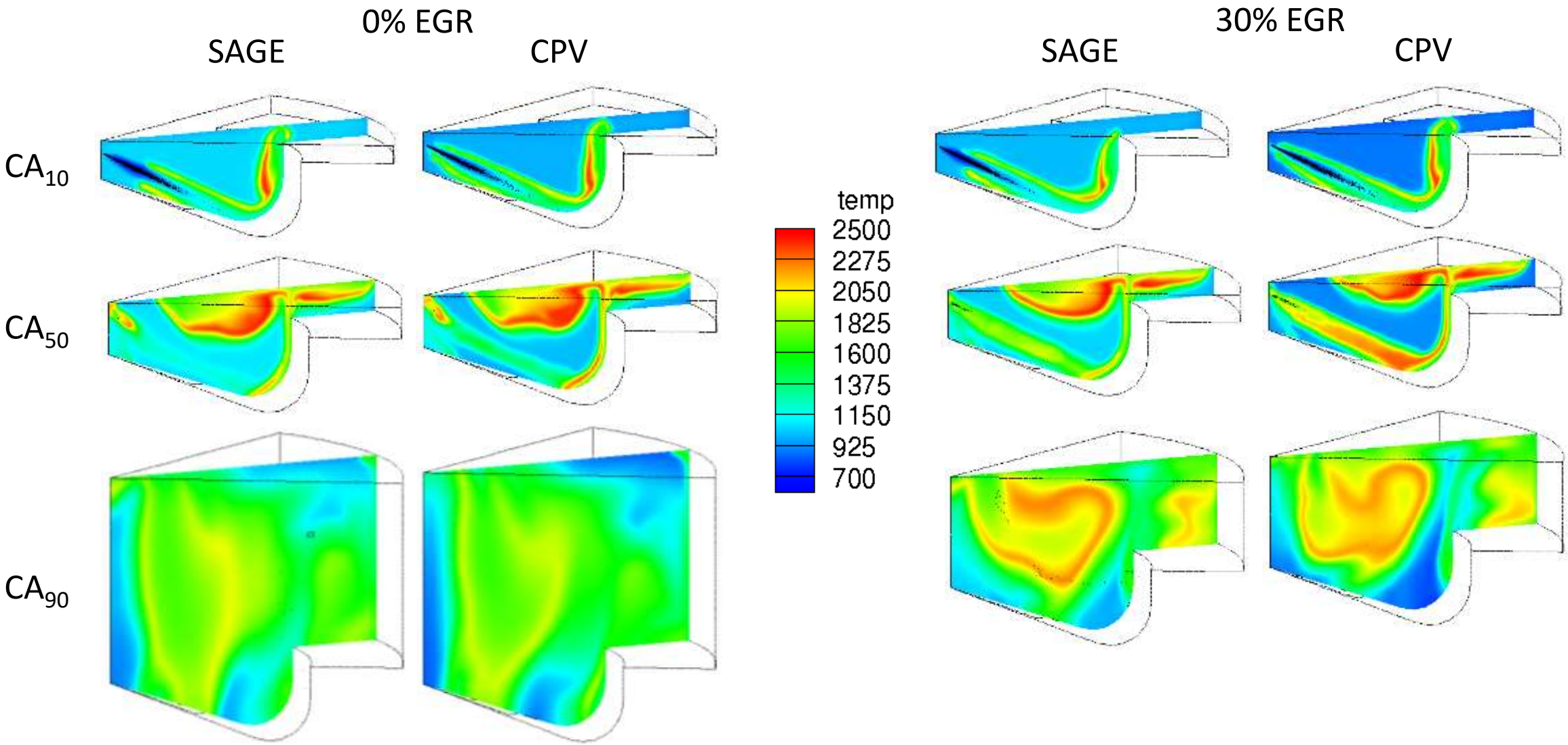
Diesel Engine Application – Combustion Prediction

- Good agreement in accumulated HR
- Good agreement in burn duration (CA_{10}, CA_{50} and CA_{90})





Diesel Engine Application – Combustion Prediction



CPU Times

- Spray A calculations are carried out on 36 cores (2017)
- Diesel engine case are carried out on 20 cores (2016)
- Speed up factor: 4 - 20 and higher depending on the number of species

		Number of Species	Chemistry solver	CPU time
Spray A case		487	SAGE	108.59 h
		487	tabulated	7.95 h
Diesel Engine case	No EGR	121	SAGE	7.66 h
		121	tabulated	2.00 h
	EGR	121	SAGE	8.23 h
		121	tabulated	2.16 h

Conclusion

Conclusion

- The Combustion Progress Variable (CPV) approach is presented
  - Model shows a reasonable good agreement to SAGE on-line chemistry solver and experiment
  - Model is applicable to Spray and DI combustion simulation
  - CPV tables are applicable over a wide range of operating conditions

- CPU times
  - Speed up of factor 4 and higher for 121 species mechanism
  - Speed up of factor more than 20 for the n-dodecane mechanism

- Next steps:
  - implement species based thermodynamics in the code
  - Soot prediction

Thanks!

CONTACT

www.logesoft.com

contact@logesoft.com