A Computationally Efficient Combustion Progress Variable (CPV) Approach for Engine Applications

Corinna Netzer[1], Harry Lehtiniemi[2], Anders Borg[2,4], Andrea Matrisciano[2,4], Adina Werner[1], 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

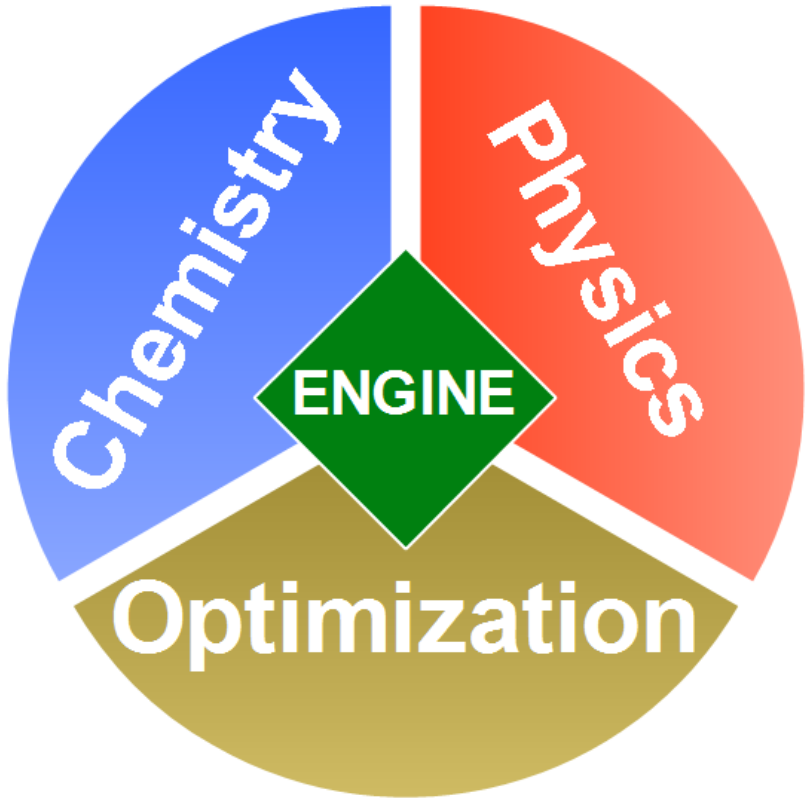
CONVERGE USER CONFERENCE Europe 2018
Bologna, Italy

Brandenburg University of Technology Cottbus - Senftenberg

LOGE LUND COMBUSTION ENGINEERING

Objective

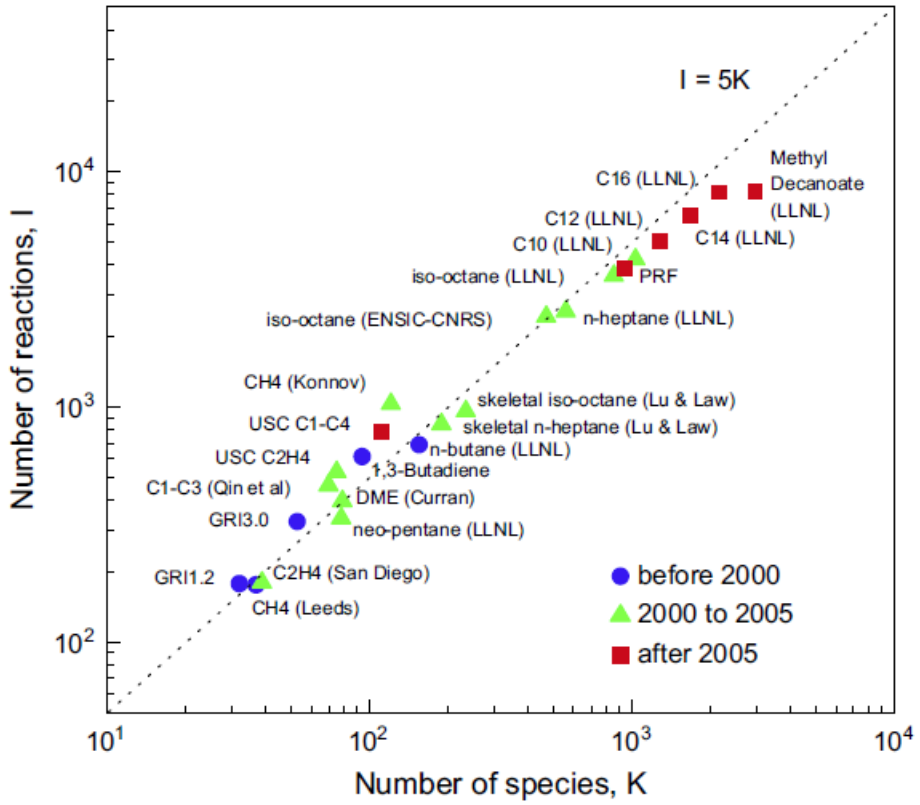
- The main target within internal combustion engine simulation is to achieve predictive results.
- Detailed chemistry schemes play a key role
  - to reproduce fuel sensitivities
    - Knocking combustion
    - ….
  - to predict emissions
    - NOx
    - Soot
    - Unburned hydrocarbons
    - ….
  - to understand new combustion concepts
    - Water injection
    - RCCI
    - …..



Source: Pasternak M. et al., SAE Technical Paper 2012-01-1072 (2012)

Objective

- Availability of detailed chemistry schemes and their complexity are increasing



Source: Liu and Law, Prog. Energ. Combust. (2009)

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:**
   - Diesel Engine
   - Spark Ignition Engine
   - CPU Times

4. **Conclusions**

THE COMBUSTION PROGRESS VARIABLE (CPV) MODEL

General Idea of the CPV (Combustion Progress Variable) Model

- The well-stirred reactor (WSR) combustion model is increasing again in popularity

- The larger the mechanism is, 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

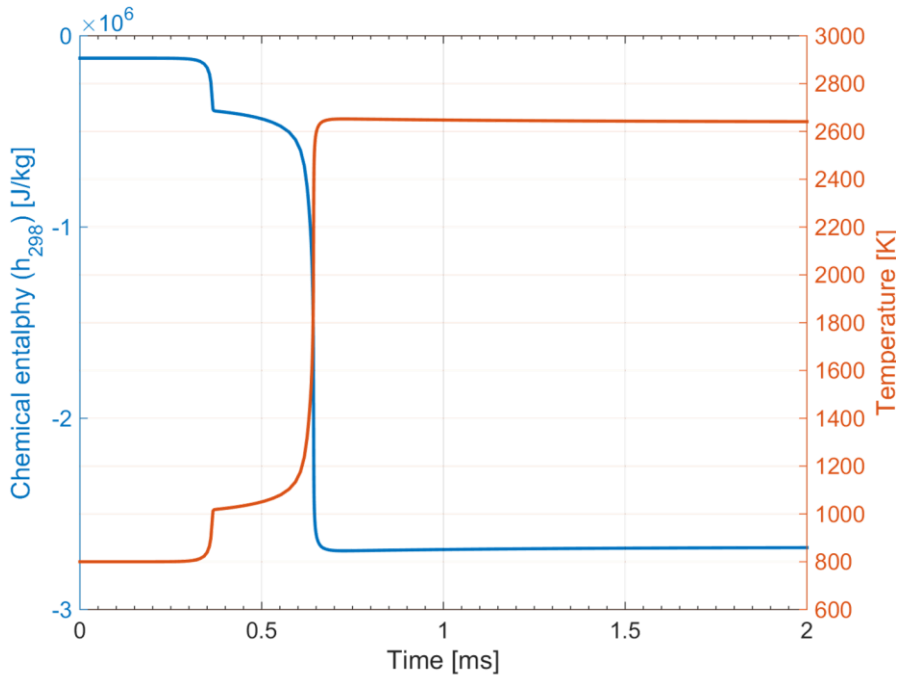
Lehtiniemi et al., Combust Sci Technol 178, 2006

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

- 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)



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.

The Chemistry Look-up Table

- 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

Table look-up parameters

- Pressure p
- Unburned Temperature T
- Equivalence ratio ϕ
- EGR amount Y_{EGR}

Info stored in the look-up table

- Progress variable source terms $\frac{dC}{dt}$
- Molar mass of the mixture M_{mix}
- Thermodynamic polynomial coefficients
- Chemical species for thermodynamics
- Any chemical species that the user decides to monitor
- Emission source terms

Fuel
O_2
N_2
CO_2
H_2O
CO
H_2
C_2H_2
C_2H_4

Soot
NO_x

The Chemistry Look-up Table

- Exemplary dimensions of a CPV table for Diesel application

Property	Range	Grid points
EGR [%]	0.0 – 40.0	5
Equivalence ratio [-]	0.2 - 4.0	19
Pressure [bar]	1.0 - 200.0	17
Unburnt temperature [K]	350.0 - 1400.0	67
Progress Variable	0.0 -1.0	15

Temperature Grid Points:
3 points in the range [350 ; 550] K
45 points in the range [560 ;1000] K
11 points in the range [1020 ;1200] K
8 points in the range [1225 ;1400] K

191 520 points

1 GB

- Table generation done via LOGEtable v1.0
  - CPU time for table generation: 3h
    on 8 parallel cores (2016)

Combustion Progress Variable Model

- The combustion model is replaced, chemistry solution from the look-up table
- Transport of passives and species by CFD code
- Communication over source subroutine

CFD Code

Transport of
- Chemical enthalpy H_{298}
- Mixture fraction Z
- Mass fraction EGR Y_{EGR}
- Species for thermodynamics
- Emissions

Extra output species are assigned as passive_nt

Table look-up parameters
- p
- T
- ϕ
- Y_{EGR}

Combustion Progress Variable Model

Combustion
Well-stirred reactor model with source terms from the CPV table

Soot
Method of Moments M_0 and M_1

NOx
Thermal NO

Update of sources
- H_{298}
- Z
- Y_{EGR}

Species / emission update

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

  - If tuning is required, it is possible to scale the chemical reaction source term

- 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

Additional transport equations (cont.)

- Thermal NO marker

$$\frac{\partial \bar{\rho} \widetilde{Y_{NO}}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{v}} \widetilde{Y_{NO}}\right) - \nabla \cdot \left(\bar{\rho} D_t \nabla \widetilde{Y_{NO}}\right) = \overline{\rho \omega_{NO}}$$

Solved by CONVERGE

Solved by CPV

- Soot moments M_0 and M_1

$$\frac{\partial \bar{\rho} \widetilde{M_r}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\boldsymbol{v}} \widetilde{M_r}\right) - \nabla \cdot \left(\bar{\rho} D_t \nabla \widetilde{M_r}\right) = \overline{\rho \dot{\omega}_r}$$

Solved by CONVERGE

Solved by CPV

- The thermal NO model can be calibrated using calibration parameters A, B, C and D. Usually it is only needed to use parameter A.

- The soot model allows for calibration through scaling source terms for:
  - Nucleation, Surface growth, fragmentation, oxidation by O_2 and oxidation by OH

APPLICATION: DIESEL ENGINE

Diesel Engine Application (1)

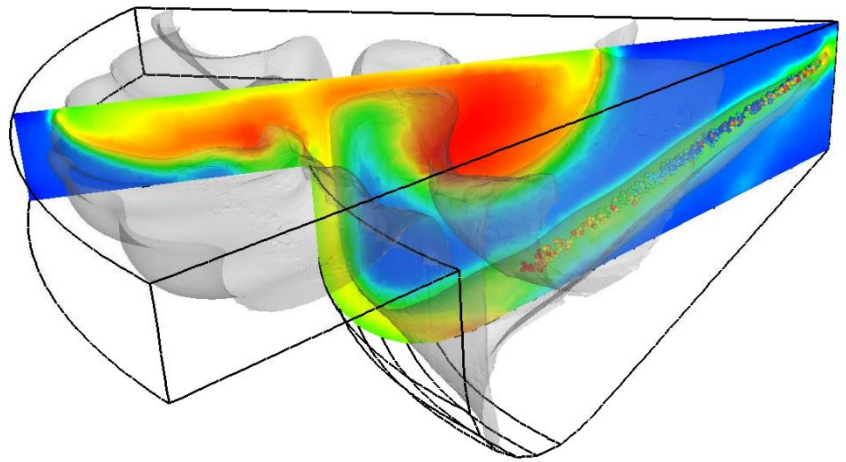
- Reaction scheme
  - Reduced n-heptane reaction scheme
    - 56 species and 206 reactions
  - Low and high temperature chemistry
  - Pathways for major engine out emissions

Seidel et al., J. Eng. Gas Turbines and Power 2017

- CPV table

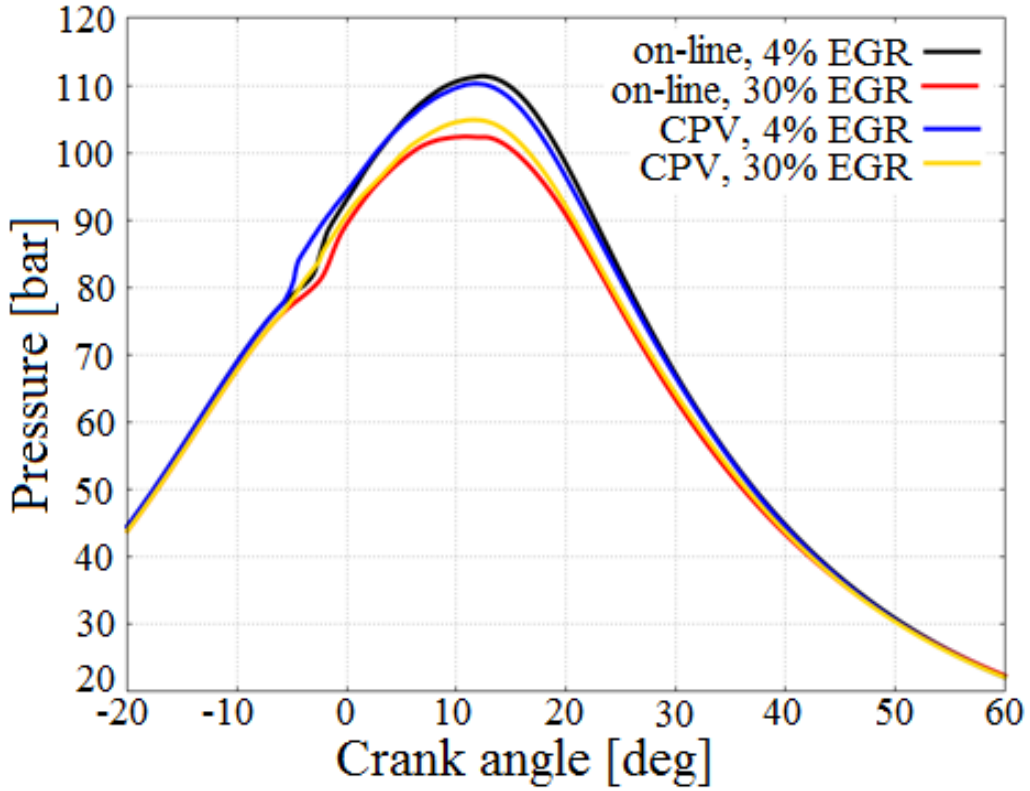
Property	Range	Grid points
EGR [%]	0.0 – 50.0	6
Equivalence ratio [-]	0.1 - 10.0	38
Pressure [bar]	1.0 - 200.0	24
Unburnt temperature [K]	300.0 - 1500.0	89

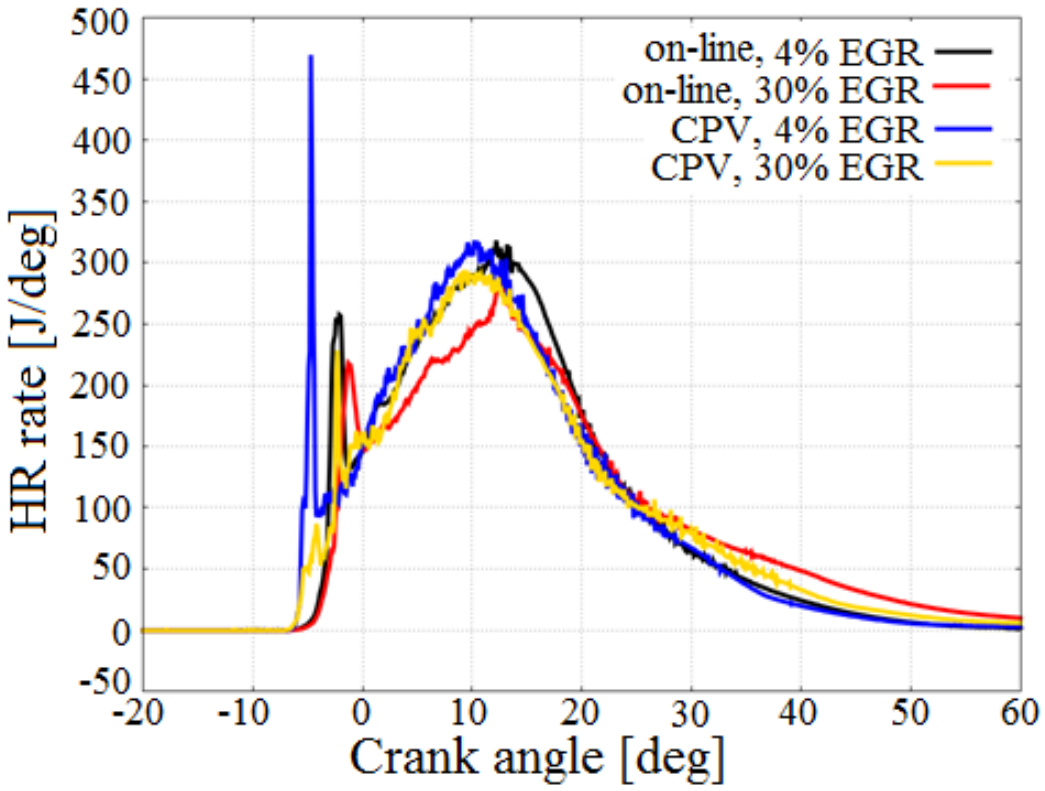
- Engine case
  - 1600 rpm
  - Single injection at 9°CA bTDC
  - EGR amount 4% and 30 %
  - Bore 137mm
  - Stroke 165 mm
  - Connecting rod 263 mm



Diesel Engine Application (1) – Combustion Prediction

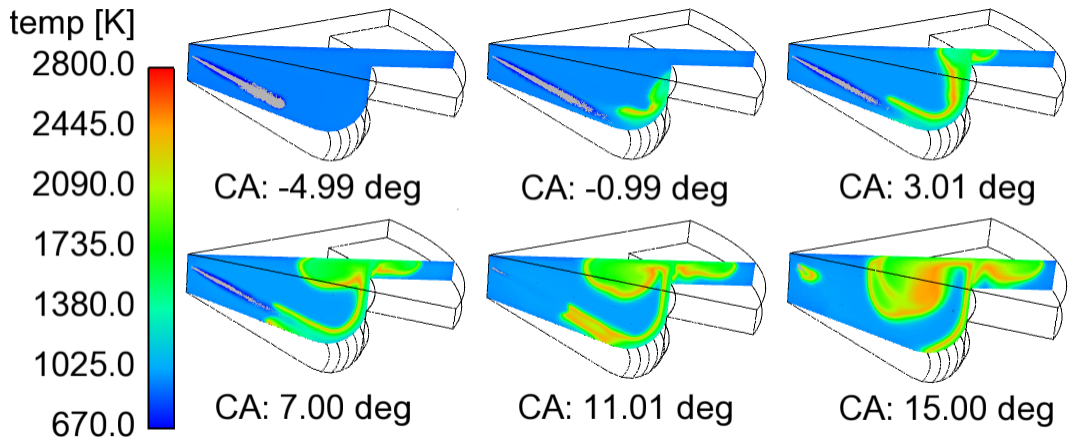
- Validation against on-line chemistry solver
  - CPV model is compared to a on-line well-stirred reactor model (LOGE API)
- EGR amount 4% and 30%

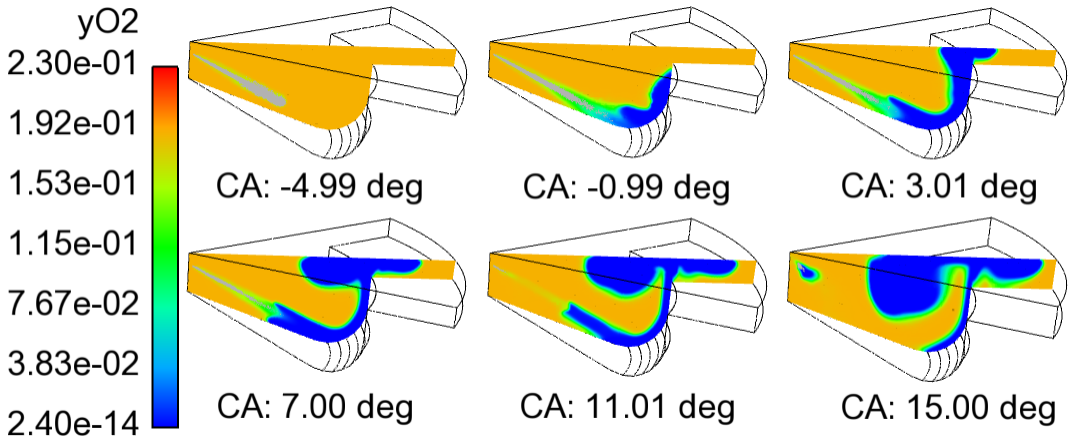




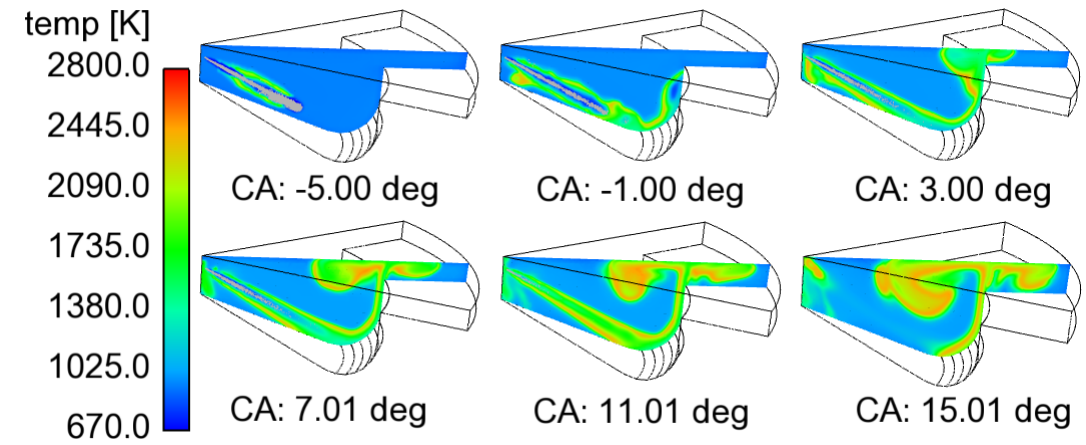
Diesel Engine Application (1) – Combustion Prediction

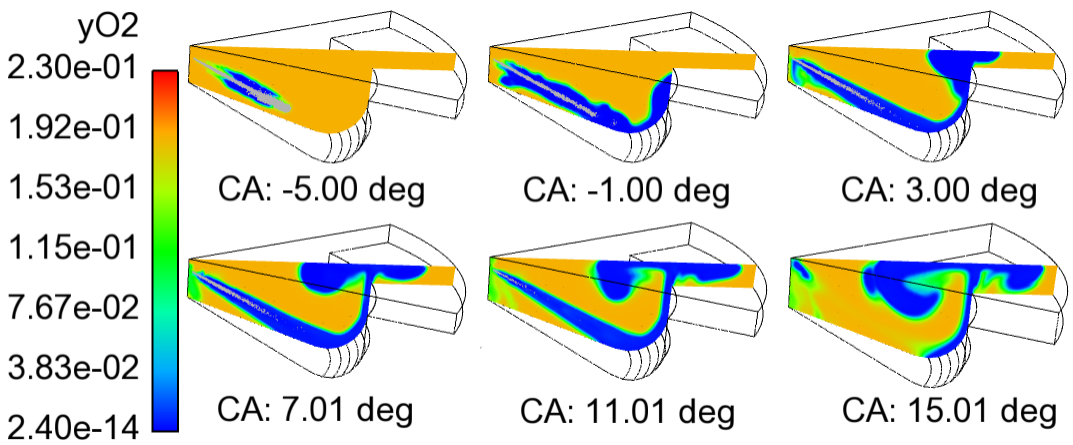
LOGE API – 30 % EGR





CPV – 30 % EGR





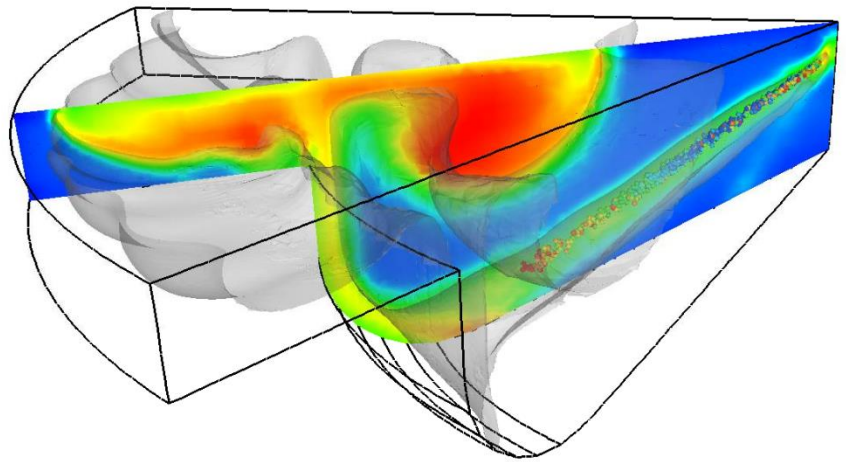
Diesel Engine Application (2)

- Reaction scheme
  - LOGEDiesel:
    - Surrogate: 75% n-Decane and 25% α-Methyl-Napthalene
    - 189 species and 2483 reactions
  - Low and high temperature chemistry
  - Pathways for major engine out emissions

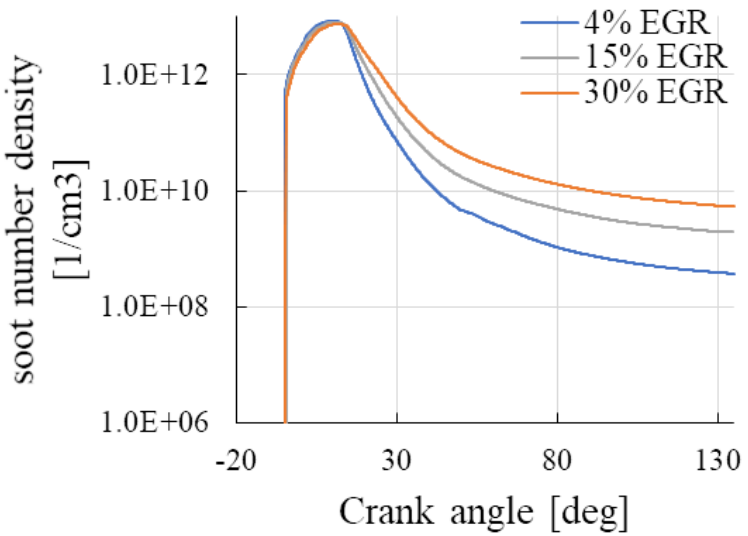
- Engine case
  - 1600 rpm
  - Single injection at 9°CA bTDC
  - EGR amount 4%, 15% and 30 %
  - Bore 137mm
  - Stroke 165 mm
  - Connecting rod 263 mm

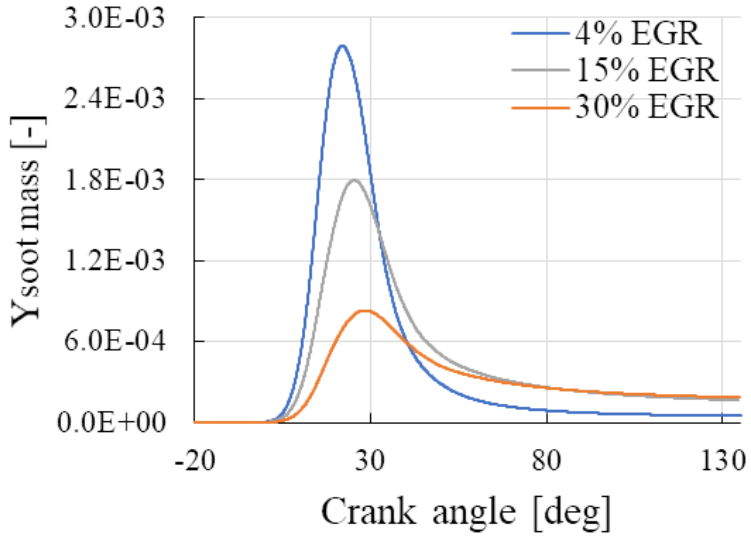
- CPV table

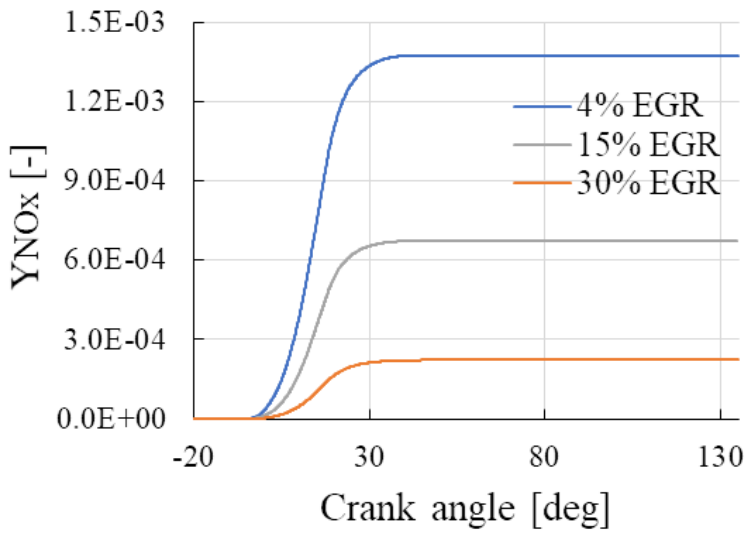
Property	Range	Grid points
EGR [%]	0.0 – 50.0	6
Equivalence ratio [-]	0.1 - 4.0	20
Pressure [bar]	1.0 - 200.0	17
Unburnt temperature [K]	300.0 - 1500.0	22

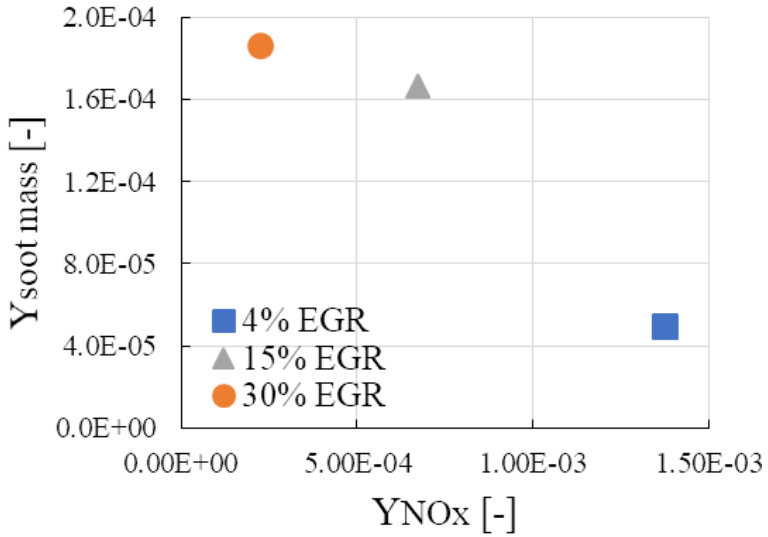


Diesel Engine Application (2) – Emissions Prediction









- Soot and NO_x prediction are as expected from literature
- 4% EGR has highest soot formation and oxidation rates
- Soot-NO_x trade-off is reasonable

LOGE LUND COMBUSTION ENGINEERING

b-tu Brandenburg University of Technology Cottbus - Senftenberg

APPLICATION: SPARK IGNITION ENGINE

Spark Ignition Engine Application

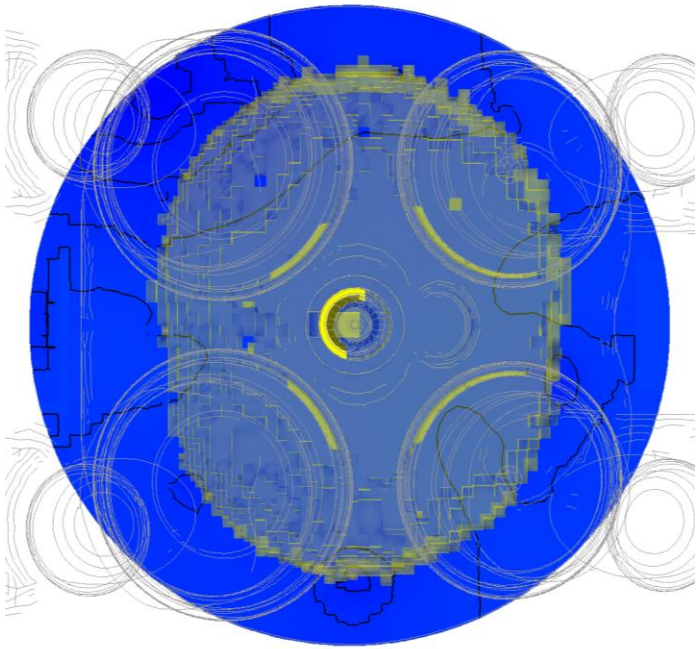
- Reaction scheme
  - PRF reaction scheme
    - Surrogate octane rating: 95
    - 48 species and 152 reactions
  - NO_x updates
  - Pathways for major engine out emissions

Yao-Dong et al. Energy and Fuels, 2012

- CPV table

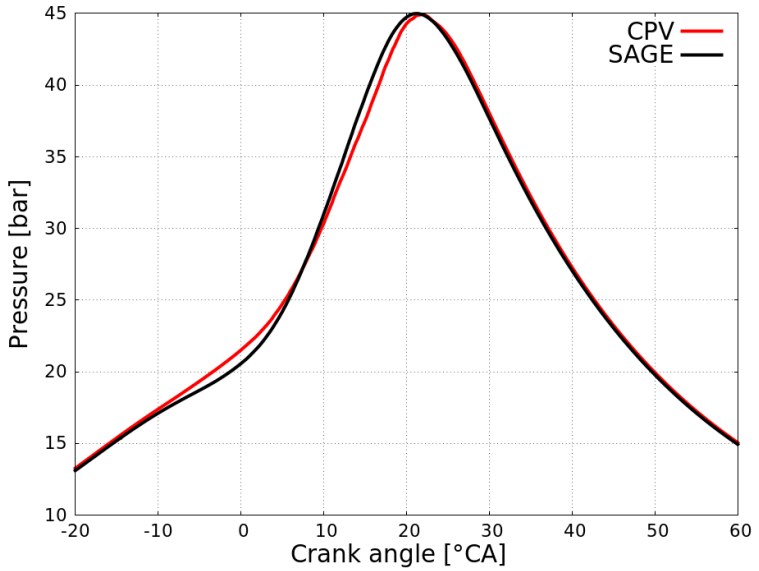
Property	Range	Grid points
EGR [%]	0.0 – 10.0	3
Equivalence ratio [-]	0.9 – 1.1	5
Pressure [bar]	1.0 - 200.0	17
Unburnt temperature [K]	300.0 - 1400.0	67

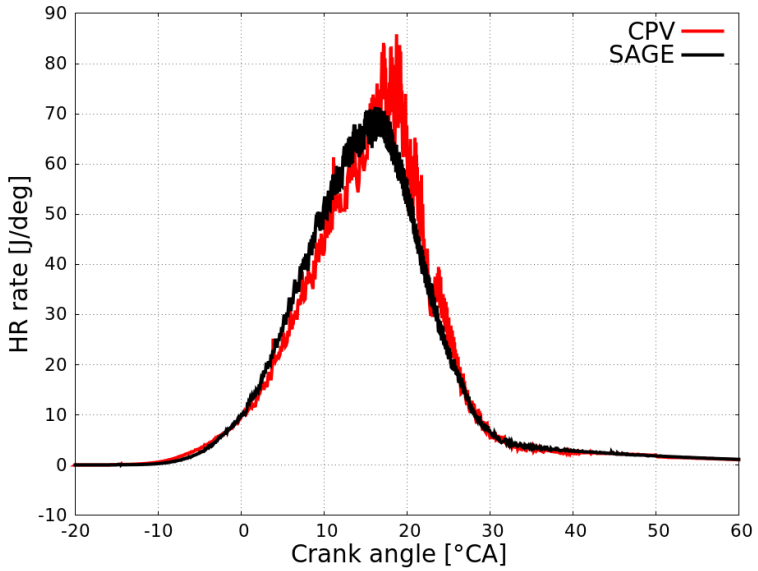
- Engine case
  - 3000 rpm
  - Spark timing 15°CA bTDC
  - Bore 86 mm
  - Stroke 90 mm
  - Connecting rod 180 mm

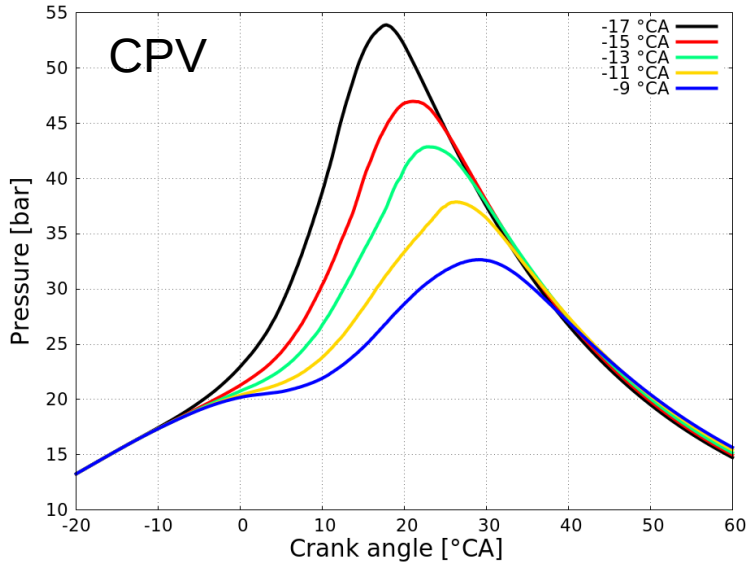


Spark Ignition Engine – Combustion Prediction

- Validation against on-line chemistry solver
  - CPV model is compared to a online well-stirred reactor model (SAGE)



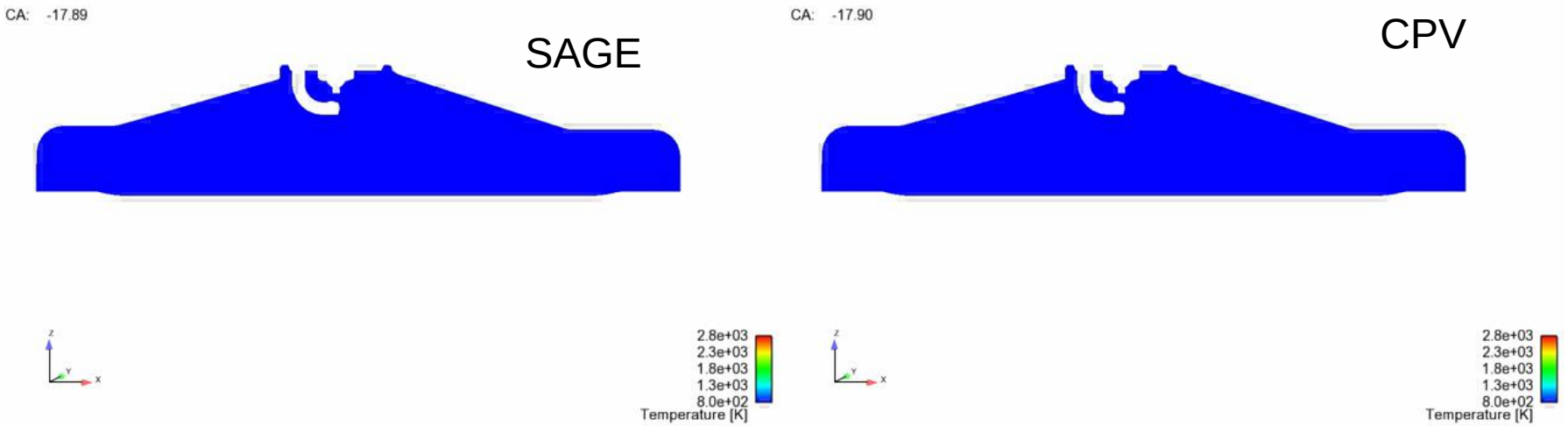




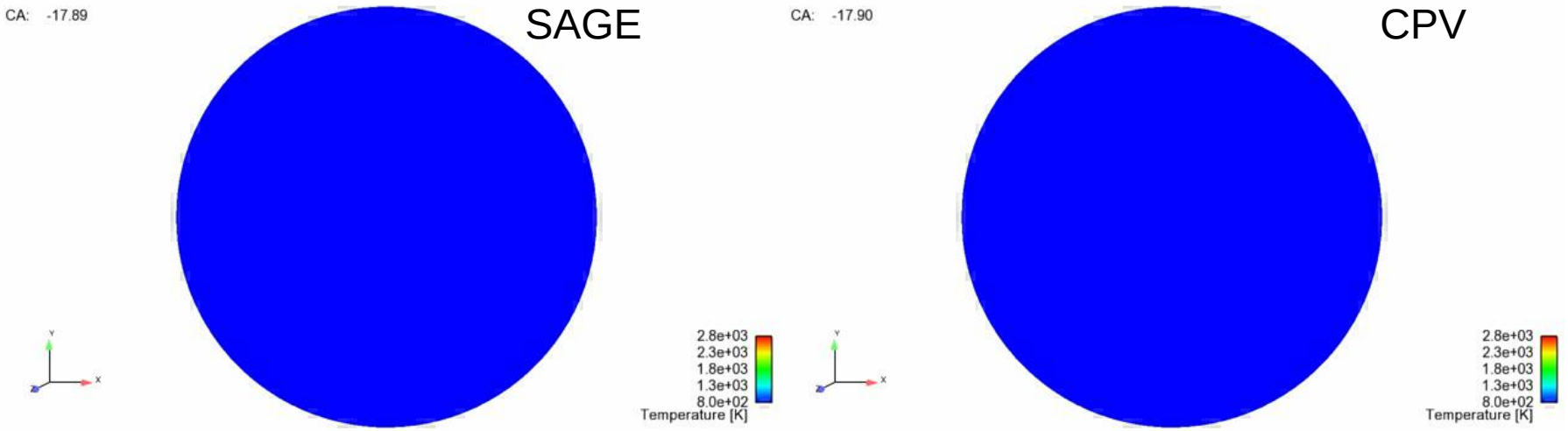
Spark Ignition Engine – Combustion Prediction

- Validation against on-line chemistry solver

View on clip plane y=0



View from top



CPU Times

- All calculations are carried out on 32 cores (2008)
- Speed up factor: 2 and higher

	Number of Species	Chemistry solver	CPU time [hours]
Diesel Sector Case	56	On-line	36.7
	56	LOGE-CPV	15.7
	189	LOGE-CPV	15.2
SI - Full Cylinder Case	48	On-line	73.8
	48	LOGE-CPV	40.1

No CPU time increase due to additional soot and NO_x model or more species

CONCLUSIONS

Conclusions

- A Combustion Progress Variable (CPV) approach is presented
  - Model shows a reasonable good agreement to on-line chemistry solver
  - Model is applicable to DI and SI combustion simulation
  - Emission prediction is physical reasonable
  - CPV tables are applicable over a wide range of operating conditions
- CPU times
  - Speed up of factor 2 for the 56 species mechanism, higher speed-up for larger mechanisms (up to factor 700)
  - Emission prediction free of CPU costs
- Next steps:
  - Updates to species treatment for thermodynamics
  - Updates to improve vaporization

THANK YOU!