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A computationally efficient combustion progress variable (CPV) approach for engine applications

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Introduction

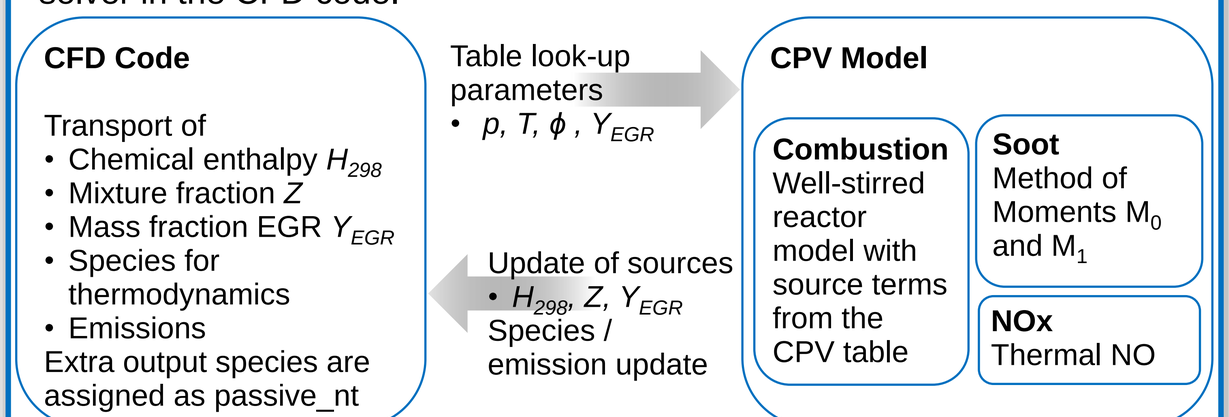
In modern Computational Fluid Dynamic (CFD) simulations of internal combustion engine detailed chemistry schemes are important, also for the prediction of soot. The more and more available complex detailed chemistry schemes including more species can obtain more accurate results. The biggest disadvantage is the high demand of computational cost due to the high number of transported scalars and the chemistry solver. The tabulated chemistry approach which use the chemical enthalpy h_{298} as a progress variable is proposed to overcome this problem.

The CPV model

The base for this approach forms the assumption that a progress variable C can be used for the reconstruction of the thermo-chemical state on the whole reaction trajectory. C is defined as a function of the chemical enthalpy h_{298}:

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

The chemistry is solved using constant pressure reactors and stored in a look-up table (CPV table). The generated loo-up replaces the chemistry solver in the CFD code.



Only 9 CPV species are transported and used to calculate the thermodynamics of the gas phase: Fuel, O_2, N_2, CO_2, H_2O, CO, H_2, C_2H_2, C_2H_4.

Reaction schemes

Table 1: CPV table ranges.

	reduced *n*-heptane		*n*-decane/ *α*-methyl-naphthalene	
Species	56		189	
Reactions	206		2483	
Property	Range	Grid points	Range	Grid points
EGR [%]	0.0 – 50.0	6	0.0 – 50.0	6
Equivalence ratio [-]	0.1 - 10.0	38	0.1 - 4.0	20
Pressure [bar]	1.0 - 200.0	24	1.0 - 200.0	17
Unburnt temperature [K]	300.0 - 1500.0	89	300.0 - 1500.0	22

The *n*-heptane mechanism is used to compare the tabulated versus on-line combustion prediction. The more complex *n*-decane/*α*-methyl-naphthalene mechanism consists 75 mass% n-decane and 25 mass% α-methyl-naphthalene is to predict emissions.

Engine case

For this study a diesel engine sector case is used (137 mm bore, 165 mm stroke and 263 mm connecting rod). The engine operates at 1600 rpm and the fuel is injected as single injection at 9° CA bTDC. The EGR amount is set to 4%, 15% and 30%.

Results and Discussion

The HR rate indicates that the CPV cases ignites earlier than the on-line chemistry cases. Further, the premixed peak of the CPV case for 4% EGR is recognizable higher than the other premixed peaks. The reason for that can be understood considering Figure 2. The CPV case ignites earlier and around the whole injection cone, whereas the on-line solution shows a clear lift-off. The reason of the early ignition is because of the use of 9 species for the thermodynamics in the CPV model only. The injected mass can either be assigned to n-heptane or to small hydrocarbons as C_2H_4, whereas in the on-line calculation several possible decomposition pathways with different contribution to the thermodynamic state are available.

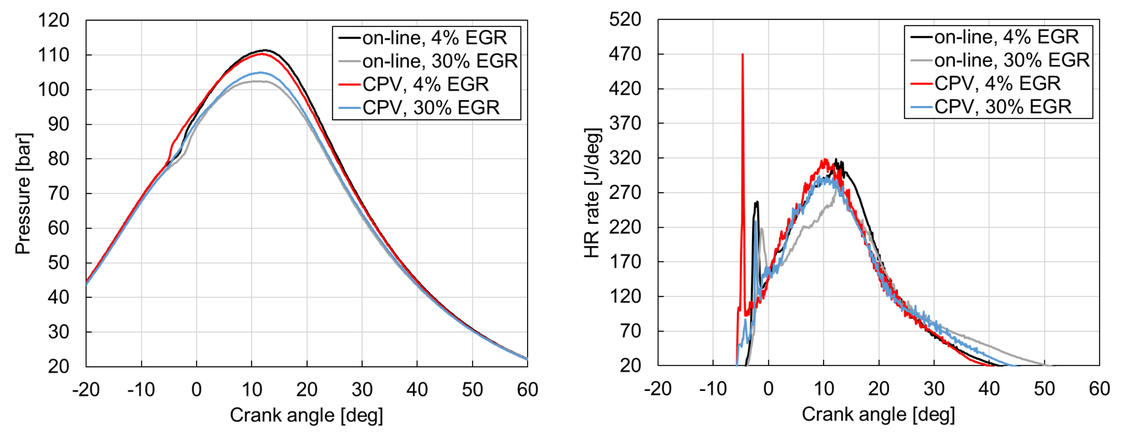


Figure 1: Pressure and Heat release (HR) rate comparison between CPV and on-line chemistry

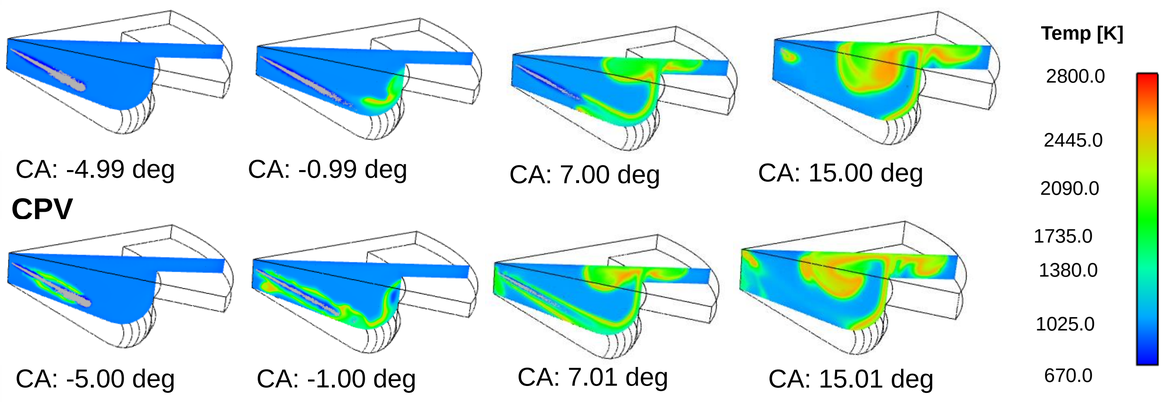


Figure 2: 3D post-processing: Temperature profiles from on-line and CPV cases with 30% EGR.

The results in figure 3 are reasonable. A low EGR amount leads first to a higher soot formation rate, but because of the higher temperatures and available oxygen and hydroxyl radicals, the soot is oxidized during expansion. As a result the soot number density and the soot mass are the lowest at (exhaust valve opening) EVO. The lower soot production by lower EGR amounts results on the other hand in a higher NOx production.

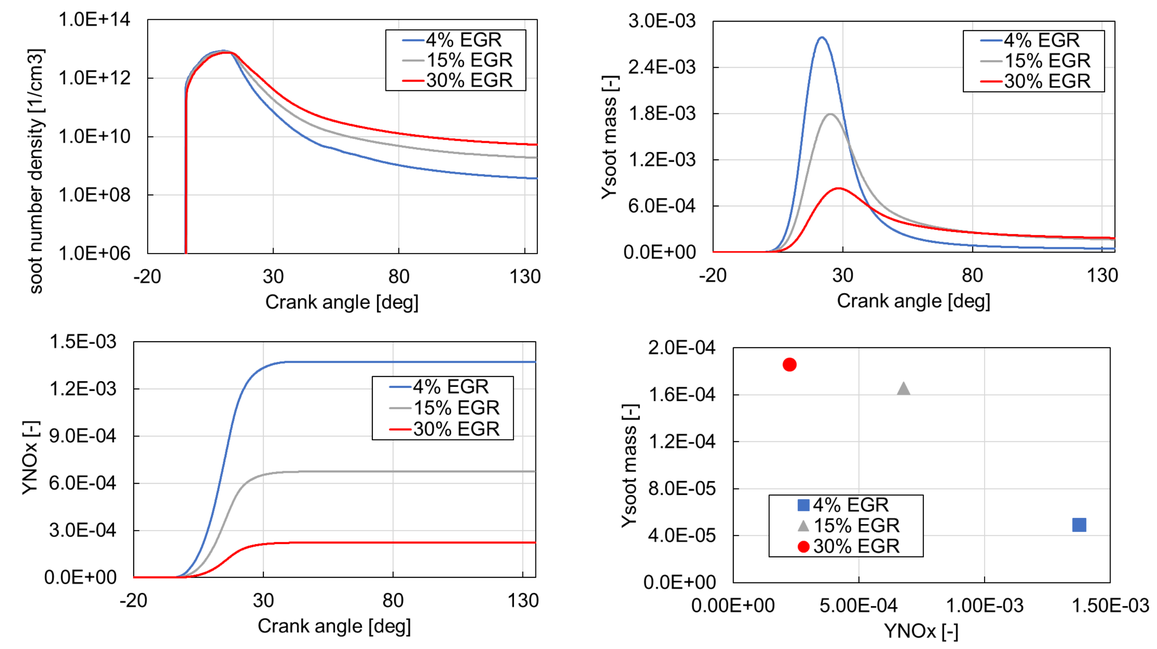


Figure 3: CPV *n*-decane/*α*-methyl-naphthalene mechanism results with different EGR amounts

Number of species	Chemistry solver	CPU time [h]
56	On-line	36.7
56	LOGE-CPV	15.7
189	LOGE-CPV	15.2

Conclusions

The combustion prediction using the CPV approach agrees reasonable with the on-line chemistry solver. Also, the emission prediction is plausible. The CPV times …

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