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Further Application of the Fast Tabulated CPV Approach

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Introduction

A reaction mechanism describes the combustion of a surrogate fuel and accounts for chemical and physical properties of the commercial fuel. The use of complex detailed reaction mechanisms in 3D Computational Fluid Dynamic (CFD) simulations can lead to a high demand of computational costs. One possible solution to reduce these costs is to use tabulated chemistry methods. In this work, two applications predicted using the detailed chemistry solver SAGE and the tabulated combustion progress variable (CPV) approach are presented. Good agreement between the two models are found for a diesel engine sector case and the Spray A from the Engine Combustion Network (ECN).

The CPV model

The CPV model assumes 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} [1]:

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

The look-up tables were generated with LOGEtable [2] using adiabatic homogeneous constant pressure reactors. The generated table replaces the chemistry solver in the CFD code [3].

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 passives

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

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

Species / emission update

CPV Model

Combustion
Well-stirred reactor model [8, 9] with source terms from the CPV table

Soot
Method of Moments M_0 and M_1 [10, 11, 12]

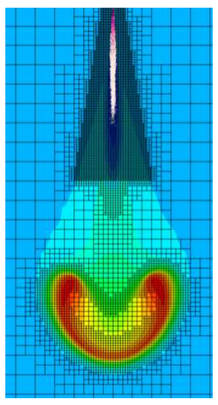
NO_x
Thermal NO

Only 19 CPV species are transported and used to calculate the thermo-dynamics of the gas phase.

Table 1: Used reaction schemes and CPV table ranges.

	***n*-dodecane** [4]		***n*-heptane** [5]	
Species	487		121	
Reactions	2331		594	
Property	Range	Grid points	Range	Grid points
EGR [%]	0.0 – 40.0	5	0.0 – 40.0	5
Equivalence ratio [-]	0.2 - 10.0	25	0.2 - 10.0	25
Pressure [bar]	1.0 - 200.0	18	1.0 - 200.0	24
Unburnt temperature [K]	250.0 - 1500.0	101	300.0 - 1500.0	89

Simulation Setup



The Spray A from the ECN [6] is modelled using the 3D CFD Code CONVERGE [7]. The chosen geometry is a cube with an edge length of 10.8 cm. The turbulence is predicted using the Reynolds Averaged Navier-Stokes (RANS) model. To different combustion models are applied: the SAGE detailed chemistry solver [7] to solve the chemistry on the fly and the CPV model [3].

Further, a diesel engine sector case (137 mm bore, 165 mm stroke and 263 mm connecting rod) is modelled. The engine operates at 1600 rpm and the fuel is injected as single injection at 9° CA bTDC. Two different cases with no EGR and 30 % EGR amount were compared.

Results and Discussion

Figure 1 shows the predicted pressure of the detailed chemistry solver SAGE and the CPV model versus the experimental pressure for Spray A. The pressure is well predicted by both combustion models. The first differences occur at 0.2 ms, where the first liquid parcels leave the fixed cell cone. The deviation between SAGE and CPV may be caused by differences in the mesh refinement and time stepping.

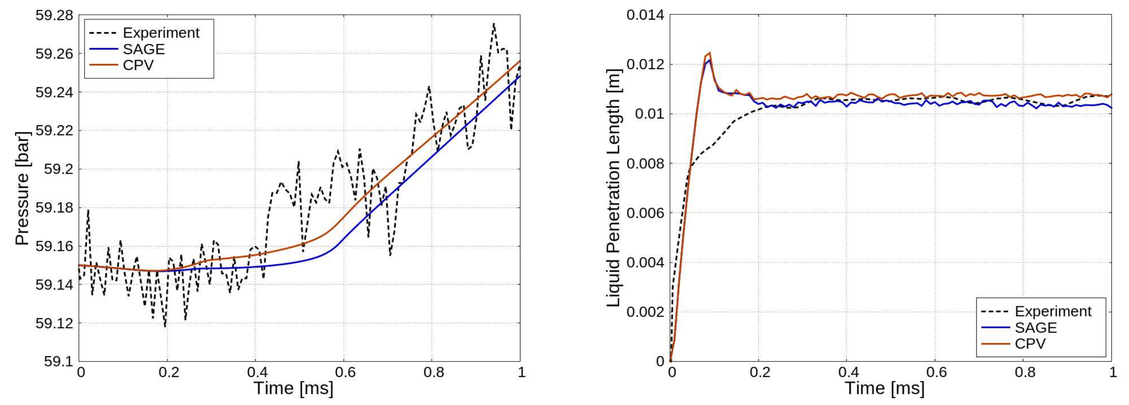


Figure 1: Comparison of the predicted pressure and liquid penetration length using SAGE and CPV versus experiment.

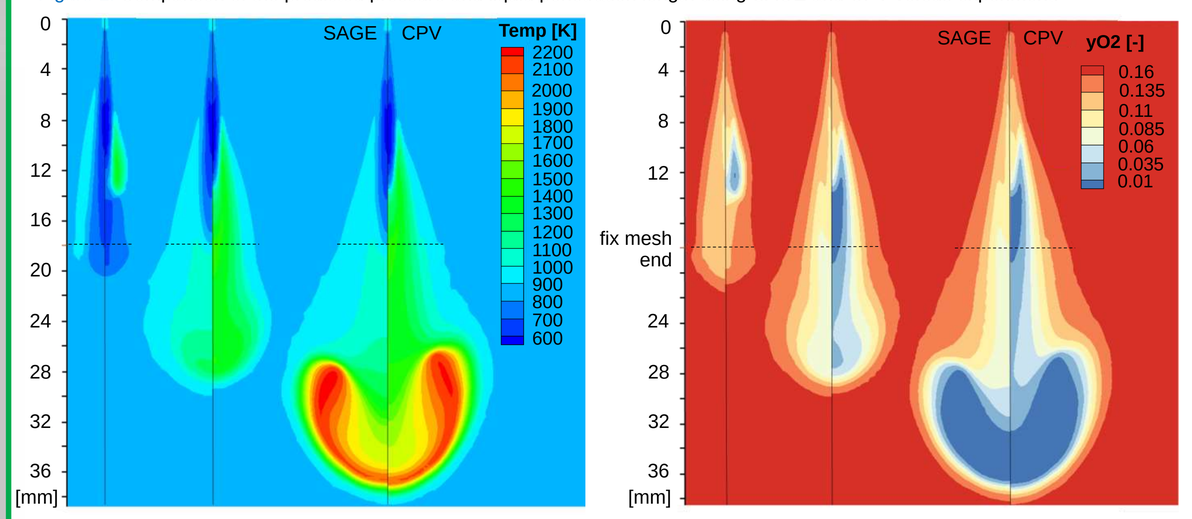


Figure 2: Temperature and O_2-mass fraction profile of SAGE (left) and CPV (right) at 0.2 ms, 0.425 ms and 0.725 ms.

Figure 2 shows the temperature and O2-mass fraction profile of SAGE and CPV at three different time steps. The overall behaviour is similar. The ignition behaviour is unexpected. Both cases ignite next to the spray cone, not at the tip of the spray. The CPV predicts higher temperatures and less O2 in the same regions. A possible reason for this discrepancy is the thermodynamic treatment within CPV, where only 19 species are available. This treatment will be investigated further in future.

Figure 3 shows the prediction of the pressure and rate of heat release (RoHR) for the engine sector case for both EGR levels and combustion models. The prediction of both combustion models agrees well. As expected, a higher EGR amount leads to a lower mean pressure and RoHR. The temperature profile (Figure 4) shows an overall good agreement.

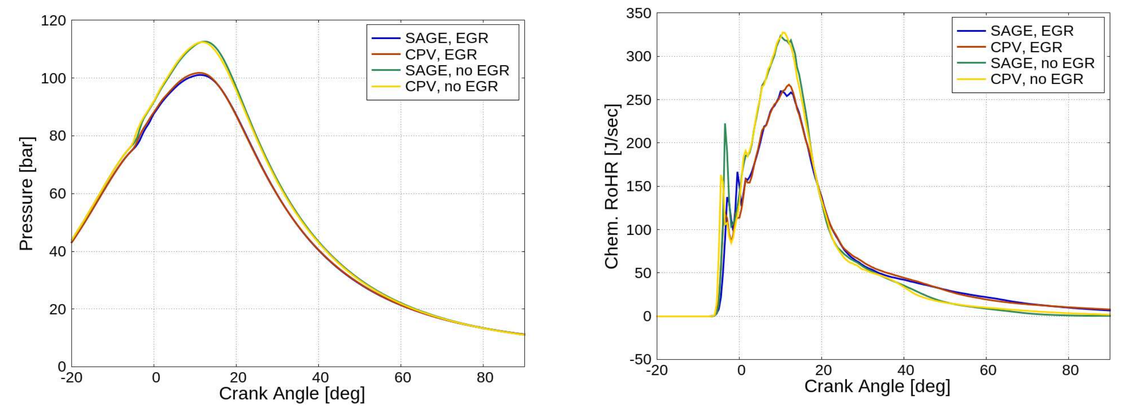


Figure 3: Predicted pressure and chemical RoHR of SAGE and CPV for different EGR amounts (no EGR: 0%; EGR: 30%).

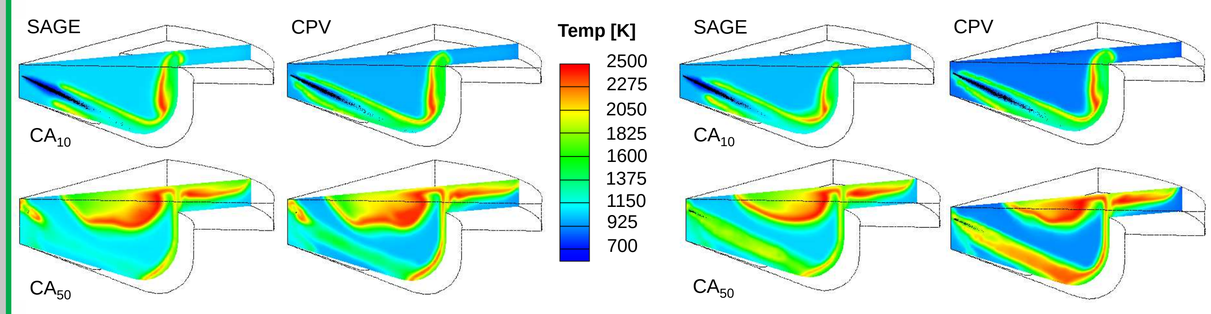


Figure 4: Temperature profile of SAGE and CPV for no EGR (left) and 30% EGR (right) at two different time steps.

Table 2: Comparison of CPU times SAGE vs CPV and 487 species vs 121 species.

Number of species	SAGE CPU time [h]	CPV CPU time [h]
487	169.98	13.74
121	7.66 / 8.23	2.00 / 2.16

Conclusions

The tabulated combustion progress variable approach leads to good and reasonable results compared to the SAGE detailed chemistry solver and the experiment. The tabulated approach decreases the CPU times by factor 13 for the n-dodecane mechanism and by factor 4 for the smaller n-heptane mechanism. Future work will include emission prediction and validation.

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