Further Application of the Fast Tabulated CPV Approach

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Abstract

A reaction mechanism describes the combustion of a surrogate fuel and accounts for chemical and physical properties of the commercial fuel. Detailed chemistry can also capture the impact of exhaust gas recirculation (EGR) and radicals or NOx in the residual gas. The use of complex detailed reaction mechanisms in 3D Computational Fluid Dynamic 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.

Introduction

The main target in modern Computational Fluid Dynamic (CFD) simulations of internal combustion engine combustion is to obtain predictive results. The use of complex detailed chemistry reaction schemes with a high number of species and reactions is indispensable to reach this aim. To overcome the disadvantage of high computational cost tabulated chemistry approaches were used. In this work, a tabulated progress variable approach based on the chemical enthalpy h_{298} is applied. The benefit of this approach is the independence of the CPU costs on the number of species and reactions in a reaction scheme.

The Combustion Progress Variable (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. The normalized reaction progress variable C is defined as a function of the enthalpy of formation at standard state (h_{298}) as follows [1]:

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

h_{298} is the current enthalpy in the cell, $h_{298,0}$ the enthalpy of formation at unburned state and $h_{298,min}$ the enthalpy of formation at the most reacted burned state, where the maximum chemical heat is released. With this approach, both low and high temperature reactions can be tracked.
The look-up tables were generated with LOGEtable [2] using adiabatic homogeneous constant pressure reactors. The look-up parameters are the unburned temperature (T_u), pressure (p), equivalence ration (Φ) and the EGR amount (Y_{EGR}). Only 19 CPV species are transported and

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used to calculate the thermodynamics of the gas phase. The generated table replaces the chemistry solver in the CFD code [3].

Reaction schemes

A n-dodecane reaction mechanism with 487 species is used for the Spray A simulation. The n-dodecane model is a skeletal scheme and uses the mechanism published in [4] as core model. For the diesel engine case a n-heptane reaction mechanism [5] with 121 species is applied. Table 1 shows the used ranges to generate the look-up tables.

Table 1: CPV table ranges for the n-dodecane and n-heptane reaction mechanism.

	n-dodecane		n-heptane	
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 - 200	18	1 – 200	24
Unburned temperature [K]	250.0 - 1400.0	101	300 - 1500	89

Simulation setup

The Spray A from the Engine Combustion Network [6] is modeled using the 3D CFD Code CONVERGE in the version 2.4.19 [7]. The chosen geometry is a cube with an edge length of 10.8 cm. The base grid has a length of 2 mm. The adaptive mesh refinement (AMR) is used to downsize cells as function of temperature and velocity. Close to the injector, the cell size is fixed to 0.125 mm. For the spray modelling the Kelvin-Helmholtz (KH) model, the dynamic drop drag model, the O'Rourke model for the turbulent dispersion and the Frossling model for evaporation are applied as implemented in Converge 2.4.19 [7]. The turbulence is predicted using the Reynolds Averaged Navier-Stokes (RANS) model and the standard k-ε-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. Combustion and turbulence models are the same as given above.

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. At this time step, 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.

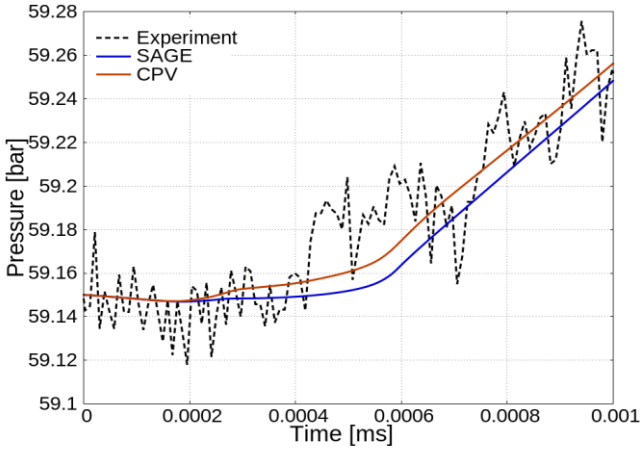

Figure 1: Comparison of the predicted pressure using SAGE and CPV versus experiment.

Figure 2 shows the temperature and O_2-mass fraction profile of SAGE (left) and CPV (right) at three different time steps. The overall behavior is similar. The ignition behavior is unexpected. Both cases ignite next to the spray cone, not at the tip of the spray. The CPV predicts higher temperatures and less O_2 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.

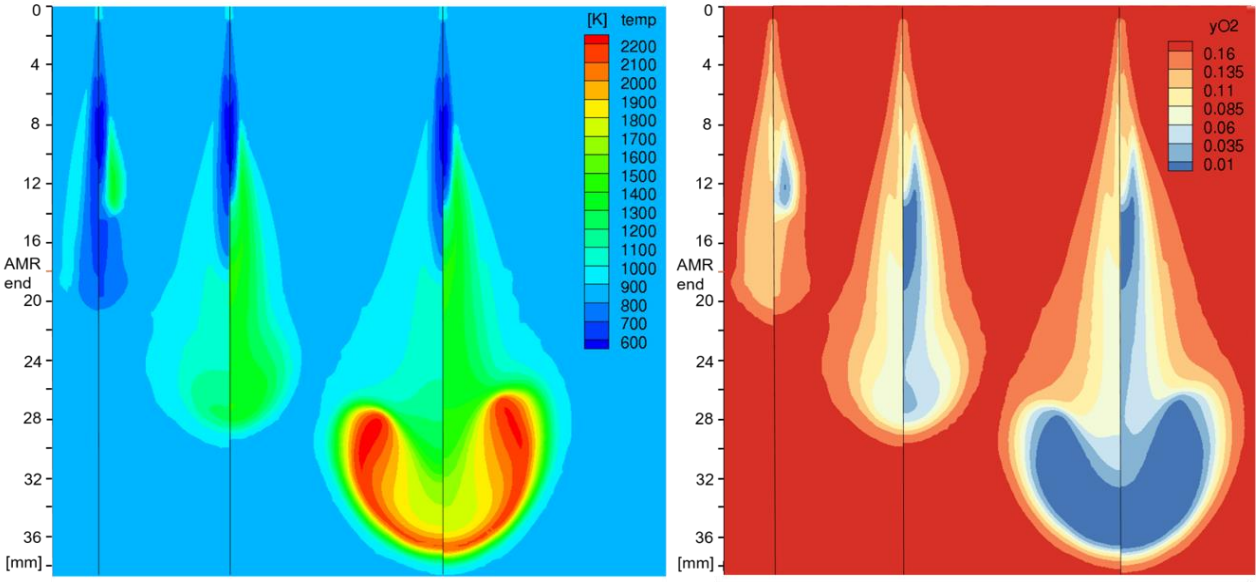

Figure 2: Temperature and O_2-mass fraction profile of SAGE (left) and CPV (right) at 0.2 ms, 0.425 ms and 0.725 ms.

Figure 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.

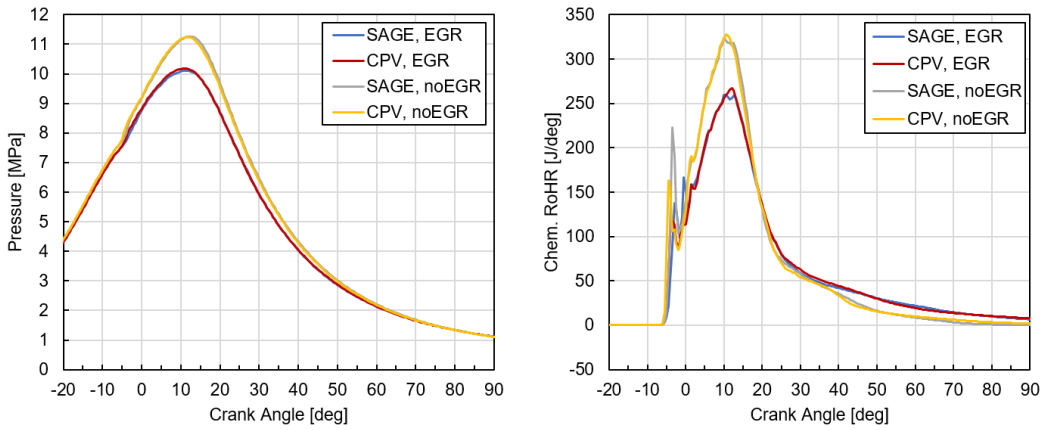

Figure 3: Predicted pressure and chemical RoHR of SAGE and CPV for different EGR amounts (no EGR: 0%; EGR: 30%).

The simulation of Spray A using SAGE and the n-dodecane mechanism has a CPU time of 170 h on 32 cores (AMD OPTERON from 2008). The use of the CPV model decreases the CPU time to 13.7 h. The CPU time of the SAGE engine sector runs is 8 h, of the CPV model 2 h.

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 120 for the n-dodecane mechanism and by factor 4 for the smaller n-heptane mechanism. Future work will include emission prediction and validation.

References

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