Preliminary study of chemistry solvers with focus on ignition in the context of turbulent buoyancy-driven reacting flows

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With the use of the EDC combustion model accounting for finite rate chemistry, the influence of the chemistry solver can be non-negligible to some extent. The present work aims to analyze the most relevant numerical schemes in order to investigate their influence on scenarios involving (buoyancy-driven) reacting flows. Here, the Ordinary Differential Equation (ODE) option is compared with the Euler Implicit (EI) approach for the chemistry solver. Four benchmark cases involving ignition (i.e., premixed combustion) of methane, hydrogen, iso-octane and n-heptane as well as a turbulent UMD line burner [1] (i.e., non-premixed combustion) scenario are considered. The UMD test case considers only methane as fuel, in order to avoid the complexity of modelling the soot formation, and the reaction mechanism is adopted from Westbrook-Dryer 2-step global mechanisms [2]. Unlike the line burner test case, which is run in a 3-D environment (flow field is available), the benchmark cases are run in a 0-D environment.

For the ignition cases, the significant difference between ODE and EI is that the latter requires more clock time to complete. Other than the hydrogen (H_2) case, the accuracy of the two is not deviating at all from the referred value, particularly when the EI chemical time scale coefficient (referred to as CTau) is set to be CTau = 1. The modification of CTau has a significant impact in reducing the clock time of the simulations, however, very high CTau values also result in loss of accuracy of the numerical simulations.

When applied to the UMD line burner case, some observable differences between the two numerical schemes, ODE and Euler Implicit (CTau = 1), are observed when examining the flow field. The Euler Implicit case shows an earlier declination of the centerline temperature than the ODE even though both reached a similar maximum centerline temperature. Consequently, the centerline velocity of the former test case is reaching a lower peak value compared to the latter. The sensitivity study on different chemistry solvers in the numerical simulations revealed that ODE is the best option in terms of both accuracy and computational cost and is recommended for use in simulations of (buoyant-driven) reacting flows.

Table 1. Comparison of computational cost with different chemistry solvers for the benchmark test case (n-heptane).

Chemistry solver	Coefficient/ODE solver	Clock time (s)	Steps	Ignite
ODE	Seulex	93	177	Yes
Euler Implicit	CTau = 1	86196	685270	Yes
	CTau = 10	44007	359004	Yes
	CTau = 100	6799	52610	Yes
	CTau = 1000	38	28	No

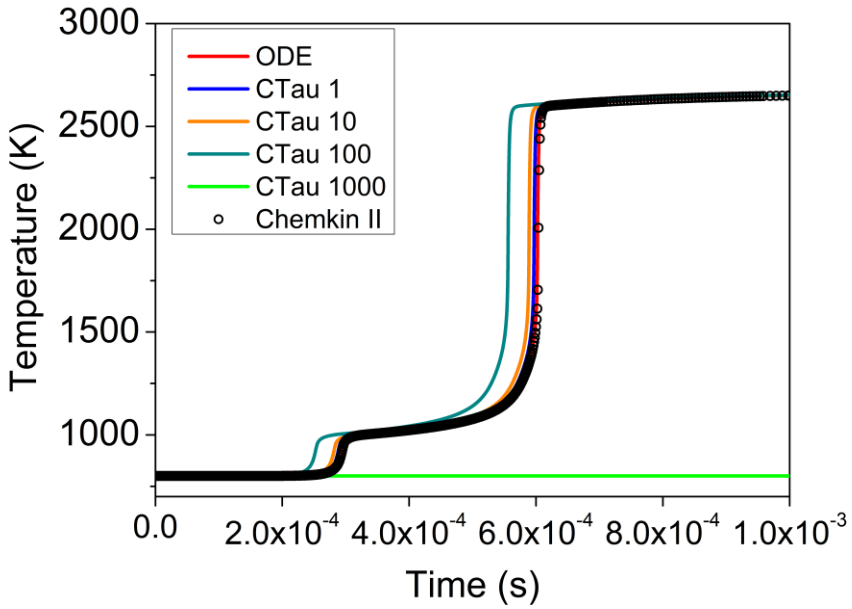

Figure 1. Simulation result of the benchmark test case (n-heptane); temperature profile across different chemistry solvers

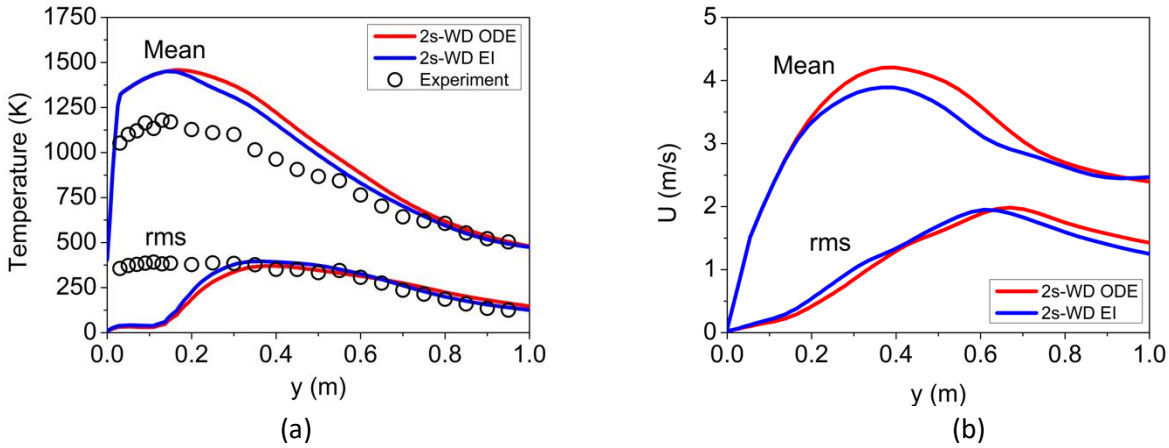

Figure 2. Mean and rms centerline (a) temperature and (b) axial velocity for UMD test case with different chemistry solvers.

References

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[2] C. K. Westbrook, F. L. Dryer, Chemical kinetic modeling of hydrocarbon combustion, Progress in Energy and Combustion Science 10 (1984) 1-57.