A Comparison of Numerical Frameworks for Modelling Homogenous Reactors and Laminar Flames

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Abstract

Five different numerical frameworks with possibilities of modelling homogenous batch reactors and laminar premixed flames are compared in terms of results consistency and performance. The considered projects are Cantera, Chemkin-II, Ansys/Chemkin-PRO, FlameMaster, and OpenSMOKE++. In this study, first, results for homogenous, isochoric, adiabatic batch reactors are compared based on test cases precisely defined in terms of numerical setup and initial conditions. All frameworks provide consistent results. Based on this agreement, the comparison is extended for premixed laminar flames. Very good agreement between Cantera, Ansys/Chemkin-Pro, FlameMaster, and OpenSMOKE++ is achieved given that the same modelling assumptions and a sufficiently accurate numerical setup are chosen by the user. Finally, Cantera, FlameMaster, and OpenSMOKE++ are compared in a process time benchmark for homogenous, isochoric batch reactors.

Introduction

Simulations of homogenous zero-dimensional reactors and one-dimensional laminar flames are the foundation upon which the analysis and the understanding of various combustion processes rest. Numerical frameworks that enable researchers to conduct such simulations are a key tool in the development of complex kinetic models [1]. Simulation results can be analyzed and compared to experimental measurements from various devices such as shock tubes, rapid compression machines, or spherical combustion chambers. Besides the stand-alone application, which usually only allows for simulating relatively simple configurations, implementations of zero- and one-dimensional simulations are often directly or indirectly incorporated to solve complex three-dimensional problems. For example, the same set of equations that describes homogenous, isobaric batch reactors can be solved within a finite rate

chemistry simulation to obtain a new gas phase composition at the end of a time step [2]. An example for an indirect incorporation would be the tabulation and lookup of simulation results as done in the flamelet approach. These examples show that the numerical frameworks for zero-dimensional and one-dimensional configurations are useful in a vast range of applications. Frequently, these applications have specific design, implementation, or feature requirements and it is not surprising that many different frameworks have evolved in the past decades. Researchers concerned with a problem from one of the above-mentioned fields are confronted with the question which of the available software packages, if any, suites their needs. This question cannot be answered universally due to users' specific aims and interests. In this work, we focus on an important prerequisite to make this decision: The consistency of results predicted by some of the most commonly used numerical frameworks. The considered free, open source projects are Cantera [3], Chemkin-II [4], FlameMaster [5], and OpenSMOKE++ [2,6]. Ansys/Chemkin-PRO (Chemkin-Pro) [7] is the only commercial software in the comparison. The presented results are intended not only for the users and developers of the presented programs, but they are also meant to serve as reliable data for the validation of other implementations. Besides accurate and consistent results, the performance in terms of process time can be an important criterion for the choice of software. Here, a comparison is carried out for two specific test cases. Comparability of process time for such a small set of test cases requires sufficiently similar numerical methods, which is given for Cantera, FlameMaster, and OpenSMOKE++ for homogenous, isochoric reactors as discussed below.

Homogeneous, Isochoric, Adiabatic Batch Reactors

The first configuration under investigation is the one for homogenous, isochoric, adiabatic reactors, which can be described by a set of ordinary differential equations (ODE) for the species mass fractions and the temperature [6]. This configuration is important as straightforward extensions for facility effects allow to simulate rapid compression machines and shock tubes. However, in the below defined test cases, such effects where not considered to ensure simple and yet precisely defined conditions for the test cases. Homogenous zero-dimensional reactors are well suited to validate the computation of the reaction kinetics and the thermodynamic species properties. The implementation of this configuration is similar in Cantera, FlameMaster, and OpenSMOKE++. All three frameworks provide the option to make use of the same solver for initial value problems, which is CVODE [8]. Therefore, this test case serves as a starting point for the comparison. The initial conditions for this test case are given in Table 1 and a small kinetic model for hydrogen-air combustion is used [9]. If CVODE is available, the employed relative and absolute tolerances are 3.0e-12 and 3.0e-14, respectively. Chemkin-II and Chemkin-Pro do not provide this option. Instead, a solver for differential algebraic equations (DAE), DASPK [4,7], is integrated. While OpenSMOKE++ integrates multiple ODE- and DAE-solvers [6], only CVODE was used in this study.

The results from all frameworks agree very well. Several species mole fractions and temperature profiles were compared. An illustration of the results is not included as it would not provide further insight due to the very small deviation of the results.

Table 1. Initial conditions for the homogenous, adiabatic, isochoric reactors.

Pressure [bar]	30.0
1000/Temperature [1/K]	0.7 – 1.5
Fuel-Air-Equivalence Ratio [-]	0.7, 1.0, 1.3

Laminar, Freely Propagating, Premixed Flames

As a second test case simulations of premixed, freely propagating, laminar flames are considered. This configuration is chosen not only because of its importance for the simulation of several experimental setups, but also because one-dimensional configurations add another important layer of complexity to the simulation. Besides different numerical methods for solving a set of partial differential equations [6], they also introduce models that account for transport phenomena. To assess the consistency of the results for this configuration, predictions for the laminar burning velocity of methane-air flames are considered over a range of fuel-air-equivalence ratios. In all simulations, the GRI3.0 kinetic model [10] is utilized and radiation is not considered. Conditions of the unburnt mixture are summarized in Table 2.

Table 2. Conditions in the unburned mixture for the premixed, laminar flames.

Pressure [bar]	1.0
Temperature [K]	300.0
Fuel-Air-Equivalence Ratio [-]	0.6 - 1.7

For one-dimensional flames, an important part of the implementation are models that account for transport phenomena. All simulations were conducted using the same mixture-averaged diffusion model and accounting for thermal diffusion, if possible. Note that the current standard version of FlameMaster implements a different thermal diffusion model than Chemkin-II, Chemkin-Pro, and OpenSMOKE++ and the implementation was extended to include the thermal diffusion model identical to the other frameworks. Cantera only allows to account for thermal diffusion, if multi-component diffusion is applied. Therefore, thermal diffusion was not accounted for in the Cantera simulations. The below presented simulations were rerun with FlameMaster and OpenSMOKE++ without thermal diffusion and it was found that the applied model reduces the burning velocity slightly by approximately 1%.

Another important factor for simulations of one-dimensional flames is the utilized grid. An insufficient number of grid points results in a poor prediction of the laminar burning velocity. Therefore, all simulations were run with at least 1200 grid points and central differences, if possible. In tests previously conducted with Cantera, it was found that this number is sufficient whereas increasing the number of grid points

beyond this value does not change the predicted laminar burning velocity significantly.

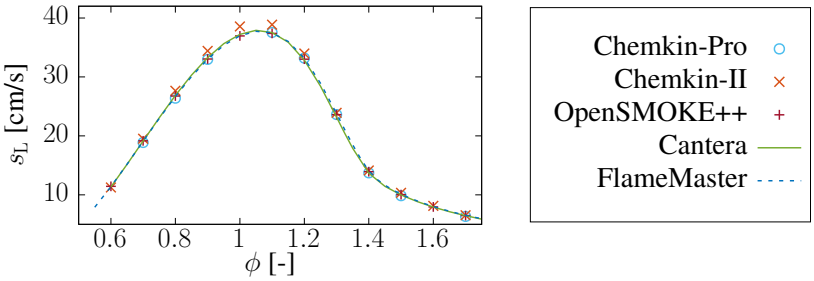

Figure 1. Flame speed of premixed, laminar flames over fuel-air-equivalence ratio.

Fig. 1 shows the predicted laminar burning velocities as a function of the fuel-air-equivalence ratio. The results from Cantera, Chemkin-Pro, FlameMaster and OpenSMOKE++ agree very well. Most of the predicted values deviate less than 0.2 cm/s from one another. Only for slightly rich mixtures, Cantera predicts a laminar burning velocity that is 0.45 cm/s lower than the other predictions. As thermal diffusion was not accounted for, it was expected that the laminar burning velocity would be slightly increased instead. The largest deviation is obtained for Chemkin-II. For near stoichiometric mixtures, the laminar burning velocities predicted by Chemkin-II are up to 1.6 cm/s higher compared to the other frameworks.

Process Time Benchmark

Finally, the performance in terms of process time required for running simulations of homogenous, isochoric, adiabatic batch reactors is compared between Cantera, FlameMaster, and OpenSMOKE++. The terms process or CPU time refer to the amount of time the central processing unit (CPU) requires for processing all instructions of a simulation. The comparability of the measured values is only given, if the numerical method is sufficiently similar. Cantera, FlameMaster, and OpenSMOKE++ all provide the option to run batch reactor simulations with CVODE [8], which means in all simulations identical numerical methods can be applied to conduct the time integration. Within the time integration, it is required to solve a system of nonlinear equations. This is done using a modified Newton method. The corresponding Jacobian evaluation can be done numerically using finite differences or analytically. A numerical evaluation is provided with CVODE and therefore available in all three frameworks. A semi-analytical evaluation of the Jacobian is already implemented in OpenSMOKE++. However, this option is only available with ODE solvers other than CVODE. In Cantera, the Jacobian is always estimated numerically. To demonstrate the impact of the Jacobian estimation, the current version of FlameMaster is extended to include analytical derivatives.

All benchmark simulations were done on an Intel Xeon CPU (E5-2650 v4 @ 2.20GHz). All frameworks were compiled with the Intel compilers. Cantera and

FlameMaster were linked against the multi-threaded version of math kernel library (MKL). OpenSMOKE++ was linked against the sequential MKL. For all test cases, the relative and absolute tolerances for CVODE are 1.0e-9 and 1.0e-16, respectively.

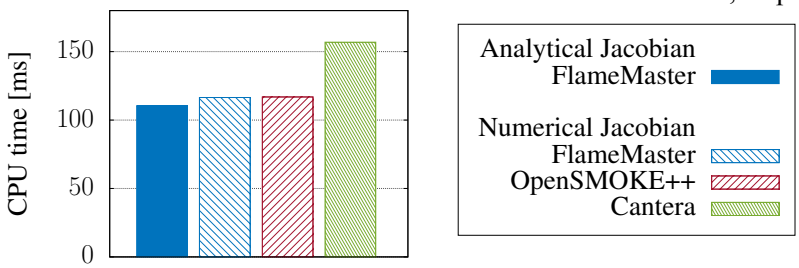

Figure 2. CPU time for simulations of isochoric reactors using a small model [10].

In the first benchmark, a stoichiometric methane-air mixture in a homogenous, isochoric batch reactor is simulated for two seconds using the GRI3.0 kinetic model [10]. The initial pressure and temperature are 30 bar and 1000 K, respectively. Fig. 2 shows that the measured CPU times are similar for all implementations. The CPU time required by FlameMaster with the analytical Jacobian evaluation is virtually the same as with the numerical evaluation.

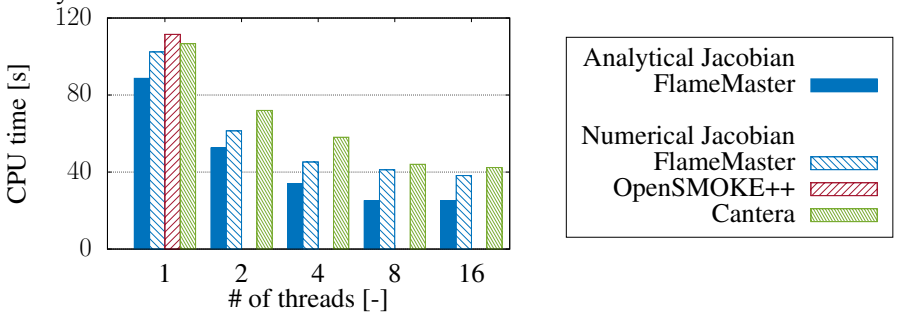

Figure 3. CPU time for simulations of isochoric reactors with a large model [1].

In the second benchmark, an isochoric reactor with a stoichiometric decane-air mixture at 30 bar and 1000 K is simulated for two seconds. The kinetic model consists of 1692 species and 5804 reactions [1]. The CPU times are shown in Fig. 3. Again, for all three frameworks, the CPU time is similar with a numerical Jacobian evaluation. The performance of FlameMaster is slightly improved with the analytical Jacobian evaluation. As Cantera and FlameMaster were linked against the multithreaded MKL, the simulations were also executed with up to 16 threads. The CPU time is clearly decreased with an increasing number of threads. The observed, significant speed up results solely from the parallelized solution of the linear system within the MKL and the remaining computation is still executed sequentially. This emphasizes the importance of the linear solver. Note that OpenSMOKE++ and the extended version of FlameMaster used here implement options for solving sparse linear systems, which are more appropriate for this test case. With these options, the CPU time for sequential execution is reduced significantly by up to a factor of 7.

Conclusions

Simulation results predicted by five commonly used numerical frameworks were compared for two representative configurations. Cantera, Chemkin-Pro, FlameMaster, and OpenSMOKE++ predict consistent results for both configurations. While the Chemkin-II results are consistent with the other frameworks for isochoric batch reactors, the predicted burning velocities for near stoichiometric conditions are slightly larger. A process time benchmark showed that the considered frameworks provide similar performance. The CPU time for the simulation of large mechanisms can be reduced with sparse or parallelized dense linear solvers.

Acknowledgment

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