

Comparison of different chemical kinetics modeling codes

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Abstract

Various codes are available to model the chemical kinetics of reactive systems, e. g. COSILAB, OpenSMOKE, Cantera, CHEMKIN, CHEMID and others. However no proper comparison is made between the performances of different codes for various cases. To assess and compare the performance of COSILAB and OpenSMOKE, we simulated different laminar combustion cases of CH₄/Air and CH₄/H₂/Air mixtures with both codes using the GRI30 mechanism and compared the obtained results. For ignition delays and mole fraction profiles in 1D flames simulations similar results are found with COSILAB and OpenSMOKE. However the laminar flame speeds obtained with the two codes differ.

Introduction

COSILAB is a commercial software developed by Rotexo. The code enables the simulation of different reactive-flow and combustion geometries and is used in different papers for combustion simulations [1].

OpenSMOKE is an open source code developed by Politecnico di Milano and can model reacting systems with detailed kinetic mechanisms [2]. Both codes are capable of simulating different combustion cases; however it is not clear whether the performance and results are the same.

Three combustion cases are simulated and compared for CH₄/Air and CH₄/H₂/Air flames. As kinetic model the GRI30 mechanism is chosen [3].

First, the ignition delay is achieved simulating a homogeneous transient system. Secondly, the mole fraction profiles of a burner-stabilized laminar flame are compared with each other. As last, the laminar flame speed obtained by freely propagating laminar flames is assessed in function of the applied equivalence ratio.

The goal is to find and explain the differences between COSILAB and OpenSMOKE results and this for different combustion cases; so that someone who needs chemical kinetics modeling code can make a reasoned decision between them.

0D-Homogeneous ignition process

Ignition delay is largely kinetically controlled in homogeneous systems. So if reliable experimental data is available, the calculated ignition delay can be used to compare the performance of both codes. The ignition delay is defined in this paper as the time of maximum pressure rise rate

CH₄/Air and CH₄/H₂/Air (70mol% CH₄ and 30mol% H₂ in the fuel) mixtures are simulated at different equivalence ratios for an adiabatic, constant-volume vessel with a starting pressure and temperature of 1 bar and 1000 K respectively.

The same ignition delays are found with COSILAB and OpenSMOKE for all the assessed possibilities (Figure 1).

To assess if the outcomes are also correct a comparison with literature is made. Zhukov et al. investigated the spontaneous ignition of CH₄/Air mixtures in a wide range of pressures using a shock tube set up [4]. We simulated two of his results and found comparable results. For a CH₄/Air mixture with an equivalence ratio of 0.5 at 1661K and 2.95atm, Zhukov et al. found an ignition delay of $101 \pm 3 \mu\text{s}$ and we simulated a value of $95.4 \mu\text{s}$. For the second case at 15.8 atm and 1628K an experimental value of $33 \pm 2 \mu\text{s}$ was

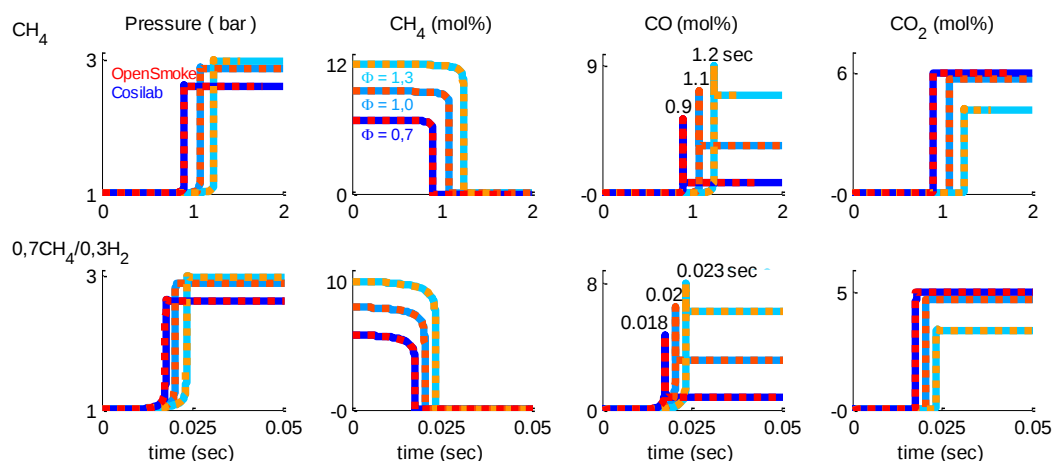


Figure 1: The ignition delays simulated with the two codes at 1 bar and 1000K, for various equivalence ratios and two mixtures CH₄/Air and CH₄/H₂/Air are in perfect agreement.

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found, while we simulated 31.2 μ s.

Donohoe et al. investigated the ignition delays of $\text{CH}_4/\text{H}_2/\text{Air}$ mixtures using a rapid compression machine [5]. He found an ignition temperature of 884K after 166.4ms for a mixture of 20mol% CH_4 and 80mol% H_2 stoichiometrically diluted with air at a pressure of 30 bar. With COSILAB and OpenSMOKE an ignition delay of 106ms is found.

Hence the performances of COSILAB and OpenSMOKE for modeling the ignition delay in homogeneous systems are similar. The same results are found with both codes and are comparable with experimental results, which also depend on the precision of used kinetic mechanism.

1D-Burner stabilized laminar flame

Burner stabilized laminar flames of CH_4/Air and $\text{CH}_4/\text{H}_2/\text{Air}$ are simulated for different equivalence ratios and pressures. The main difference between flames is the presence of H_2 , allowing to assess if the Soret effect is implemented the same way in both codes.

The mass flux is set at 0.066 kg/s/m² and the same temperature profile is implied at all the simulations discussed.

A steady Newton numerical method is used in COSILAB, with a relative tolerance of 1e-5 and an absolute tolerance of 1e-7 to solve the equations. The default values for relative and absolute tolerance are 1.19e-5 and 1e-10 respectively for OpenSMOKE.

The starting grid for both codes contains 13 points. Grid adaption is done in both codes by defining the allowed curvature and gradient in the outcomes. In COSILAB the adaptive gridding is based on all variables, while in OpenSMOKE the grid is only adapted in function of the temperature. The curvature parameter in COSILAB is 5e-1 and the gradient parameter is 2e-1. Adaptive gridding is applied in COSILAB until the curvature and gradient parameters are met, then a last time the differential equations are solved and a final solution is obtained.

In OpenSMOKE we use the default values for grid adaption in our simulations. Grid stabilization regarding the gradient value is obtained after 5 adaptations, leading to a difference of less than 5e-7K between consecutive points in the temperature profile.

Time stepping in OpenSMOKE is defined as the end time interval up to which the equations have to be solved. Meaning, a large number is needed to reach steady-state conditions. In our simulations 1e5 is used for this.

In COSILAB more time stepping parameters can be specified. The minimum time step size is set to 1e-12 and the maximum size is 1e5. For the end time a value of 1e5 is set.

The temperature profile and some mole fraction profiles for the CH_4/Air flame are displayed in Figure 2. The absolute differences between the results obtained by OpenSMOKE and COSILAB, multiplied with a factor 10 to be visible, are also displayed as grey areas. Negative values mean that the mole fractions obtained with OpenSMOKE are higher than the COSILAB solution.

The results of COSILAB and OpenSMOKE for the mole fraction profiles of a stoichiometric CH_4/Air flame at 1atm are shown in Figure 2,a. The absolute difference is less than 1% for most of the cases. The highest difference is found for the H_2O_2 species where the absolute difference is around 6.4% of the simulated mole fraction value.

Some of the experiments to validate kinetic parameters are designed at low pressure. Therefore we simulated a stoichiometric CH_4/flame at 0.07 bar and again there are no differences between the two simulation codes (Figure 2, b).

To get convergence with COSILAB at this low pressure an intermediate solution has to be set as starting profile. OpenSMOKE was able to run the simulation with only 19 starting points.

COSILAB was able to simulate the CH_4 combustion at a pressure as low as 0.05 bar, where OpenSMOKE did not converge. Possible solutions to let OpenSMOKE work at a pressure of 0.05 bar, are increasing the number of starting points of the simulation and/or changing the adaptive gridding and the time stepping. Further work is needed in this case.

Changing the equivalence ratio to a lean (0.7) or a rich (1.3) CH_4/Air flame has no effect on the performance of both codes. No substantial differences between the codes results are found (Figure 2, c and d).

If we look to the $\text{CH}_4/\text{H}_2/\text{Air}$ flame results, again no considerable differences are found between the results of COSILAB and OpenSMOKE (Figure 3).

In both codes the Soret effect is properly captured, as we can see for the mole fraction profiles H_2 and H which are similar.

A simulation of the mole fraction profiles for a stoichiometric CH_4/Air flame at 1 atm takes around 20s in COSILAB, while OpenSMOKE needs 30 to 40s.

Unlike the CH_4/Air flame, the target of 0.05bar for the low pressure simulations is met with both COSILAB and OpenSMOKE.

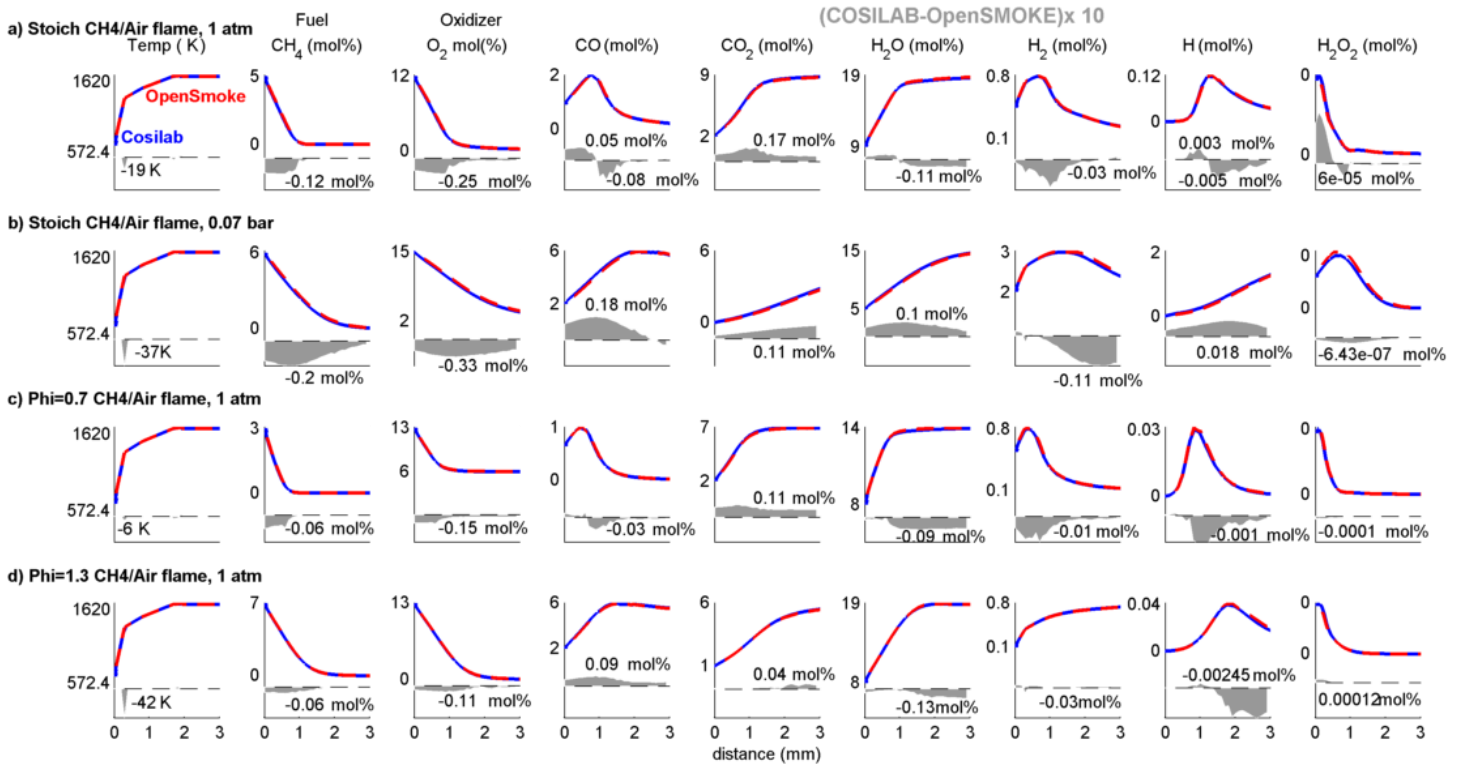


Figure 2: The mole fraction profiles for some species obtained with COSILAB (blue) and OpenSMOKE (red) for a CH_4/Air flame at different equivalence ratios and pressures are similar. The grey areas show the absolute difference between the two obtained results, multiplied by 10 to be visible. The absolute difference is mostly lower than 1% of the calculated mole fraction.

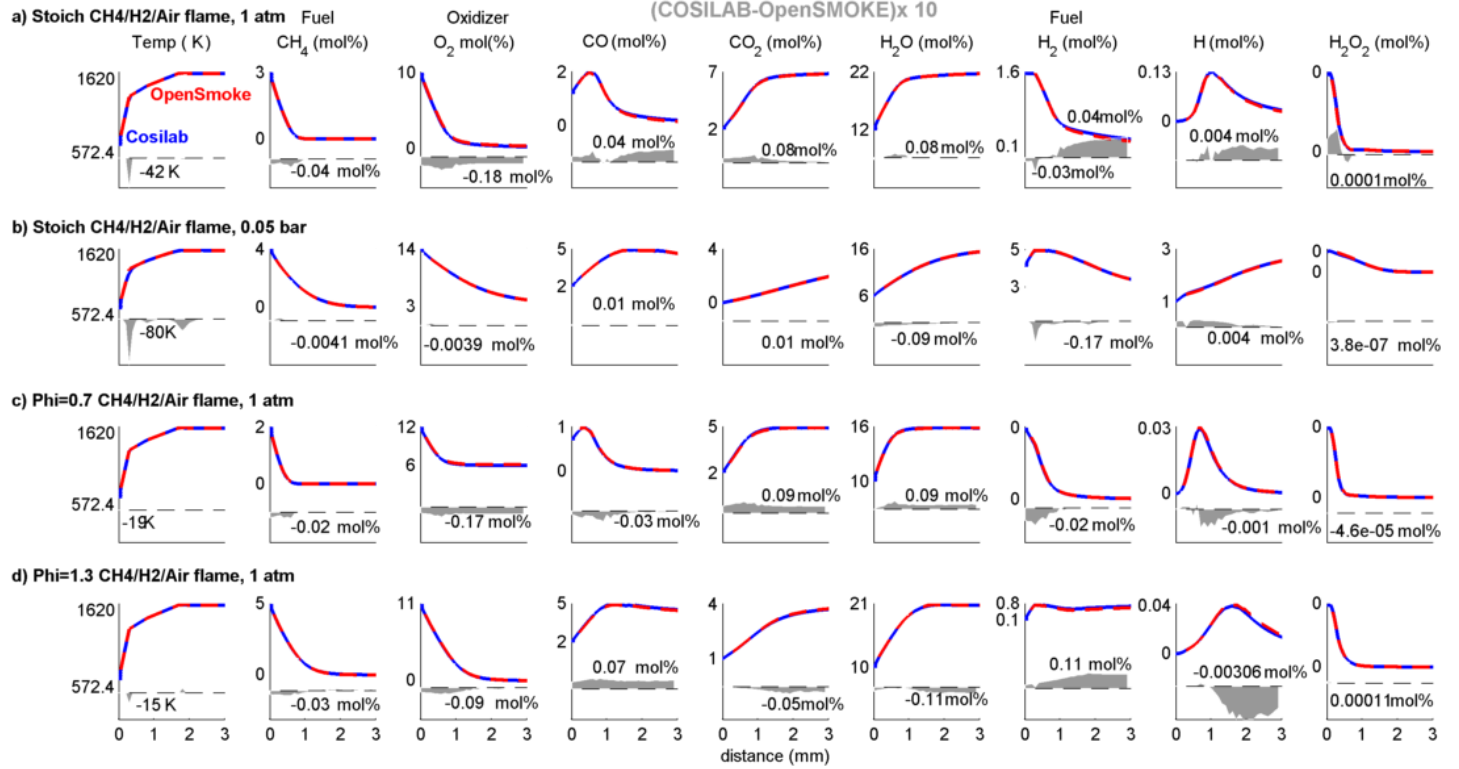


Figure 3: The mole fraction profiles for some species obtained with COSILAB (blue) and OpenSMOKE (red) for a $\text{CH}_4/\text{H}_2/\text{Air}$ flame at different equivalence ratios and pressures are similar. The grey areas show the absolute difference between the two obtained results, multiplied by 10 to be visible. The absolute difference is mostly lower than 1% of the calculated mole fraction.

1D- Freely propagating flame

The laminar flame speed is the speed of an unstretched laminar flame through the mixture of unburned reactants. The speed only depends on the composition of the fuel and the applied temperature and pressure.

Here again the performance of COSILAB and OpenSMOKE can be compared with literature values.

The numerical solver has to be changed from a steady Newton method to an unsteady one in COSILAB to get a solution. This solution can then be used as a starting value for a steady simulation. In OpenSMOKE no changes are needed. Also the time stepping and grid adaptations settings stay the same in both codes.

Next to the initial values for temperature (300K), pressure (1atm) and the composition of the fuel air mixture (CH_4/Air), both codes require flame fixing parameters. In COSILAB you need to give a value for the “excess temperature”, which has to be at least 50K. In the COSILAB manual a temperature of 100K is advised. This temperature is used to set a first gradient for the numerical method. The spatial point where COSILAB fixes the flame is at 1/3 of the grid by default.

OpenSMOKE has two parameters that have to be defined before simulation: “#FlameSpeedIndex” and “#FlameSpeedTemperature”. The “#FlameSpeedIndex” is the grid point at which the flame is stabilized; this point lays around 1/3 of the number of grid points. If you have 10 grid points to start with the “#FlameSpeedIndex”-value can be either 3 or 4.

The “#FlameSpeedTemperature” is the temperature fixed at the “#FlameSpeedIndex” grid point. In the OpenSMOKE examples a temperature 12 to 15 K higher than the inlet temperature is advised.

In Figure 4 the laminar flame speeds calculated with the advised flame fixing parameters are given. The laminar flame speeds obtained with OpenSMOKE are in general higher than the values found with COSILAB.

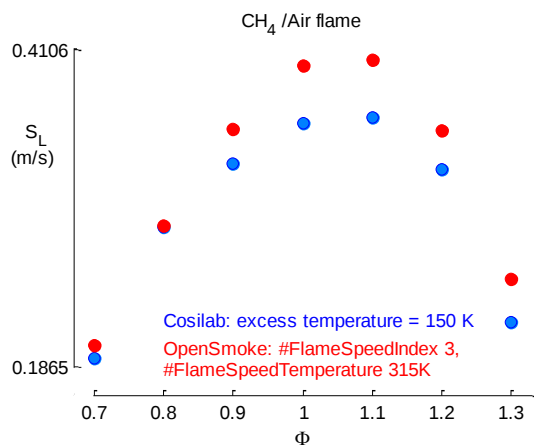


Figure 4: The laminar flame speeds for a CH_4/Air flame at 1atm in function of the equivalence ratio. Only for an equivalence ratio of 0.8 the COSILAB outcome (blue) is the same as the OpenSMOKE

Since the only parameters that can be changed are the flame fixing parameters, the influence of them is assessed. The “excess temperature” in COSILAB is set to 50K, 100K and 150K. For OpenSMOKE the “#FlameSpeedIndex”-value is changed to 4 and the “#FlameSpeedTemperature” is increased to 350 and 450K.

In Figure 5 the influence of the “excess temperature” on the derived laminar flame speed in COSILAB is visualized. With an equivalence ratio of 0.7 and 1.3 the outcomes derived with different “excess temperatures” are similar, however at other ratios there is some variation. Both 50K and 150K gives higher laminar flame speed at an equivalence ratio value of 1 and 1.1 in comparison with the advised value of 100K. However at an equivalence ratio value of 0.8 and 1.2 it is reversed. Hence there is no clear trend in the obtained laminar flame speed in function of the applied “excess temperature”.

From the OpenSMOKE results it appears that the “#FlameSpeedIndex”-value has only a minor influence on the derived laminar flame speed (Figure 6). Changing the place where the flame front is fixed, does not affect the obtained laminar flame speed. However changing the “#FlameSpeedTemperature” from 315K to 350 and 450K influences derived laminar flame speed, just like in COSILAB (Figure 7). In most cases the laminar flames speed increases if the “#FlameSpeedTemperature” increases.

Comparison with experimental data is needed to select good starting values for the flame fixing parameters (Figure 8)[6]. In overall, the OpenSMOKE and COSILAB code result in laminar flame speed values comparable to experimental values. However no conclusion about performance can yet be made, since the influence of the different numerical method, time stepping, grid adaptations and flame fixing values is not clear.

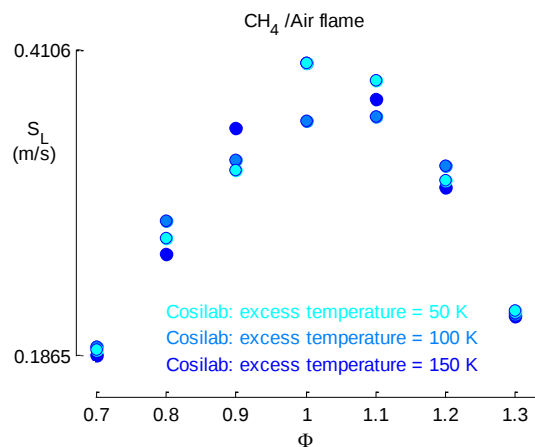


Figure 5: The laminar flame speeds in function of the equivalence ratio is influenced by the flame fixing parameters. The outcomes for COSILAB differs with the excess temperature applied

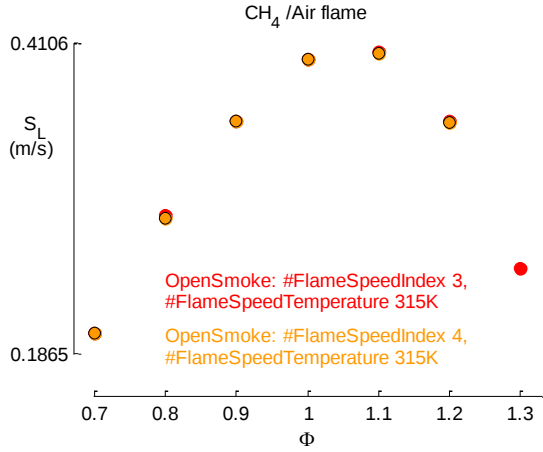


Figure 6: Changing “#FlameSpeedIndex” has no influence on the laminar flame speed calculations. The grid point in which the flame front is fixed can be changed from 3 to 4, without changing the flame speed

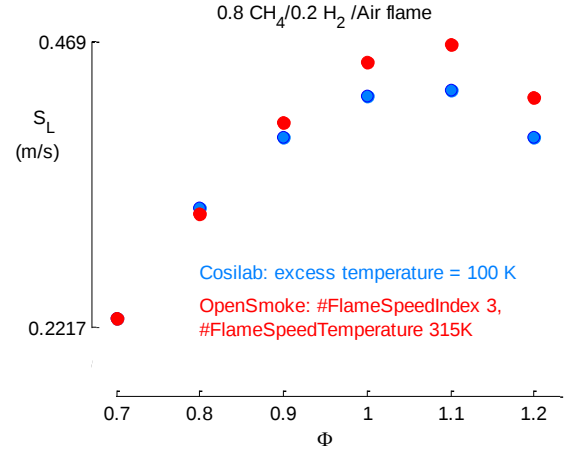


Figure 9: The laminar flame speeds derived with OpenSMOKE for a 0.8CH₄/0.2H₂/Air flame are higher for flames with an equivalent ratio between 0.9 and 1.2 compared with COSILAB results.

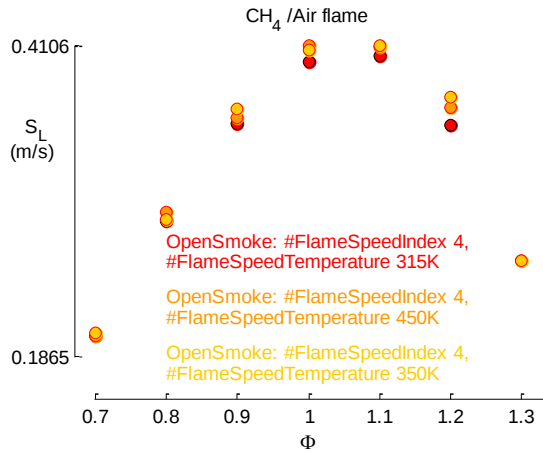


Figure 7: The laminar flame speeds calculated with OpenSMOKE are influenced by “#FlameSpeed-Temperature”. Increasing the “#FlameSpeed-Temperature” results in a higher laminar flame speed.

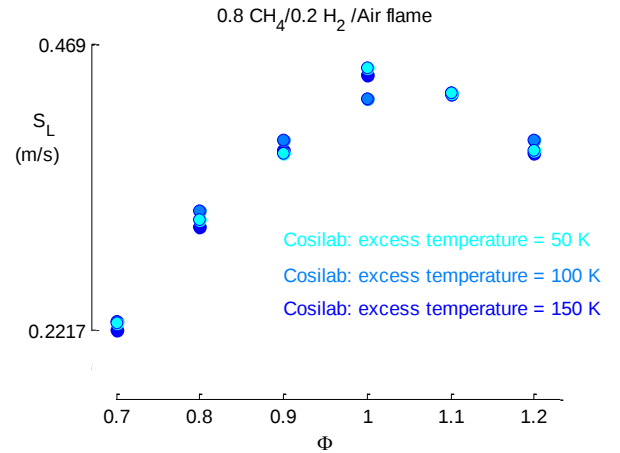


Figure 10: Varying the “excess temperature” while simulating a 0.8CH₄/0.2H₂/Air flame with COSILAB results in different laminar flame speeds, except for an equivalence ratio value of 1.1.

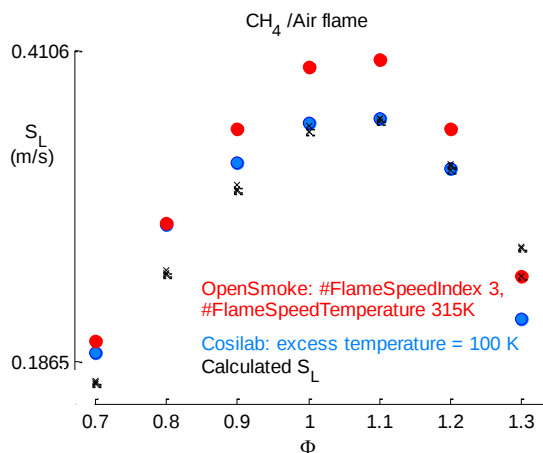


Figure 8: The COSILAB and OpenSMOKE outcomes for laminar flame speeds are comparable to calculated values from the literature [6].

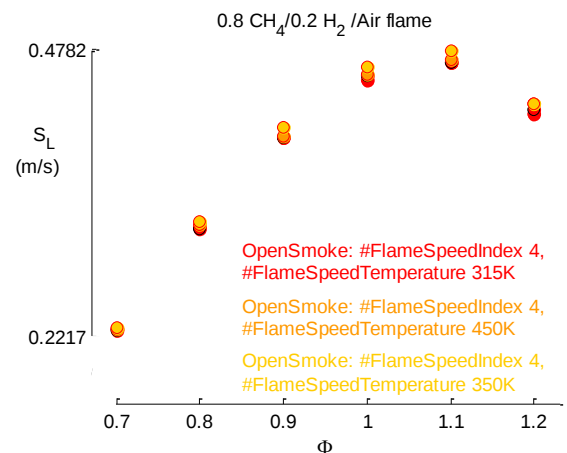


Figure 11: If the “#FlameSpeedTemperature” is increased to 350 and 450K in a 0.8CH₄/0.2H₂/Air flame modeled with OpenSMOKE, the obtained laminar flame speeds increase slightly.

The same laminar flame speed calculations are done for a 0.8CH₄/ 0.2H₂/Air flame with an inlet temperature of 298K and an inlet pressure of 1bar (Figure 9-11).

In Figure 9 the laminar flame speeds found with COSILAB and OpenSMOKE for the advised flame fixing parameters are shown. The OpenSMOKE results are higher in comparison with the COSILAB results. The flame fixing parameters influence the laminar speeds outcomes, as also found for the CH₄/Air flame (Figure 10 and 11).

If we compare the simulations with experimental results, we see that both codes simulations approach the experimental results (Figure 12) [7]. A further investigation of the influence of the numerical method, time stepping, grid adaptations and flame fixing values on the obtained laminar flame speed is needed.

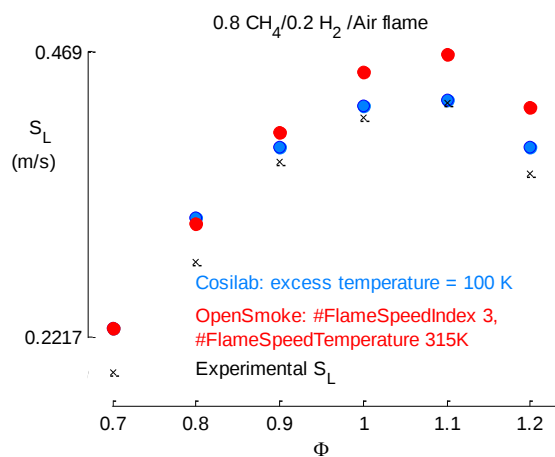


Figure 12: The laminar flame speeds for a 0.8 CH₄/0.2H₂/Air simulated by COSILAB and OpenSMOKE approach the experimental results.

Conclusions

The COSILAB and OpenSMOKE codes have similar performance to calculate ignition delays and mole fraction profiles, however when the laminar flame speed is calculated using freely propagating flames there is a difference between them. Further investigation of the influence of the code settings in terms of numerical method, time stepping, grid adaptation and flame fixing is needed before a conclusion about performance can be drawn.

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