Freely propagating flame velocity of CH4–air

Background

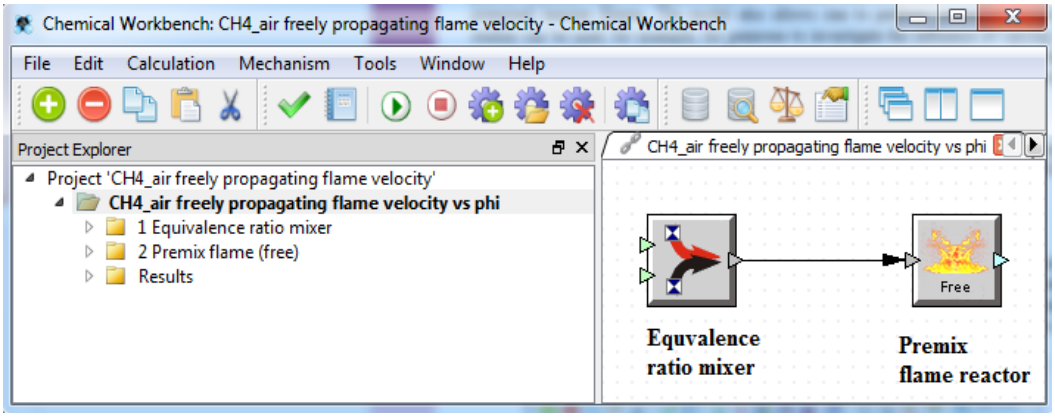
The laminar combustion properties are of fundamental importance for analyzing and predicting the performance of many combustion systems and practical combustors, such as internal combustion engines and gas turbines. The freely propagating laminar flame model is developed for modeling the behavior characteristics of the steady, adiabatic, freely propagating one-dimensional premixed laminar flames. The model also allows one to perform parameter studies. Parameter studies can be used to investigate the influence of varying input data of operating conditions such as input flow properties (species concentration and temperature) and pressure on the laminar burning velocity. Several parameters can be varied simultaneously.

Problem statement

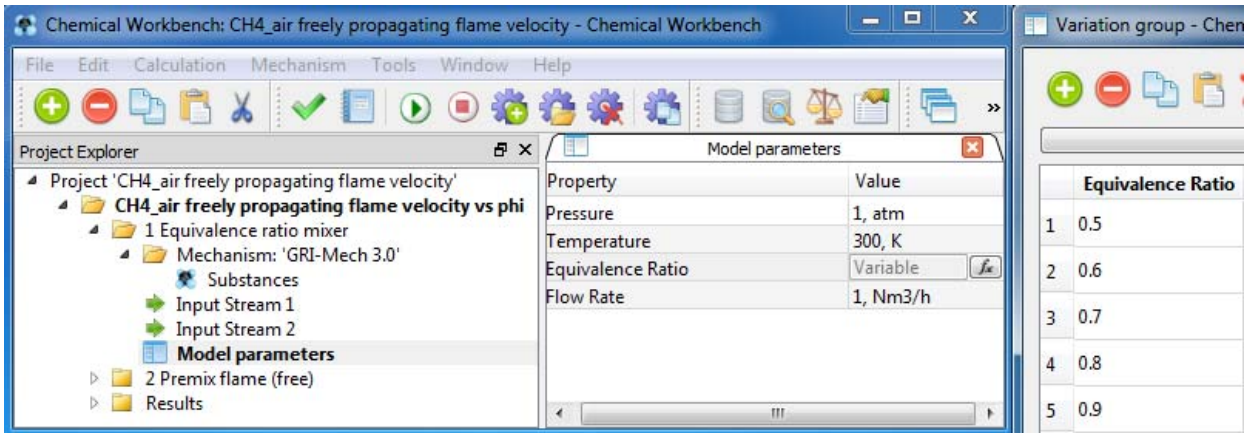
It is required to calculate the freely propagating flame velocities as function of equivalence ratio for the premixed methane-air laminar flames. Initial temperature of methane-air is 300K, pressure 1, 10, 20 atm. Mixture equivalence ratio - 0.6 – 1.8.

Problem setup in Chemical Workbench

This example includes the calculation of the propagation velocities of free flame at φ = 0.6 – 1.8, at T_0=300 K, P =1, 10, 20 atm. To calculate the flame velocities as well as temperature and main concentrations behavior during the combustion of methane-air mixture at different equivalence ratios φ, we use the chain of two reactors – **Equivalence Ratio Mixer** and **Premixed Flame Reactor**, available in Chemical Workbench.



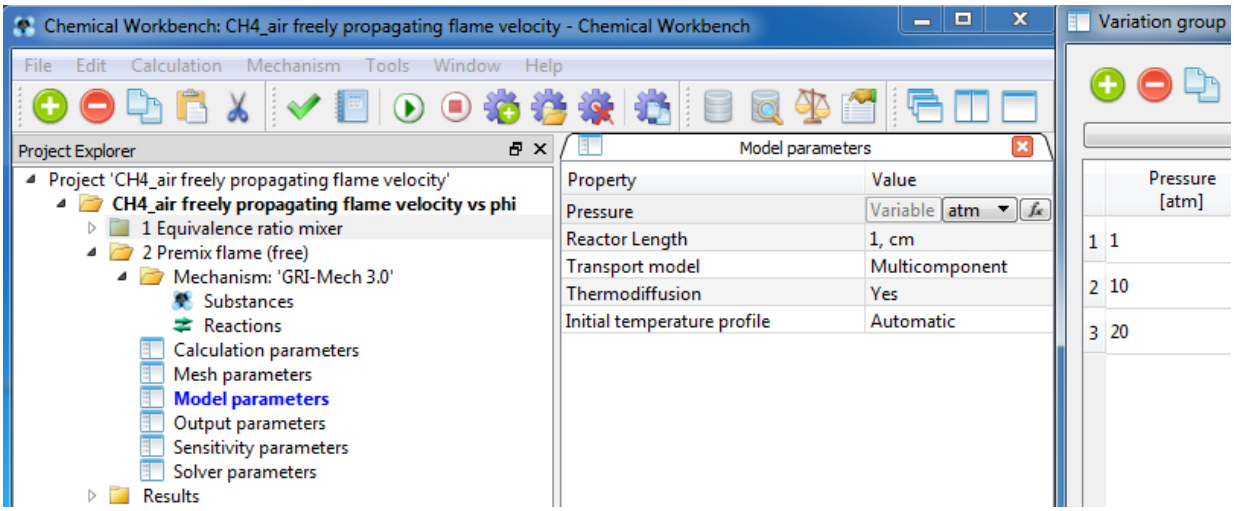
The first reactor **Equivalence Ratio Mixer** calculates composition of initial mixture at given φ. The mixture CH_4-air is inputted in this reactor - **Input Stream 1** - Fuel (CH4), **Input Stream 2** – oxidizer (air). This model requires kinetic mechanism. In this case the mechanism GRIMech-3.0 is taken. The Mechanism is loaded from KintechDB database, which is tightly integrated with Chemical Workbench.



Premixed Flame Reactor requires the following data:

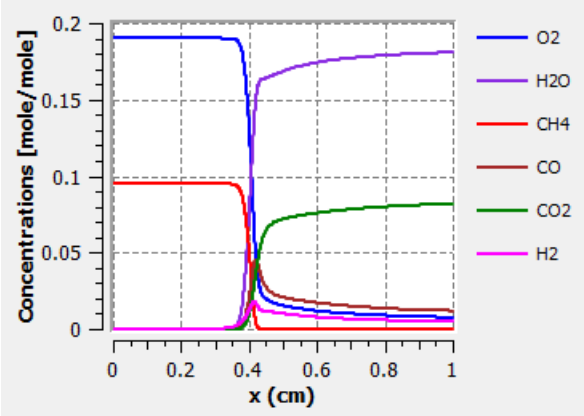
•Mechanism,
•Model parameters,
•Calculation Parameters,
•Solver parameters.

The minimum number of input parameters, related with numerical method implementation, is required. The initial guess to the temperature profile and intermediate species concentrations are not required and estimated automatically. This simplifies setup of laminar flame simulation

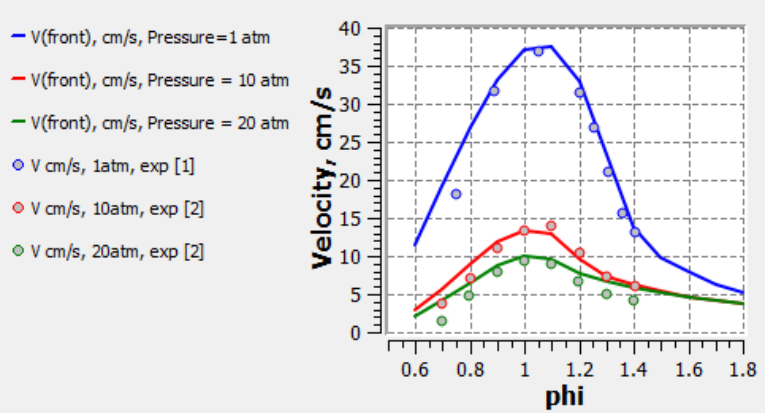


Results

Simulated results are shown at below pictures. Experimental results are taken from [1], [2].



Main concentrations of stoichiometric CH4 + air flame at standard conditions (298 K, 1 atm).



Laminar burning velocities of CH_4 + air flames at temperature 300 K and pressures 1, 10, 20 atm for φ = 0.6- 1.8.

Next steps

This example can be extended further

1.Run sensitivity analysis to identify reactions, which affect laminar burning velocity most of all

2.Compare predictions of different chemical kinetic mechanisms, available in KintechDB database, for conditions of interest for you

References

1. Vagelopoulos, C.M. and Egolfopoulos, F.N., Direct experimental determination of laminar flame speeds. Proc. Combust. Inst. 27:513–519 (1998).

2. Rozenchan G., Zhu D. L., Law C. K., and Tse S. D., Outward Propagation, Burning Velocities, and Chemical Effects of Methane Flames up to 60 atm, Proc. Combust. Inst. 29: 1461–1469 (2002).