Freely propagating flame velocity of CH4–air vs. pressure

Background

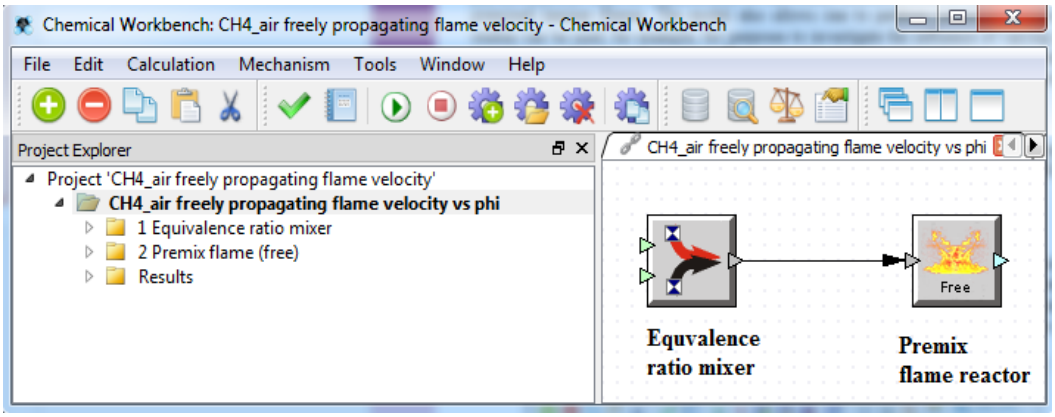
The laminar combustion properties are of fundamental importance for analyzing and predicting the performance of many combustion systems and practical combustors, such as internal combustion engines and gas turbines. The freely propagating laminar flame model is developed to model the behavior of the steady, adiabatic, freely propagating one-dimensional premixed laminar flames. The model also allows one to perform parameter studies. Parameter studies can be used, for example, to assess how the ambient conditions affect the laminar flame speed. This is a typical task encountered in internal combustion engines design, where the pressure is varying during the combustion of the fuel-air mixture

Problem statement

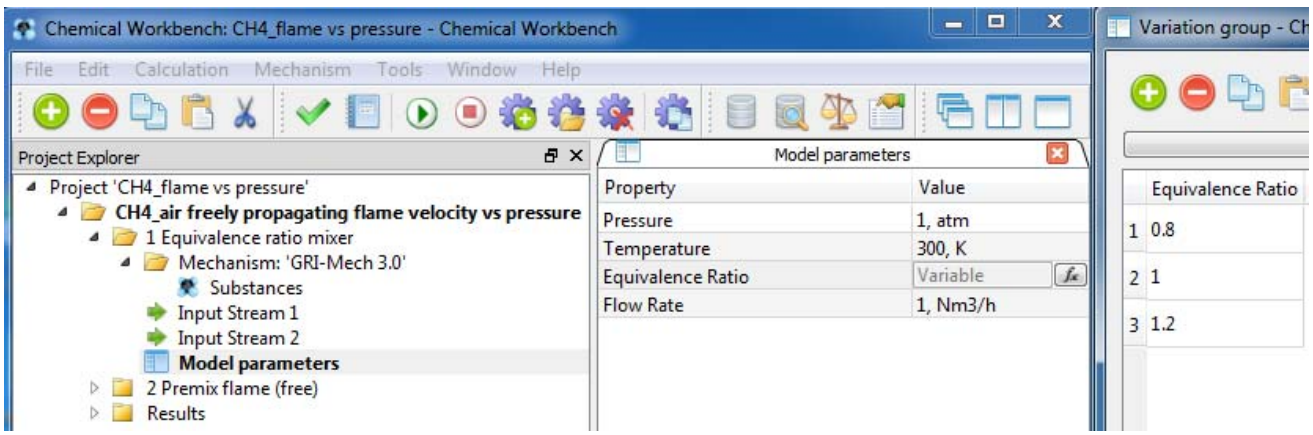
It is required to calculate the freely propagating flame velocities as function of pressure at fixed equivalence ratio for the premixed methane-air laminar flames. Initial temperature of methane-air is 300K, pressure 1- 20 atm. Mixture equivalence ratio - 0.8, 1, 1.2.

Problem setup in Chemical Workbench

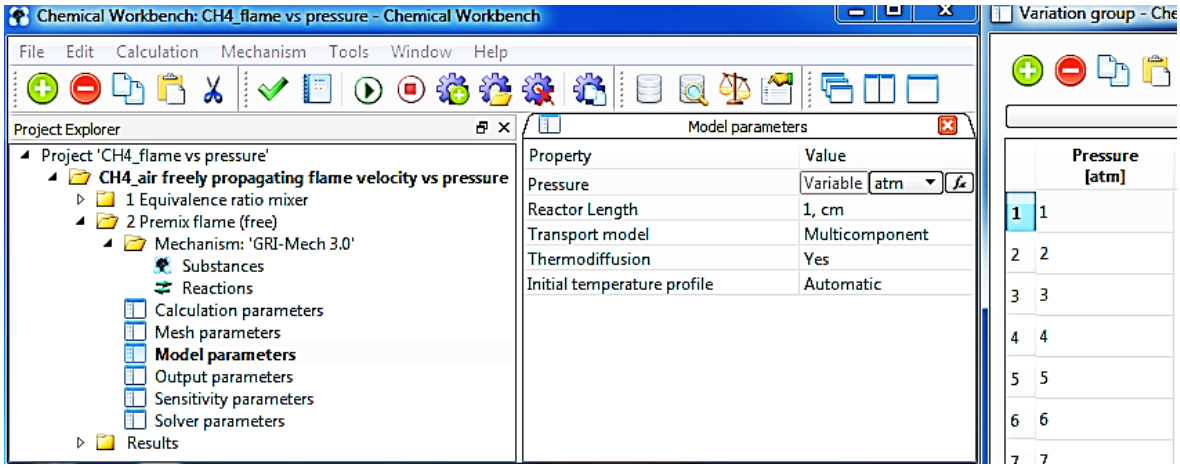
This example includes the calculation of free propagation flame velocities of at φ= 0.8, 1, 1.2 at To=300 K, P =1-20 atm. To calculate flame velocities as well as temperature and main concentrations behavior during the combustion of methane-air mixture at different equivalence ratios φ, we use the chain 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 of CH_4-air is inputted in this reactor - **Input Stream 1** - Fuel (CH_4), **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.

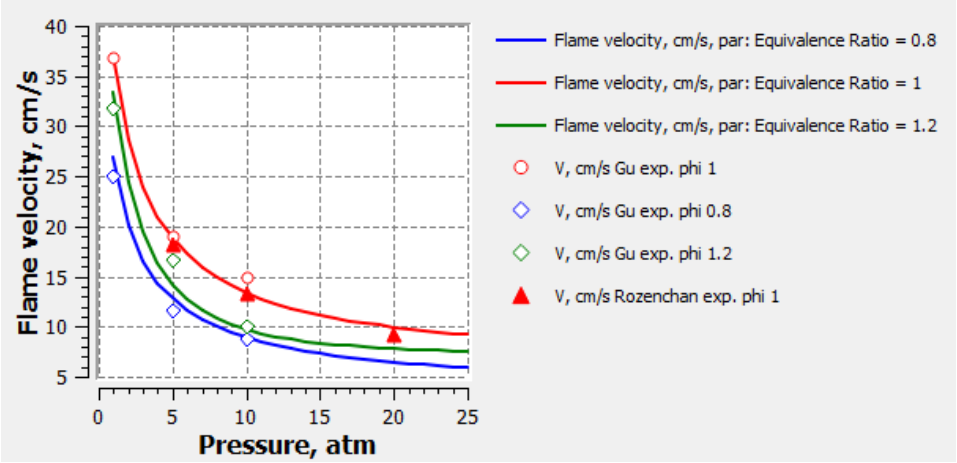


Premixed Flame Reactor demands setting the next:
•Mechanism,
•Model parameters,
•Calculation parameters
•Solver parameters
The minimum number of input parameters, related with numerical method implementation, is required. Particularly, no initial guess on temperature profile and intermediate species concentrations is required. This simplifies setup of laminar flame simulation



Results

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



Laminar burning velocities of CH_4 + air flames as a function of pressure for fixed equivalence ratios 0.8, 1, 1.2 at temperature 300 K.

Next steps

This example can be extended further
1.Run sensitivity analysis to identify reaction paths, 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. Gu XJ, Haq MZ, Lawes M, Woolley R. Laminar burning velocity and Markstein lengths of methane-air mixtures. Combustion and Flame 2000;121:41-58.
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).