KINTECH LABORATORY

Freely propagating flame velocity of CH4-air

Background

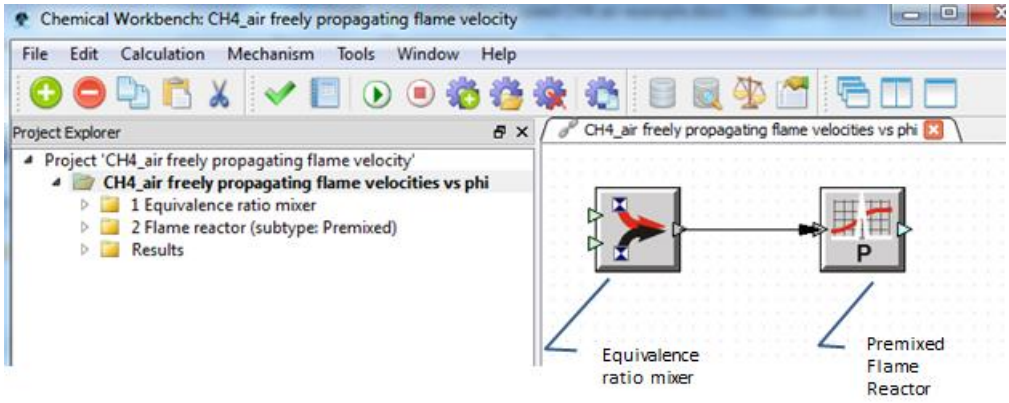
The laminar combustion properties are of fundamental importance for analyzing and predicting the performance of many experimental combustion systems and practical combustors, such as internal combustion engines. The freely propagating laminar flame model is destined for modeling the physicochemical behavior 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, for example, for purposes 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

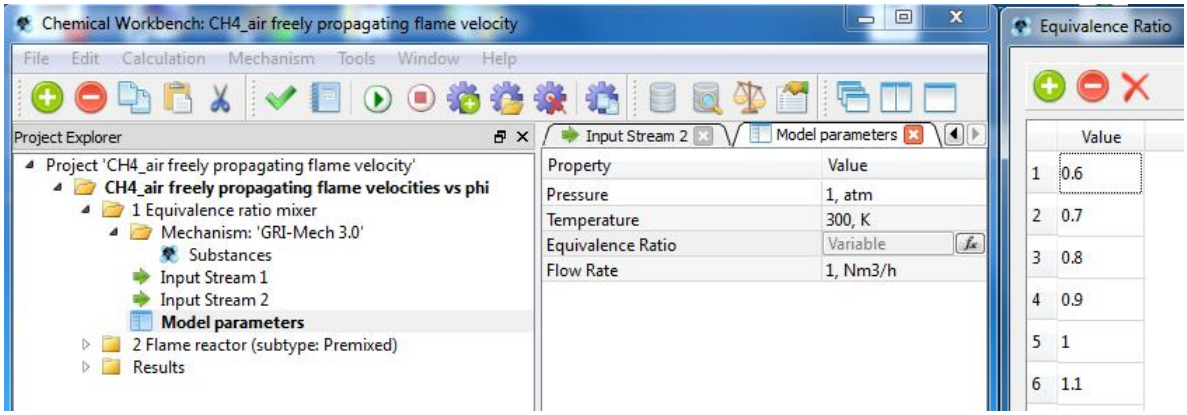
It is required to calculate the freely propagating flame velocities as function of equivalence ratio for the premixed methane-air laminar flames. Initial temperature of methane-air is 300K, pressure 1, 10, 20 atm. Mixture equivalence ratio - 0.6 – 1.8.

Problem setup in Chemical Workbench

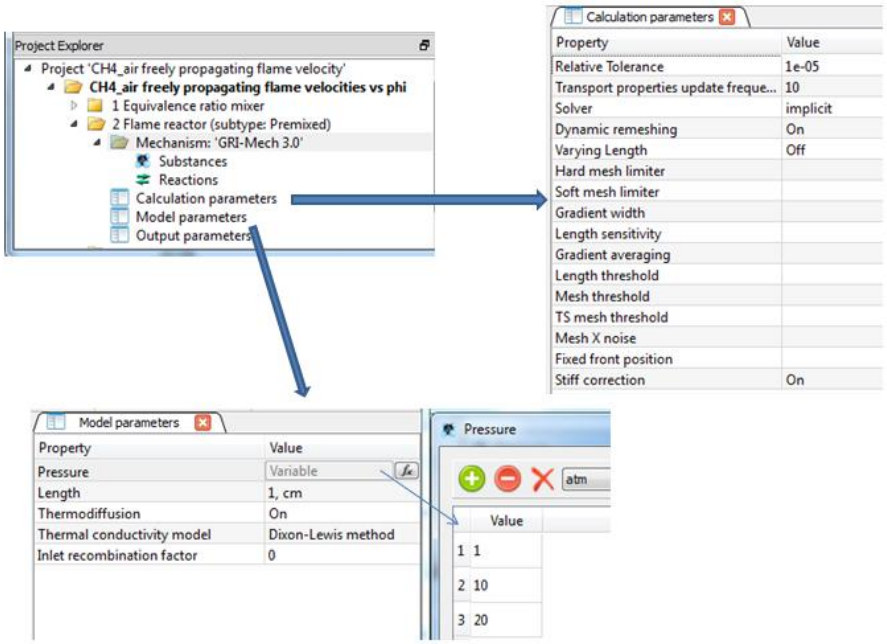
This example includes the calculation of free propagation flame velocities of at phi=0.6 – 1.8 at To=300 K, P =1, 10, 20 atm. To calculate freely propagating flame velocities , temperature and main concentrations behavior during the combustion of methane-air mixture at different phi, we use the chain 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 phi. The mixture of CH4-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 and provide kinetic mechanisms elaborated by Kintech or taken from available data . Pressure, initial temperature and equivalence ratio are given in **Model parameters**.



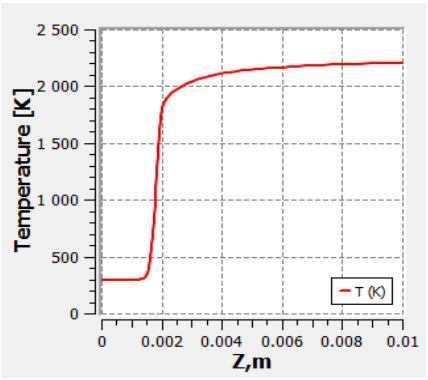
Premixed Flame Reactor demands setting the next: Mechanism, Calculation parameters, Model parameters.



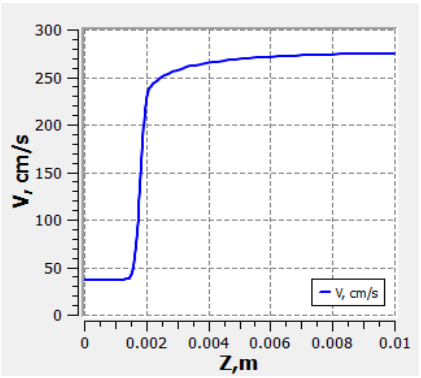
Experimental data can be included in **Results/External data** tables for validation of calculated results.

Results

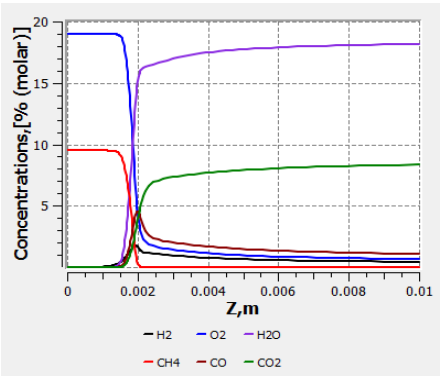
Simulated results are shown at below pictures. Experimental results are taken from [1], [2].



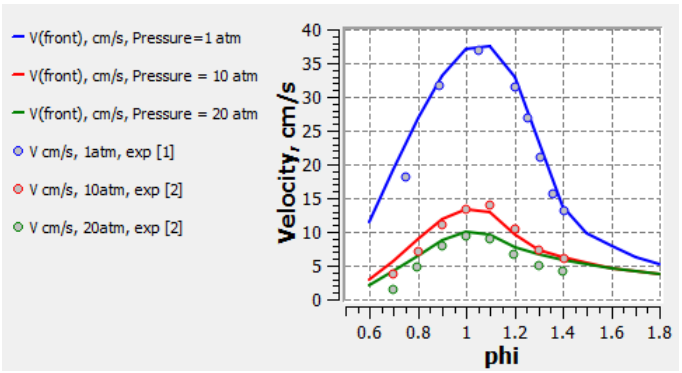
Temperature of stoichiometric CH4 + air flame at standard conditions (298 K, 1 atm).



Laminar burning velocity of stoichiometric CH4 + air flame at standard conditions (298 K, 1 atm).



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 phi = 0.6-1.8.

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).