Methane opposed–flow diffusion flame.

Background

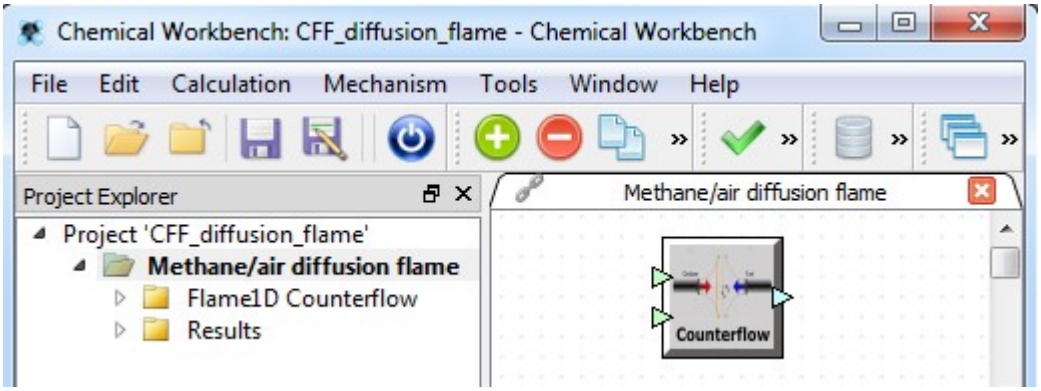
Combustion of non-premixed fuel-air mixtures is widely used in industrial and transportation combustion systems. Very often the modeling of these systems rely on the concept of counterflow flames with specified strain rates. These flames are also widely used as experimental facilities for generating data for chemical kinetic mechanisms validation.
This example demonstrates how the non-premixed counter-flow flame can be modeled in frame of Chemical Workench software.

Problem statement

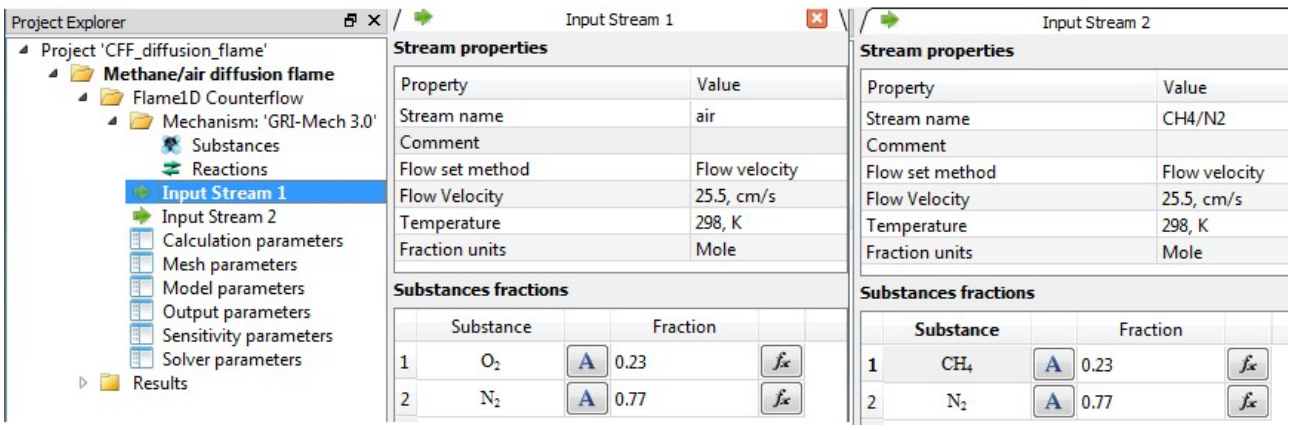
It is required to reproduce the experimentally obtained structure of methane-air counter-flow diffusion flame, which include species and temperature profiles. The fuel and oxidizer streams respectively consist of 23% methane in nitrogen, and 23% oxygen in nitrogen, both by volume, The experimental setup consists of two convergent nozzle burners with 14 mm exit diameters, placed as 13 mm apart. Exit velocities of the gases at the nozzle exits are kept equal 25.5 cm/s.

Problem setup in Chemical Workbench

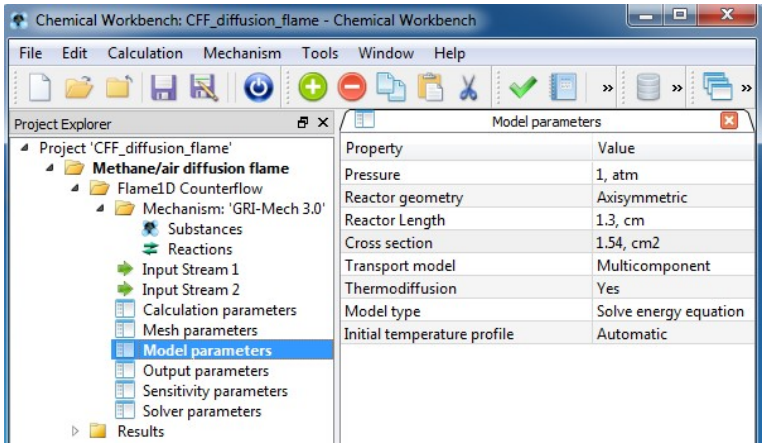
This example includes the calculation of velocity, temperature and major species profiles across the flame. Calculations were performed in the axisymmetric configuration with one atmosphere pressure and 300 K upstream temperature. To calculate gas velocities, temperature and main concentrations behavior during the combustion of methane - air mixture, **Diffusion Counterflow Flame Reactor** was used in frame of Chemical Workbench. For validation of calculated results experimental data from [1] were used.



Mixture of CH_4 and air is fed in **Diffusion Counterflow Reactor as follows**: air in **Input Stream 1**, methane/N2 mixture in **Input Stream 2**. The detailed kinetic mechanism GRIMech 3.0 was loaded from KintechDB database.

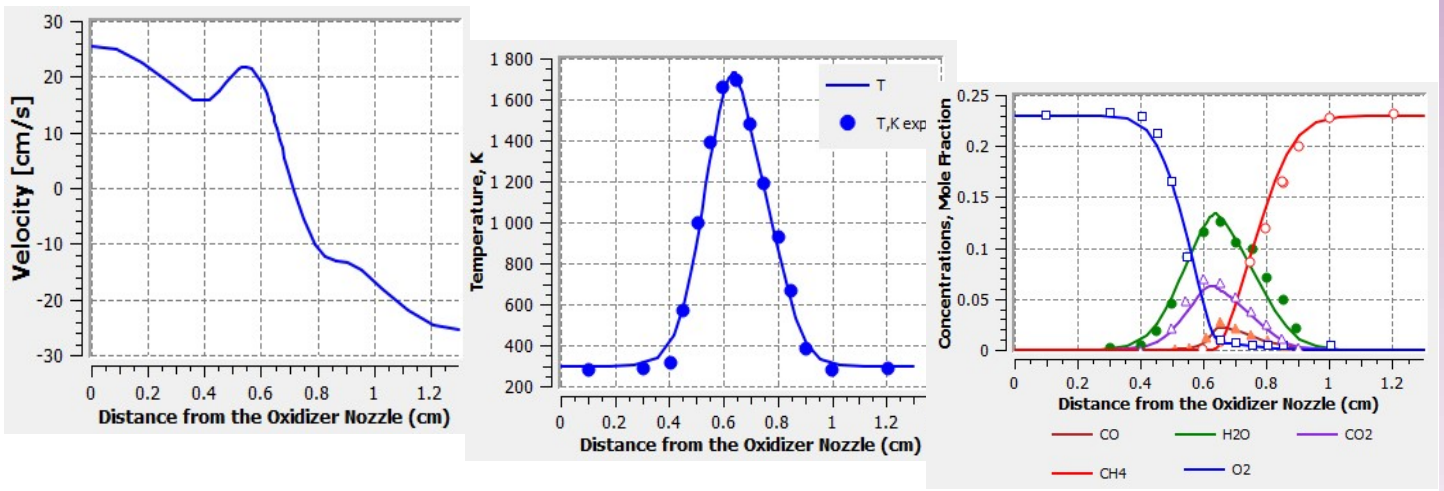


Diffusion Counterflow Reactor requires setting the follwoingdata:
•Mechanism,
•Model parameters (pressure, burners distance, burners cross-sections, transport model, etc.),
•Calculation paremeters (solver accuracy)
•Solver parameters (convergence criteria, mesh refinement, etc.)
The minimum number of input parameters, related with numerical method implementation, is required. This simplifies setup of diffusion flame simulation.



Results

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



Comparison between experimental and computed temperature and major species profiles. Lines denote computational results and symbols denote experimental data.

Next steps

This example can be extended further
1.Run sensitivity analysis to identify reaction paths, which affect diffusion velocity most of all
2.Compare predictions of different chemical kinetic mechanisms, available in KintechDB database, for conditions of interest for you

References

1. Sung C J, Liu J B, Law C K. Structure response of counterflow diffusion flames to strain rate variations. Combust Flame, 1995, 102: 481– 492.