

Introduction

In order to improve hydrogen production in an ethanol reformer it is necessary to understand what happens inside it.

Also, a numerical model can simulate different work conditions avoiding the necessity of doing a lot of experiments.

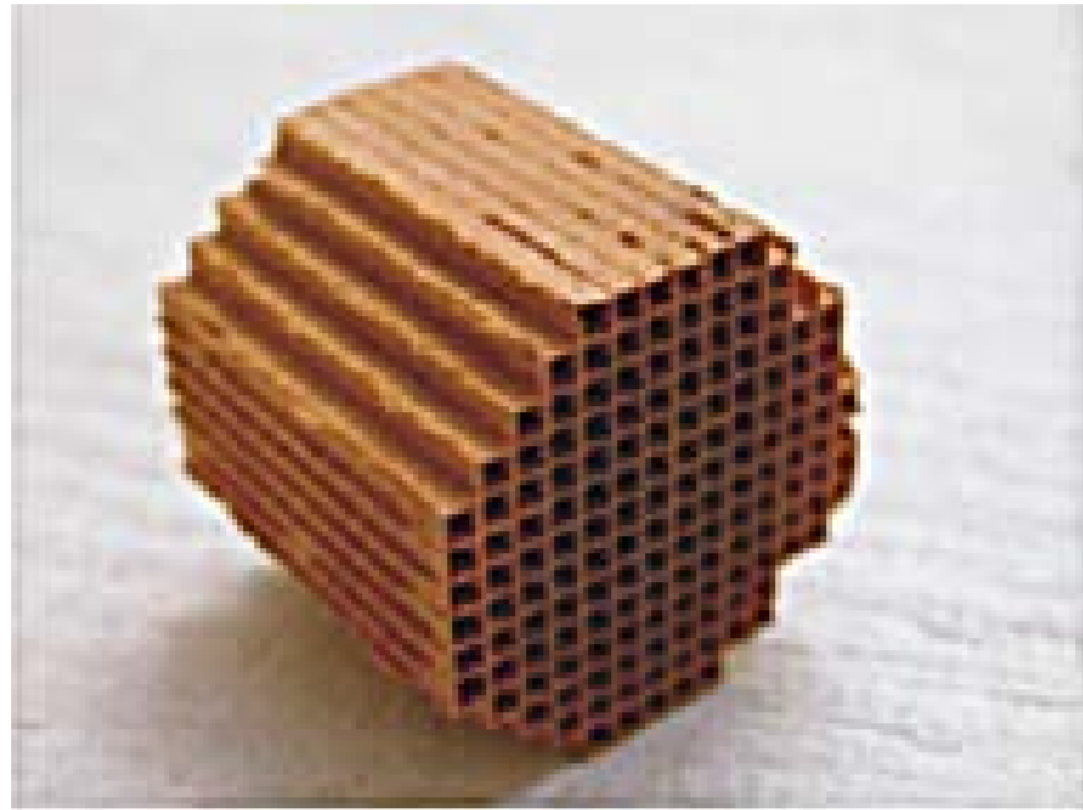
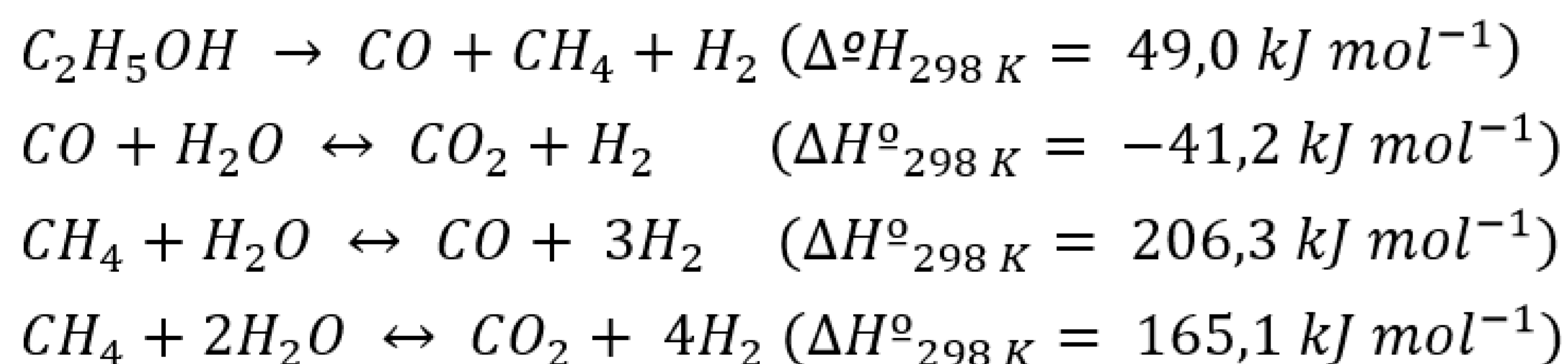


Figure 1. Ethanol reformer used in the experimental data¹

Computational Methods

To simulate the reformer it has been necessary to use 4 physics interfaces: heat transfer, CFD (laminar flow), chemistry and transport of concentrated species.

For the chemical reactions that take place inside the reformer only the main ones have been modeled:



The reaction rates have been modeled using Arrhenius expressions, where the activation energies have been obtained from [1] and the pre-exponential factors have been calculated using COMSOL Multiphysics®.

Transport and thermodynamic species expressions have been obtained using CHEMKIN extracted from [2].

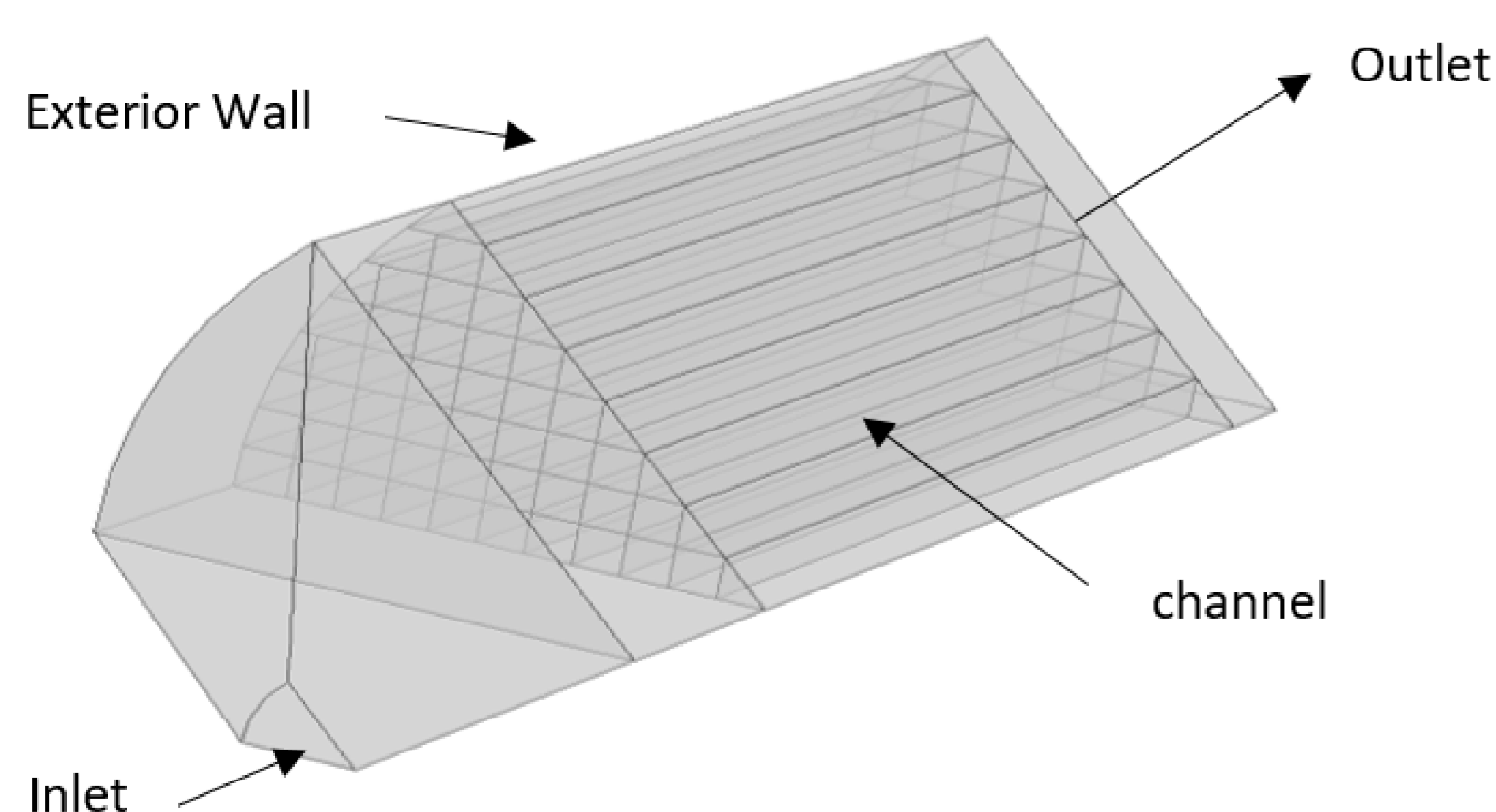


Figure 2. Geometry modelled

Results

The simulated model has been contrasted with a real experimental data showed below.

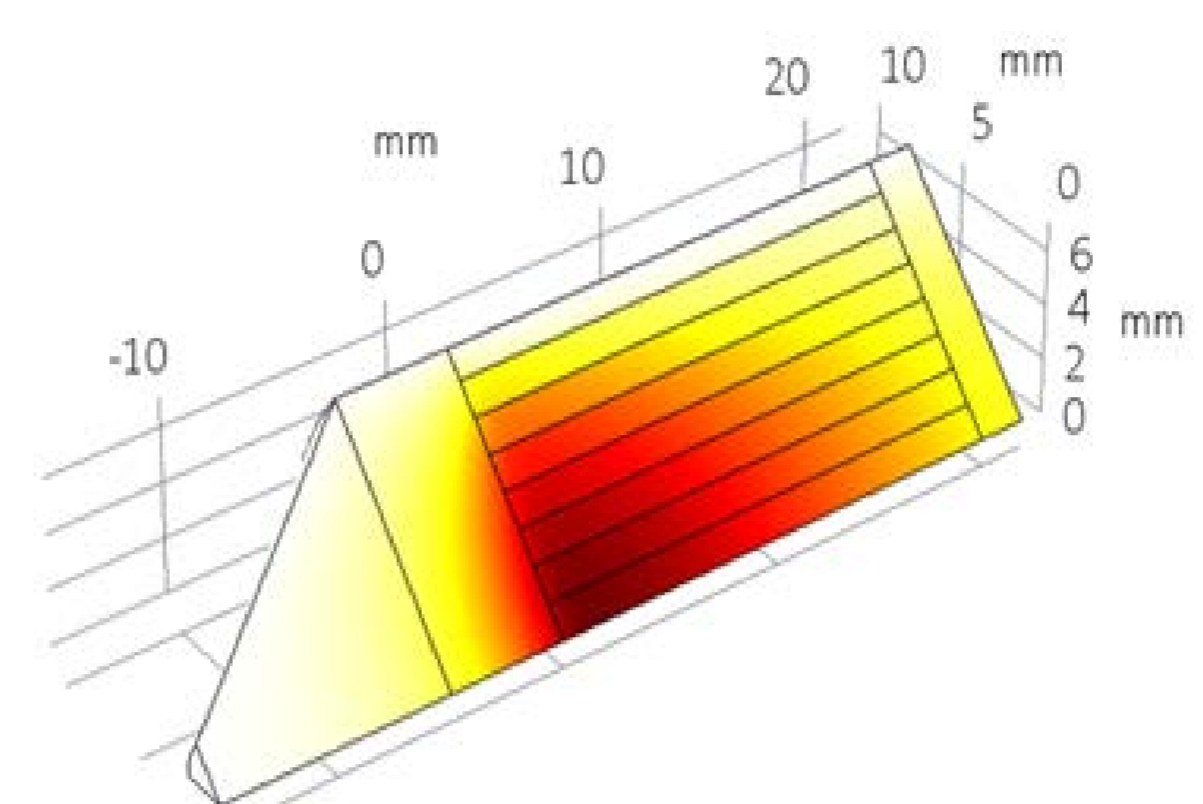


Figure 3. Temperature field (K), 950 K operating temperature and 6 bars pressure

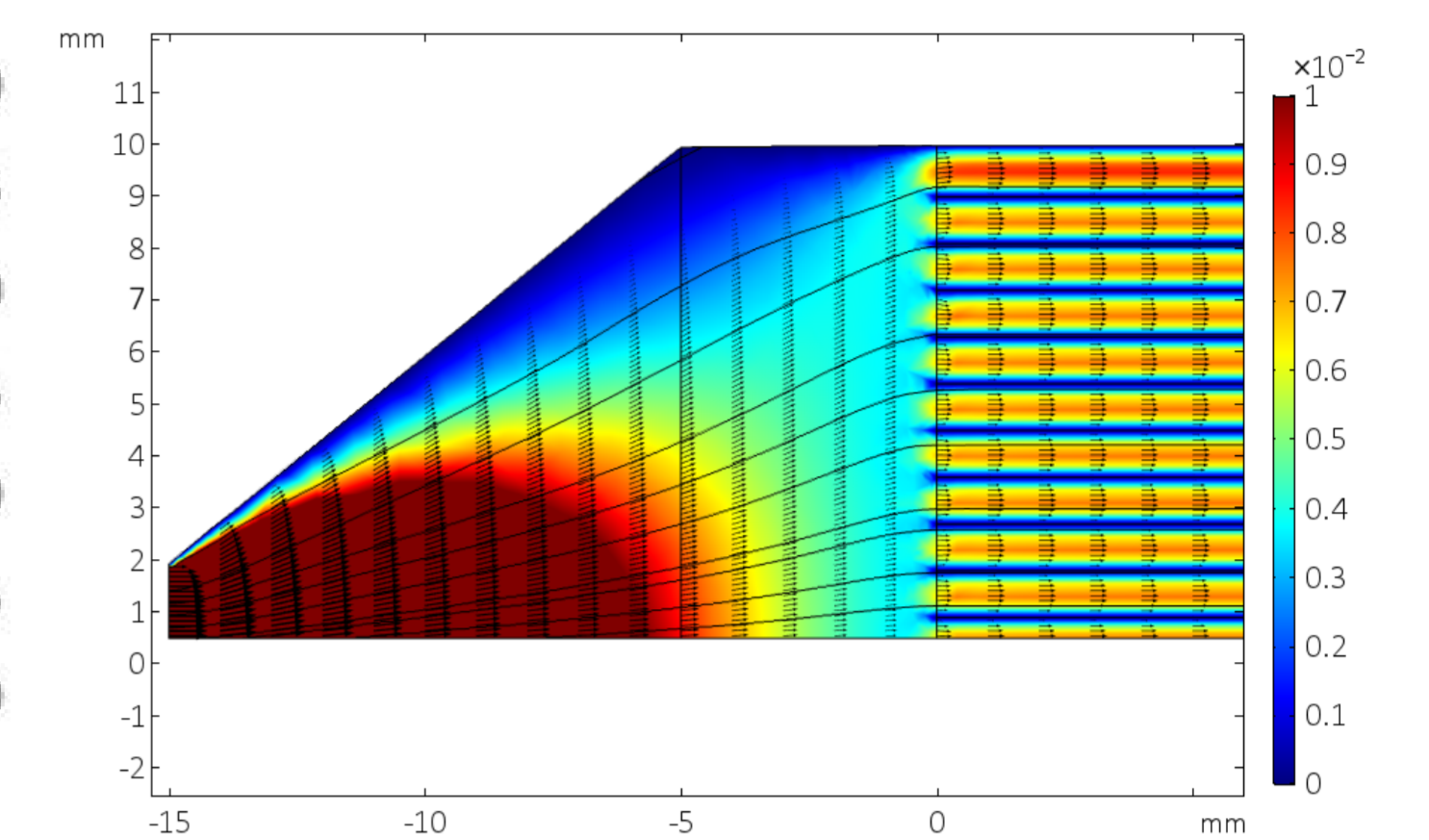


Figure 4. Velocity field (m/s), 825 K operating temperature and 3 bars pressure

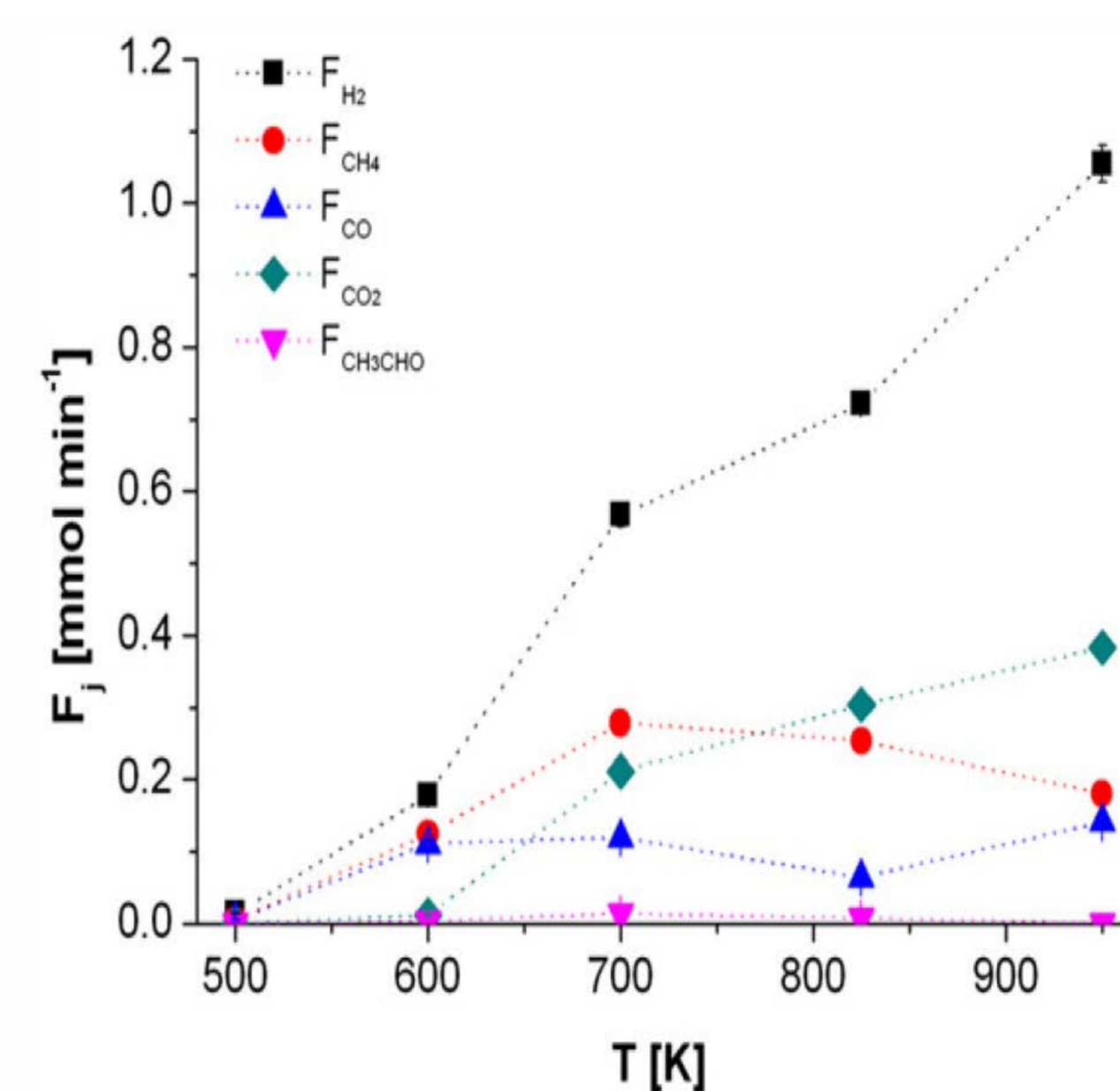


Figure 5. Experimental exit flow rates at 3 bar¹

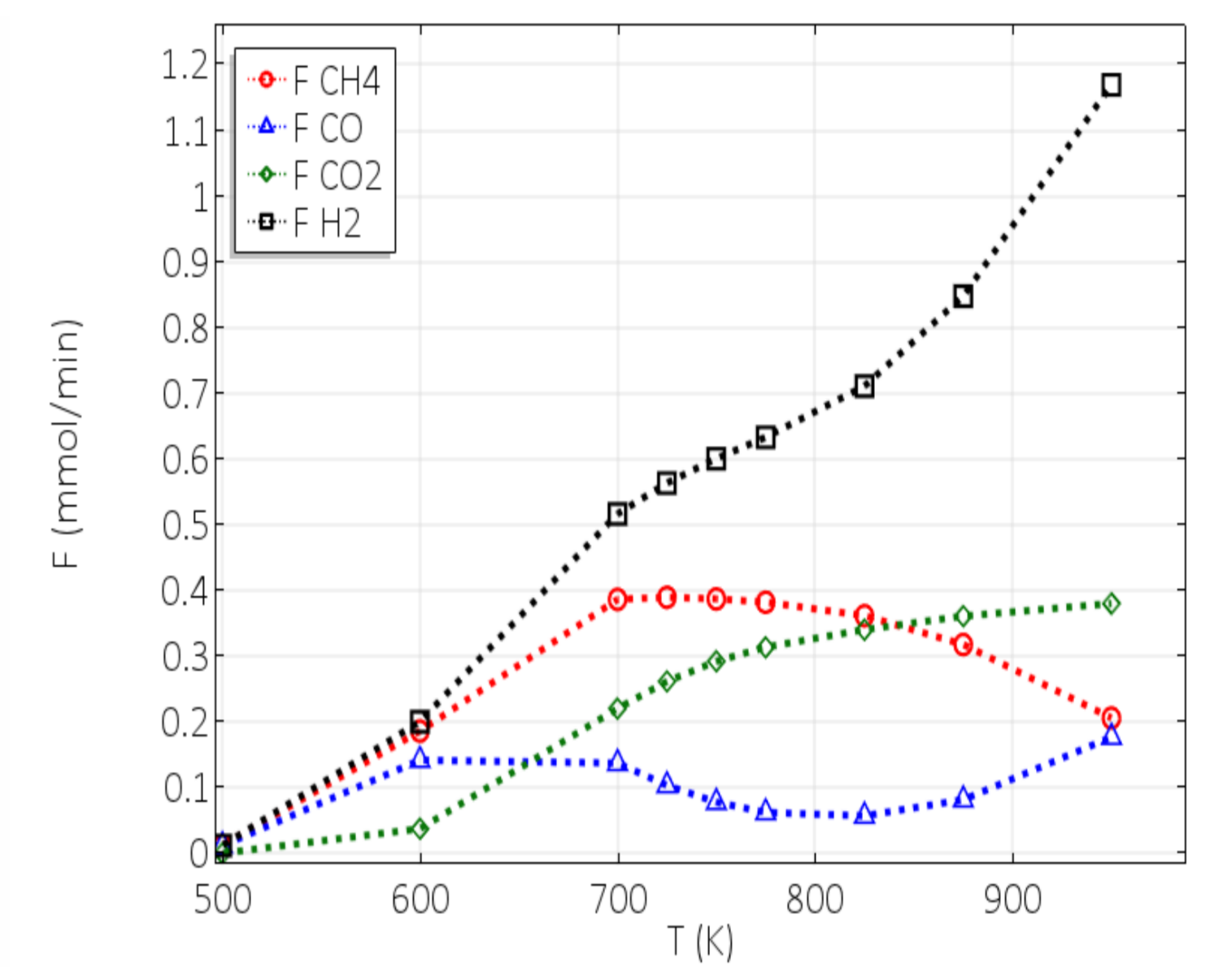


Figure 6. Simulated exit flow rates at 3 bar

Conclusions

The 3D model is accurate enough to show a similar behavior compared to the experimental data. The developed numerical model allows for a better understanding of reformers since there are not a lot of 3D models published.

Future work will consist on how to increase the efficiency of the reformer and optimize external heat necessary to produce hydrogen.

References

1. E. López, J. Llorca, N. J. Divins, A. Anzola, S. Schbib, D. Borio, "Ethanol Steam Reforming for Hydrogen Generation over Structured Analysis". International Journal of Hydrogen Energy, 38, 4418-4428, 2013.
2. "Chemical-Kinetic Mechanisms for Combustion Applications", San Diego Mechanism web page, Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego (<http://combustion.ucsd.edu>).