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The Energy Institute
College of Earth & Mineral Sciences

Simulation of H_2-O_2 Constant Volume Combustion using Comsol Multiphysics™

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EGEE 520: Mathematical Methods

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Agenda

- Introduction
- Governing Equations
- Solution using Comsol Multiphysics™
- Model Validation
- Parametric Study
- Summary

Introduction

- Hydrogen oxidation is the most studied kinetic mechanism; simulation models predict performance with extremely high accuracy.
- Hydrogen combustion study has become of supreme importance due to the advances in fuel cell technology (fuel of the future?).
- From the thermodynamic fundamental perspective, hydrogen combustion exhibits the lowest irreversibility among current combustion systems. This means superior thermal and second-law efficiencies.
- Ultimate goal of this project is to analyze irreversibility during hydrogen combustion at constant volume, and develop a simulation tool for optimization of performance.

Governing Equations(1)

- Conservation of Mass:

$$\frac{\partial \rho^g}{\partial t} + \frac{1}{a}\frac{1}{r^2}\frac{\partial}{\partial r}(\rho^g r^2 V_r) = 0.$$

- Conservation of Energy:

$$\frac{\partial}{\partial t}(\rho^g C_p^g T^g) + \frac{1}{a}\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \rho^g C_p^g T^g V_r) = \frac{1}{a^2}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \rho^g C_p^g \alpha^g \frac{\partial T^g}{\partial r}\right) + \dot{S}_E$$

- Conservation of Species:

$$\frac{\partial}{\partial t}(\rho^g C_J) + \frac{1}{a}\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \rho^g C_J V_r) = \frac{G}{a^2}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \rho^g D^g \frac{\partial C_J}{\partial r}\right) + \dot{S}_C$$

(1) Hiwase, 1998

Solution in Comsol Multiphysics™ (1)

- 2D geometry and coupled Fluid-Chemical Reactions sub-model:
  - Convection and Diffusion (Mass Conservation)
  - Convection and Conduction (Energy Conservation)
  - Incompressible Navier-Stokes (Momentum Conservation)

- Assumptions:
  - Reaction between hydrogen and oxygen occurs according to the "forward-only" 7-steps reaction model developed by the NASA Langley Research Center.
  - Hydrogen and oxygen are fully mixed in a constant volume combustion chamber. No flows are considered before or after chemical reaction.
  - Combustion is initiated by the effect of temperature, which is always above the autoignition temperature for H_2-O_2 (860K).
  - Effect of pressure is not considered in the kinetic combustion model.
  - Combustion chamber is thermally insulated (adiabatic combustion).

Solution in Comsol Multiphysics™ (2)

- Kinetic Model for Hydrogen Oxidation:

$H_2 + O_2 \rightarrow 2OH$
$H + O_2 \rightarrow OH + O$
$OH + H_2 \rightarrow H_2O + H$
$O + H_2 \rightarrow OH + H$
$2OH \rightarrow H_2O + O$
$H + OH \rightarrow H_2O$
$2H \rightarrow H_2$

$$\frac{dC_{H2}}{dt} = -k_1 \cdot C_{H2} \cdot C_{O2} - k_3 \cdot C_{OH} \cdot C_{H2} + k_7 \cdot C_H \cdot C_H - k_4 \cdot C_O \cdot C_{H2}$$

$$\frac{dC_{O2}}{dt} = -k_1 \cdot C_{H2} \cdot C_{O2} - k_2 \cdot C_H \cdot C_{O2}$$

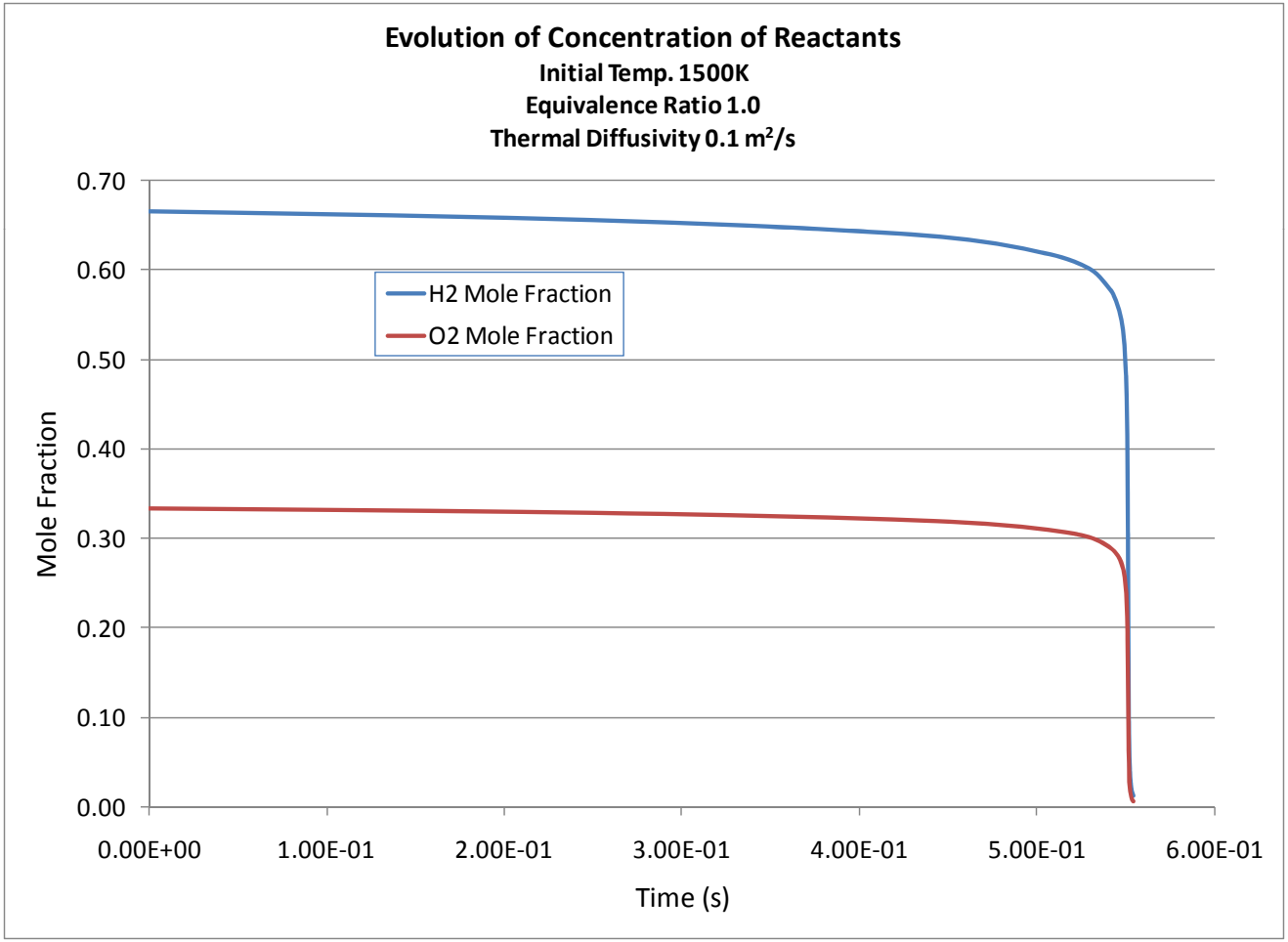
$$\frac{dC_{H2O}}{dt} = k_3 \cdot C_{OH} \cdot C_{H2} + k_5 \cdot C_{OH} \cdot C_{OH} + k_6 \cdot C_H \cdot C_{OH}$$

$$\frac{dC_{OH}}{dt} = 2k_1 \cdot C_{H2} \cdot C_{O2} + k_2 \cdot C_H \cdot C_{O2} - k_3 \cdot C_{OH} \cdot C_{H2} + k_4 \cdot C_O \cdot C_{H2} - 2k_5 \cdot C_{OH} \cdot C_{OH} - k_6 \cdot C_H \cdot C_{OH}$$

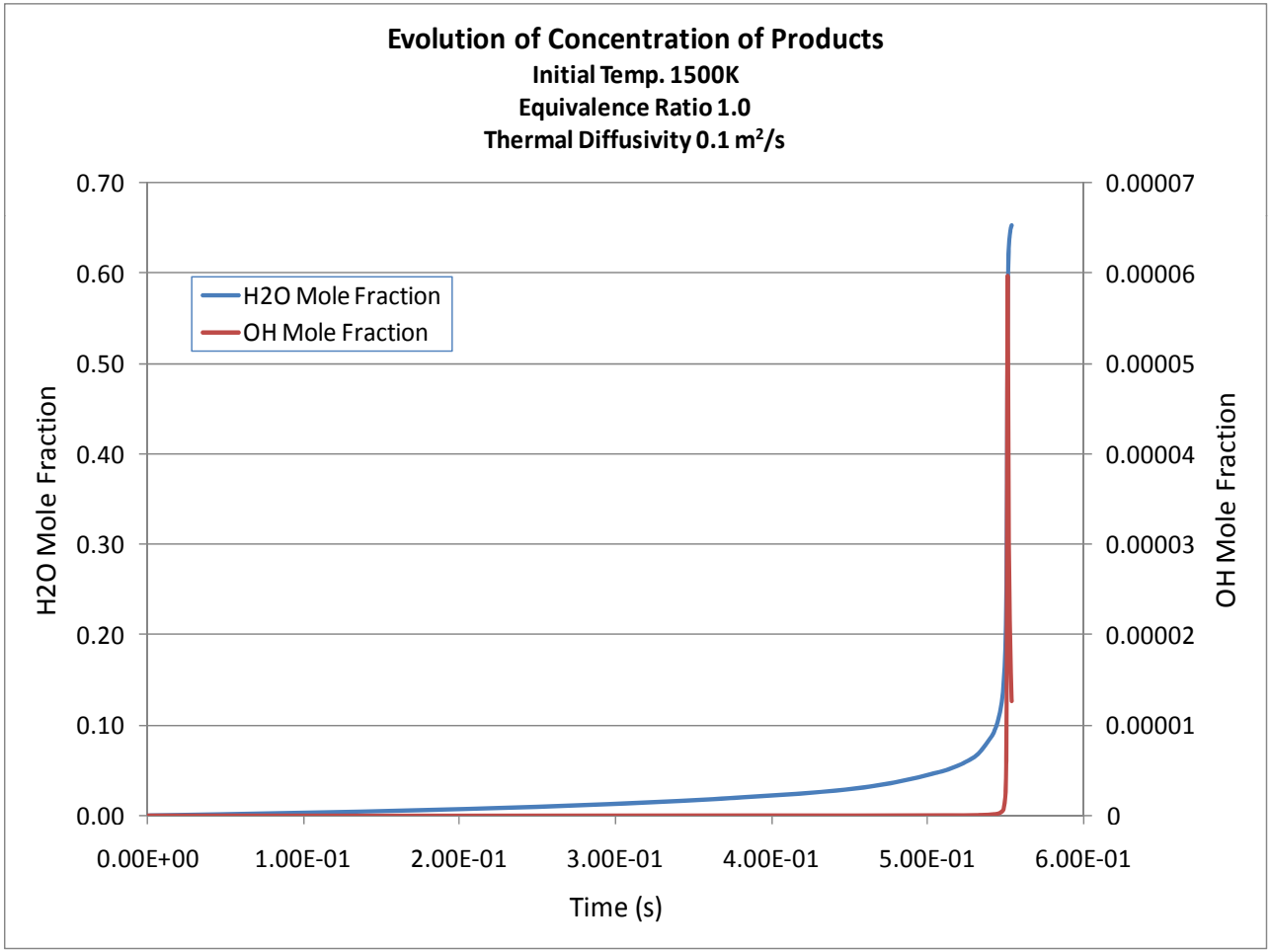
$$\frac{dC_H}{dt} = -k_2 \cdot C_H \cdot C_{O2} + k_3 \cdot C_{OH} \cdot C_{H2} + k_4 \cdot C_O \cdot C_{H2} - k_6 \cdot C_H \cdot C_{OH} - 2k_7 \cdot C_H \cdot C_H$$

$$\frac{dC_O}{dt} = k_2 \cdot C_H \cdot C_{O2} - k_4 \cdot C_O \cdot C_{H2} + k_5 \cdot C_{OH} \cdot C_{OH}$$

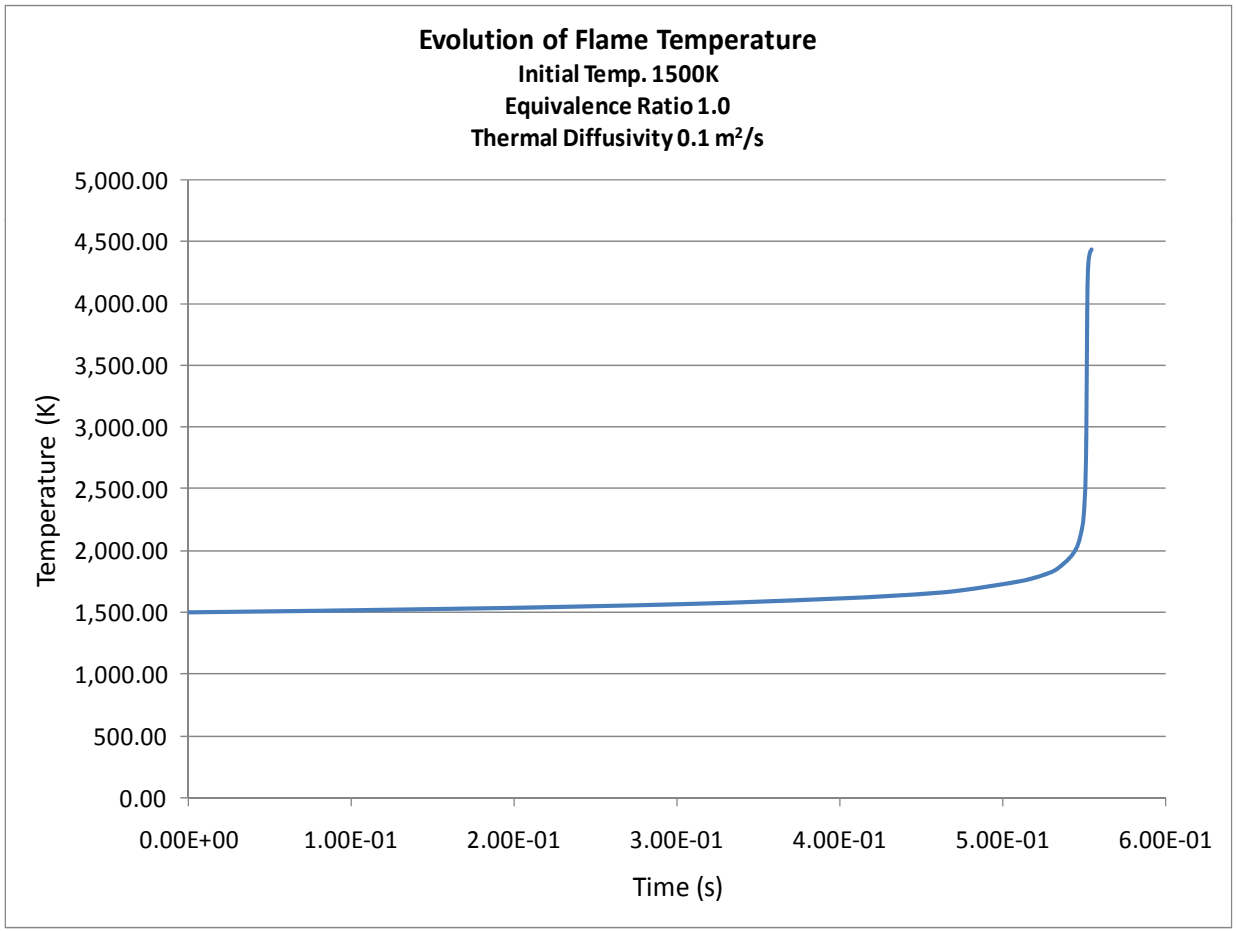
Solution in Comsol Multiphysics™ (3)



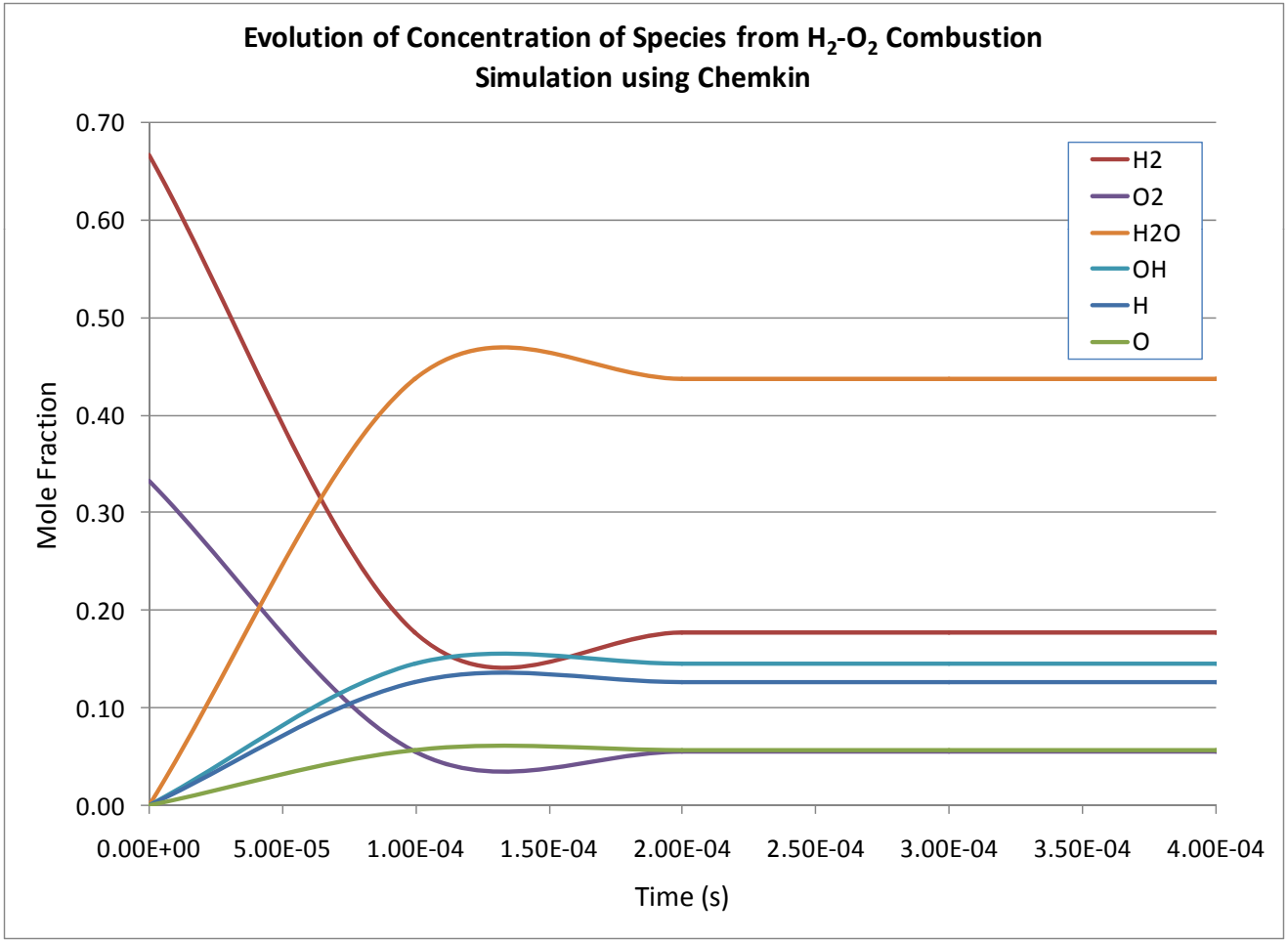
Solution in Comsol Multiphysics™ (4)



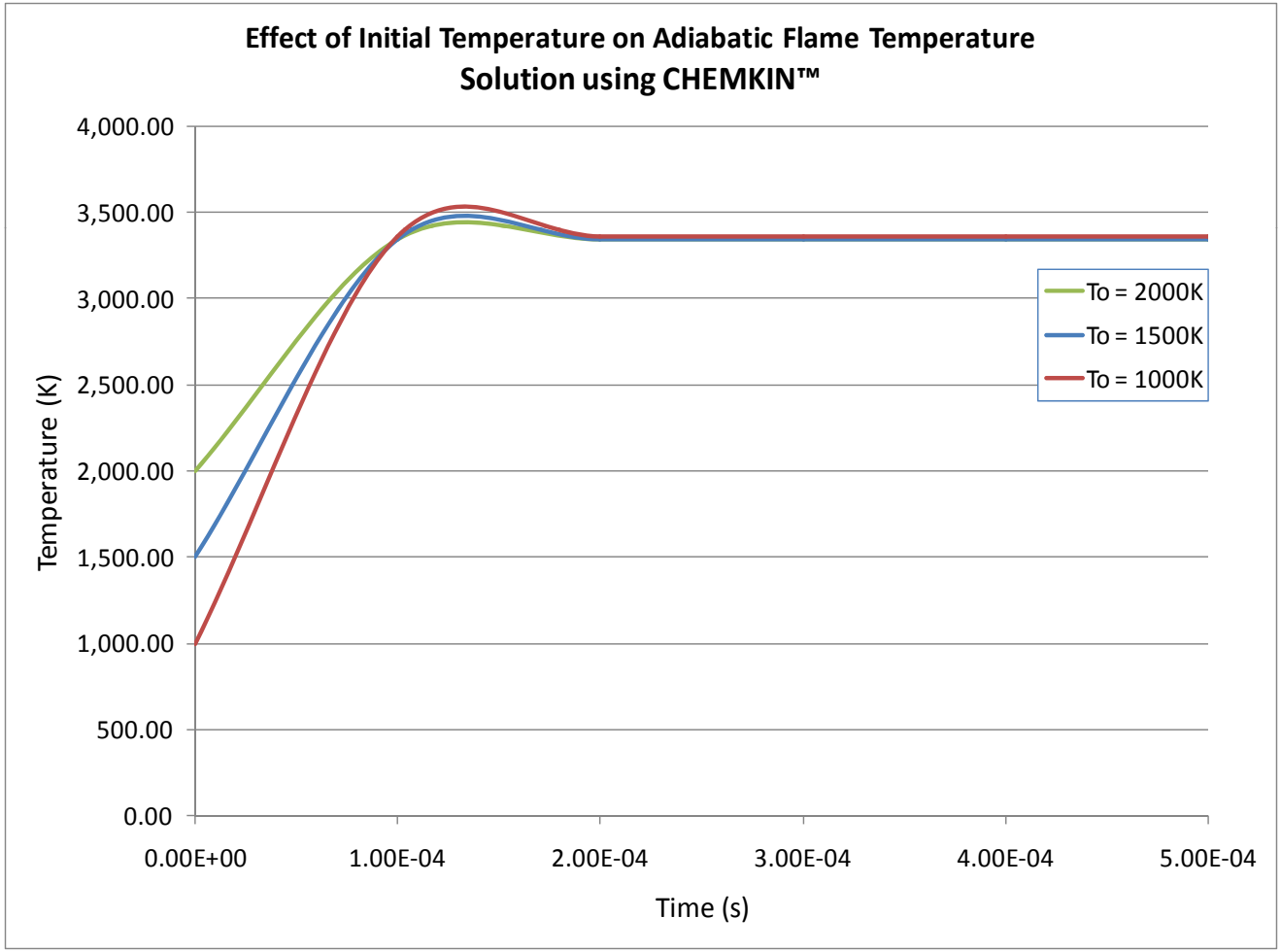
Solution in Comsol Multiphysics™ (5)



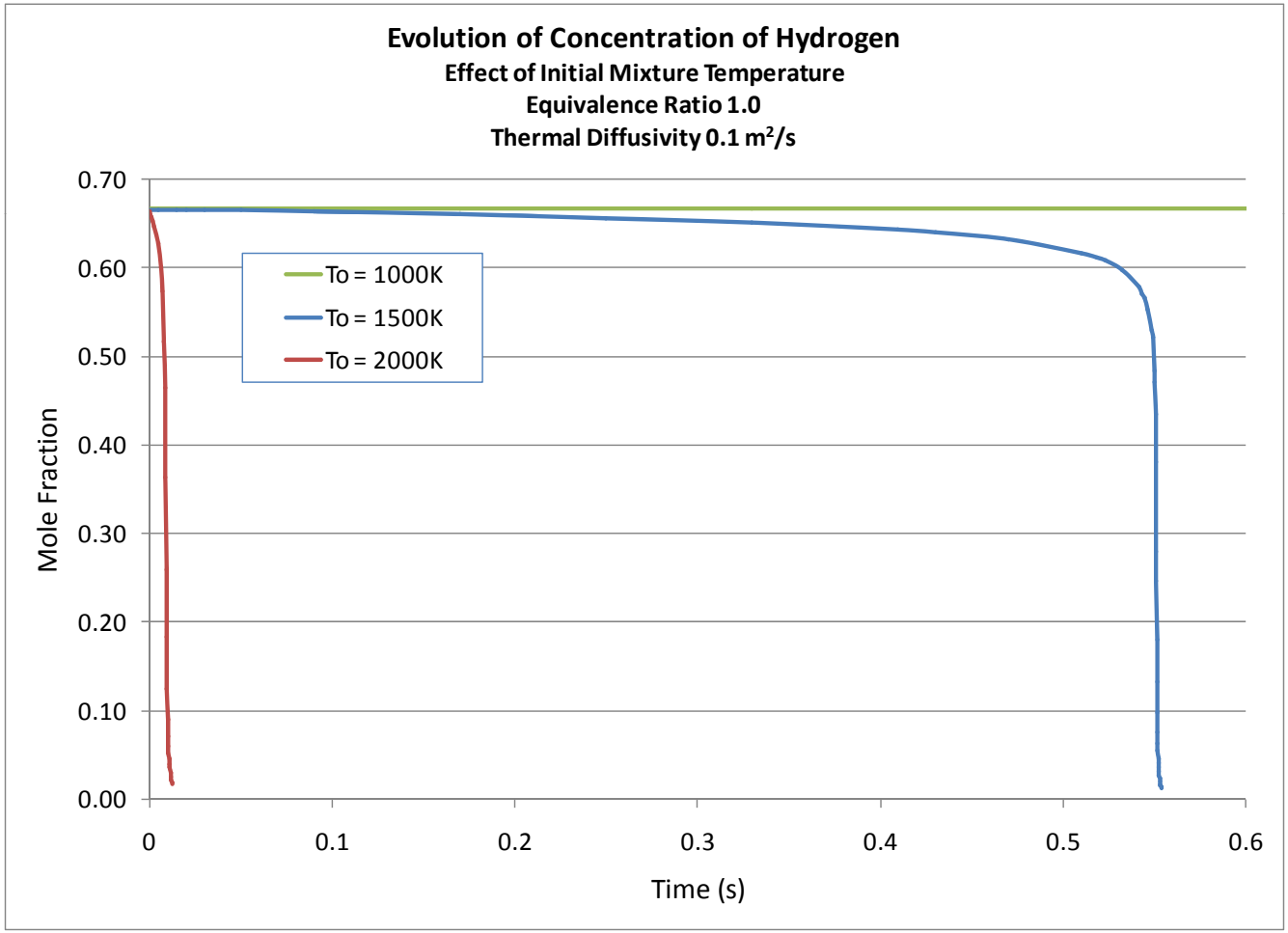
Validation – Solution using CHEMKIN™



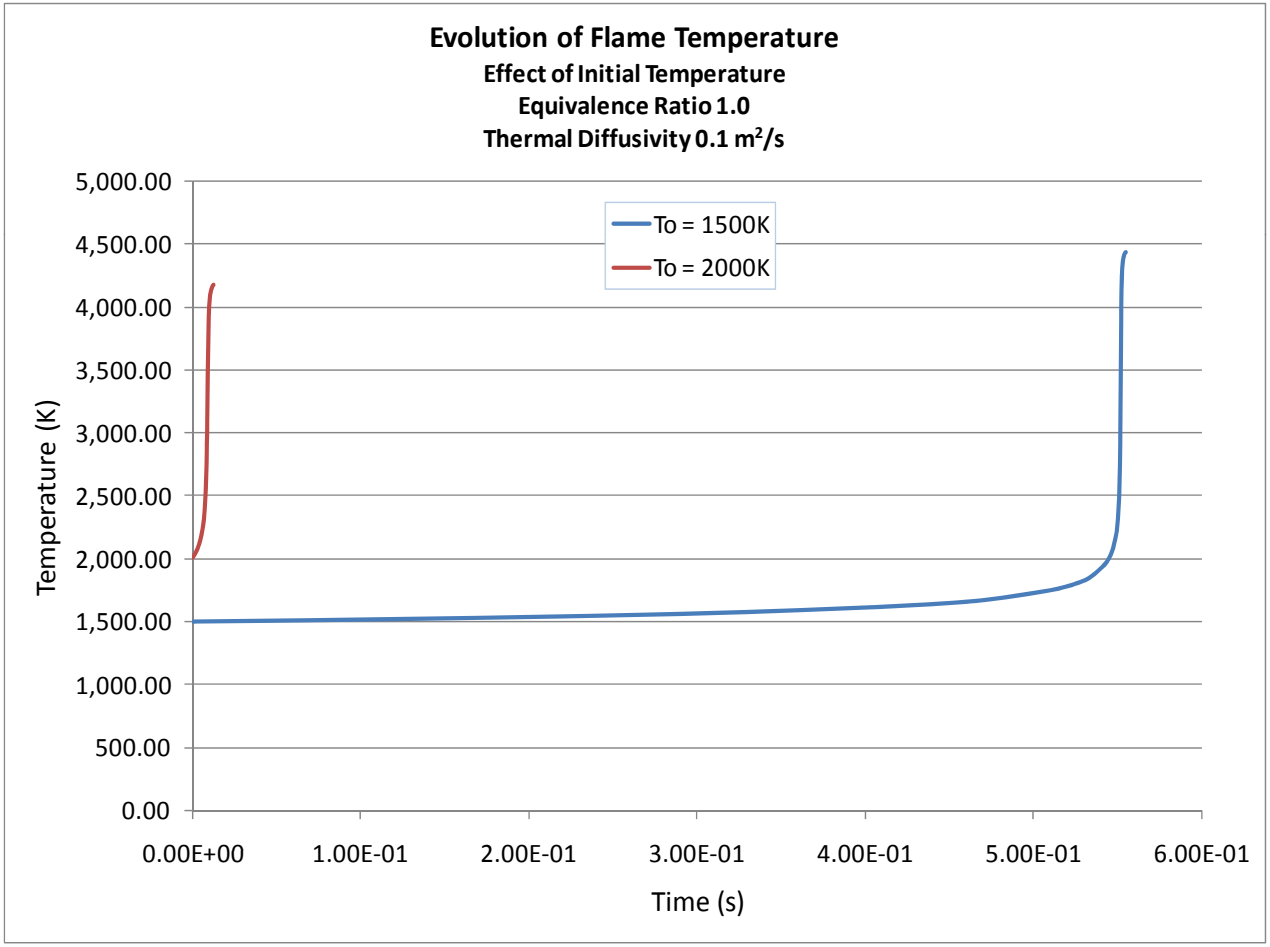
Validation – Solution using CHEMKIN™ (2)



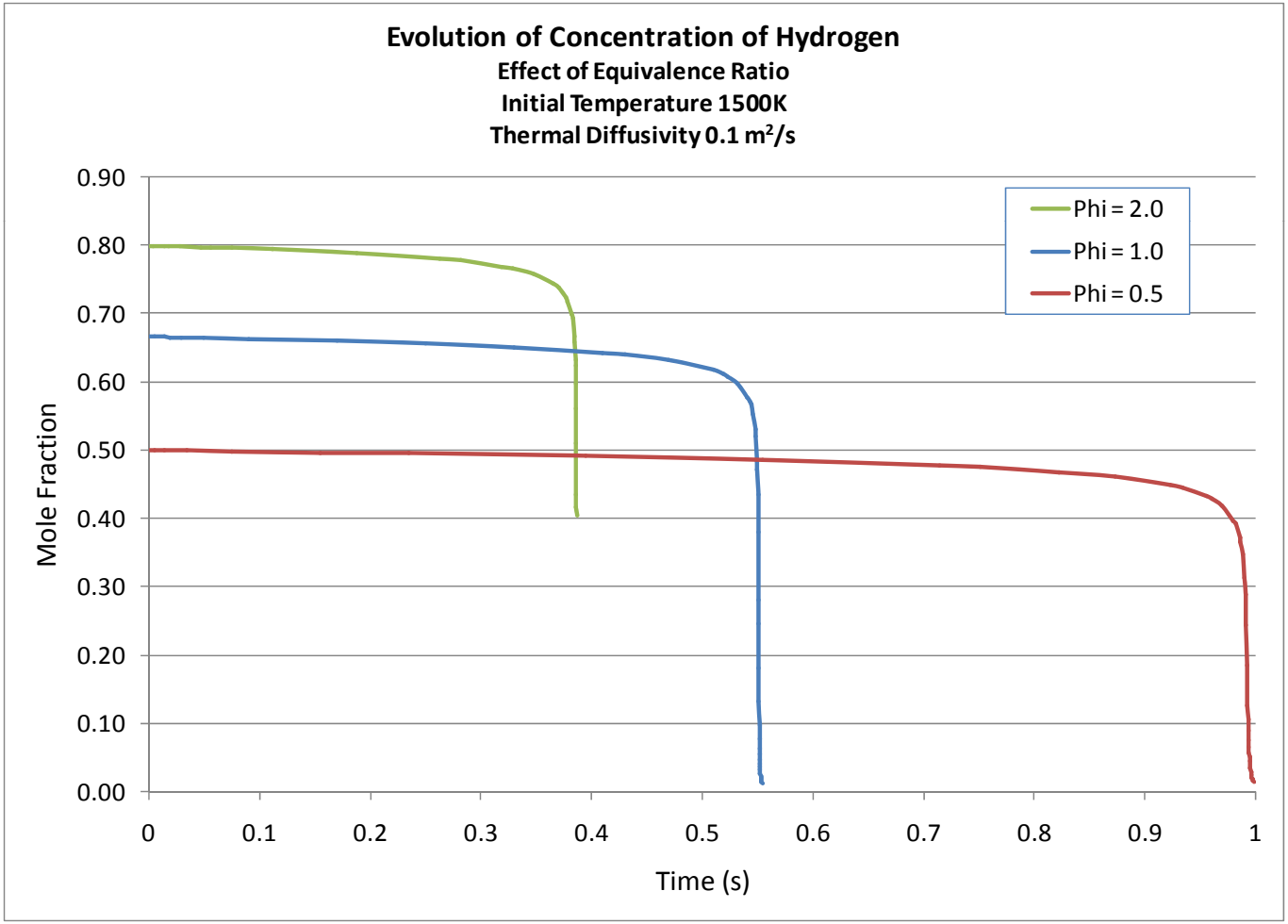
Parametric Study – Effect of Temperature



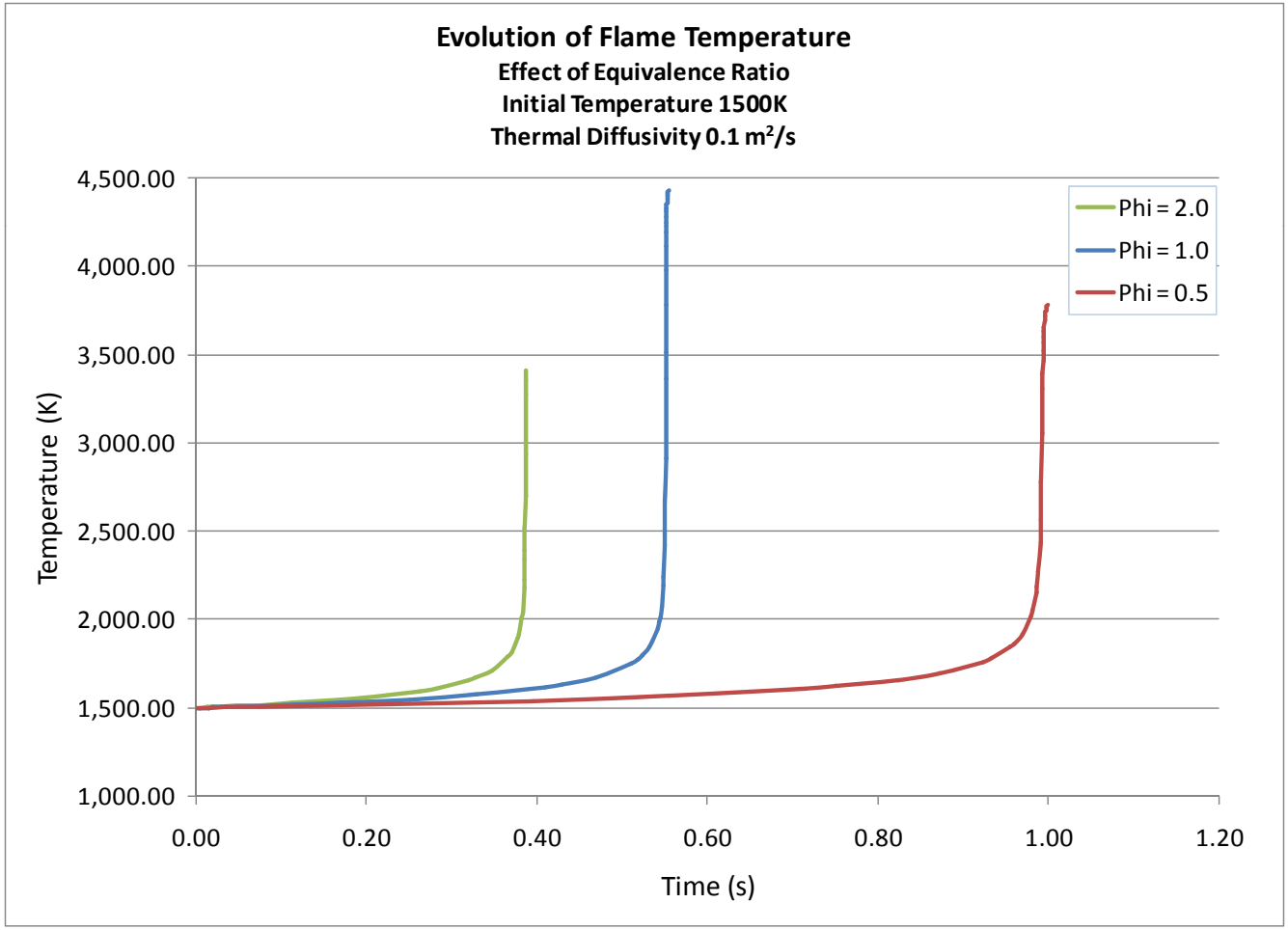
Parametric Study – Effect of Temperature (2)



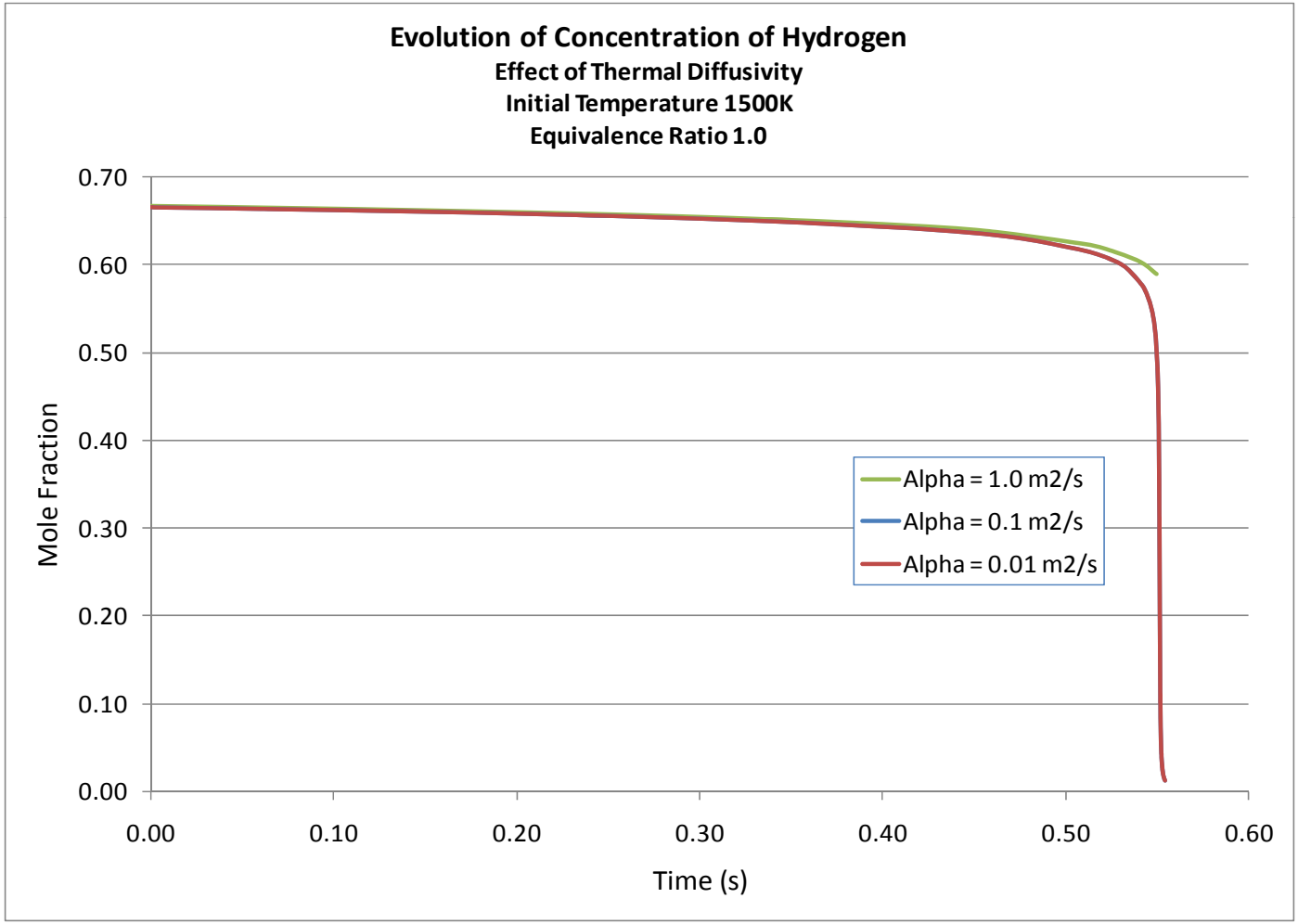
Parametric Study – Effect of Equivalence Ratio



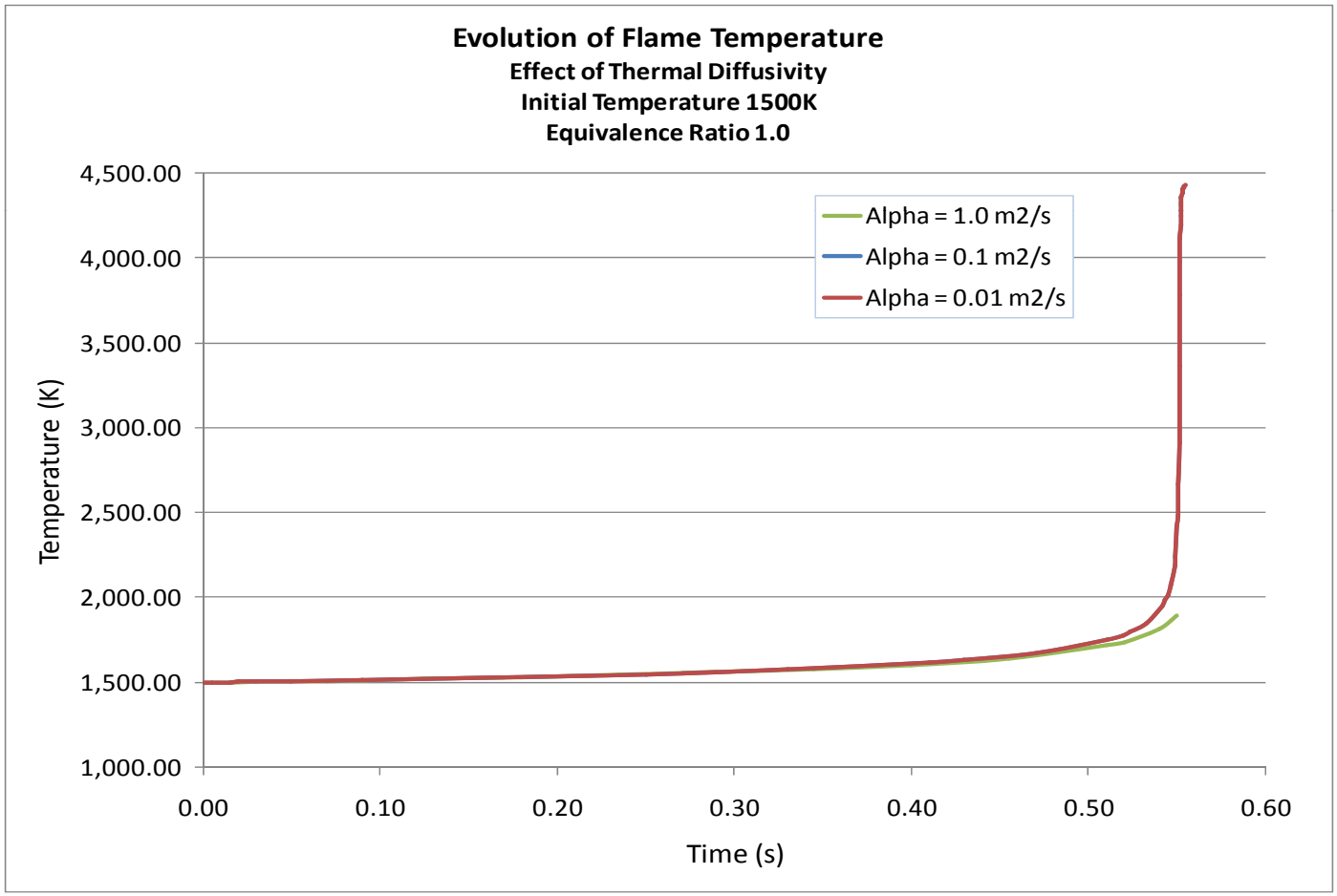
Parametric Study – Effect of Equivalence Ratio (2)



Parametric Study – Effect of Thermal Diffusion



Parametric Study – Effect of Thermal Diffusion (2)



Summary

- The model in Comsol Multiphysics™ does not capture the features of the real system as predicted by CHEMKIN™ in terms of species profiles and adiabatic flame temperatures.
- The parametric study exhibits correct trends in terms of the effects of initial mixture temperature, equivalence ratio and thermal diffusivity.
- Further refinement of the model and higher computational capabilities are needed to reproduce experimental kinetic data, analyze heat and mass transfer in complex (open, non-adiabatic) systems and simulate the full performance 3D geometries.
- Entropy generation and lost available work calculations were not considered as the model lacks physical meaning, and processes of heat and mass transfer could not be successfully included. This remains as part of future work to be considered by next students.