Simulation of H$_2$-O$_2$ Constant Volume Combustion using Comsol Multiphysics™

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

- Conservation of Energy:
  \[
  \frac{\partial}{\partial t} \left( \rho^g C_p^g T^g \right) + \frac{1}{a \ r^2} \frac{\partial}{\partial r} \left( r^2 \rho^g C_p^g T^g V_r \right) = \frac{1}{a^2 r^2} \frac{\partial}{\partial r} \left( r^2 \rho^g C_p^g \alpha^g \frac{\partial T^g}{\partial r} \right) + \dot{S}_E
  \]

- Conservation of Species:
  \[
  \frac{\partial}{\partial t} (\rho^g C_J) + \frac{1}{a \ r^2} \frac{\partial}{\partial r} (r^2 \rho^g C_J V_r) = \frac{G}{a^2 r^2} \frac{\partial}{\partial r} \left( r^2 \rho^g D^g \frac{\partial C_J}{\partial r} \right) + \dot{S}_C
  \]

\(^{(1)}\) 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 H₂-O₂ (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:

\[
\begin{align*}
\frac{dC_{\text{H}_2}}{dt} &= -k_1 \cdot C_{\text{H}_2} \cdot C_{\text{O}_2} - k_3 \cdot C_{\text{OH}} \cdot C_{\text{H}_2} + k_7 C_{\text{H}} \cdot C_{\text{H}} - k_4 C_{\text{O}} \cdot C_{\text{H}_2} \\
\frac{dC_{\text{O}_2}}{dt} &= -k_1 \cdot C_{\text{H}_2} \cdot C_{\text{O}_2} - k_2 C_{\text{H}} \cdot C_{\text{O}_2} \\
\frac{dC_{\text{H}_2O}}{dt} &= k_3 C_{\text{OH}} \cdot C_{\text{H}_2} + k_5 C_{\text{OH}} \cdot C_{\text{OH}} + k_6 C_{\text{H}} \cdot C_{\text{OH}} \\
\frac{dC_{\text{OH}}}{dt} &= 2k_1 \cdot C_{\text{H}_2} \cdot C_{\text{O}_2} + k_2 C_{\text{H}} \cdot C_{\text{O}_2} - k_3 C_{\text{OH}} \cdot C_{\text{H}_2} + k_4 C_{\text{O}} \cdot C_{\text{H}_2} - 2k_5 C_{\text{OH}} \cdot C_{\text{OH}} - k_6 C_{\text{H}} \cdot C_{\text{OH}} \\
\frac{dC_{\text{H}}}{dt} &= -k_2 C_{\text{H}} \cdot C_{\text{O}_2} + k_3 C_{\text{OH}} \cdot C_{\text{H}_2} + k_4 C_{\text{O}} \cdot C_{\text{H}_2} - k_6 C_{\text{H}} \cdot C_{\text{OH}} - 2k_7 C_{\text{H}} \cdot C_{\text{H}} \\
\frac{dC_{\text{O}}}{dt} &= k_2 C_{\text{H}} \cdot C_{\text{O}_2} - k_4 C_{\text{O}} \cdot C_{\text{H}_2} + k_5 C_{\text{OH}} \cdot C_{\text{OH}} 
\end{align*}
\]

- Chemical Reactions:

\[
\begin{align*}
\text{H}_2 + \text{O}_2 &\rightarrow 2\text{OH} \\
\text{H} + \text{O}_2 &\rightarrow \text{OH} + \text{O} \\
\text{OH} + \text{H}_2 &\rightarrow \text{H}_2\text{O} + \text{H} \\
\text{O} + \text{H}_2 &\rightarrow \text{OH} + \text{H} \\
2\text{OH} &\rightarrow \text{H}_2\text{O} + \text{O} \\
\text{H} + \text{OH} &\rightarrow \text{H}_2\text{O} \\
2\text{H} &\rightarrow \text{H}_2
\end{align*}
\]
Solution in Comsol Multiphysics™ (3)

Evolution of Concentration of Reactants
Initial Temp. 1500K
Equivalence Ratio 1.0
Thermal Diffusivity 0.1 m²/s

- H2 Mole Fraction
- O2 Mole Fraction
Solution in Comsol Multiphysics™ (4)

Evolution of Concentration of Products
Initial Temp. 1500K
Equivalence Ratio 1.0
Thermal Diffusivity 0.1 m²/s
Solution in Comsol Multiphysics™ (5)

Evolution of Flame Temperature
Initial Temp. 1500K
Equivalence Ratio 1.0
Thermal Diffusivity 0.1 m²/s
Validation – Solution using CHEMKIN™

Evolution of Concentration of Species from H₂-O₂ Combustion Simulation using Chemkin

- H₂
- O₂
- H₂O
- OH
- H
- O

Mole Fraction

Time (s)

0.00E+00 5.00E-05 1.00E-04 1.50E-04 2.00E-04 2.50E-04 3.00E-04 3.50E-04 4.00E-04

0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70
Validation – Solution using CHEMKIN™ (2)

Effect of Initial Temperature on Adiabatic Flame Temperature
Solution using CHEMKIN™

- To = 2000K
- To = 1500K
- To = 1000K
Parametric Study – Effect of Temperature

Evolution of Concentration of Hydrogen
Effect of Initial Mixture Temperature
Equivalence Ratio 1.0
Thermal Diffusivity 0.1 m²/s

Time (s)
Mole Fraction
0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70

To = 1000K
To = 1500K
To = 2000K
Parametric Study – Effect of Temperature (2)

Evolution of Flame Temperature
Effect of Initial Temperature
Equivalence Ratio 1.0
Thermal Diffusivity 0.1 m²/s

Time (s)
0.00E+00 1.00E-01 2.00E-01 3.00E-01 4.00E-01 5.00E-01 6.00E-01

Temperature (K)
0.00 500.00 1,000.00 1,500.00 2,000.00 2,500.00 3,000.00 3,500.00 4,000.00 4,500.00 5,000.00

To = 1500K
To = 2000K
Parametric Study – Effect of Equivalence Ratio

Evolution of Concentration of Hydrogen
Effect of Equivalence Ratio
Initial Temperature 1500K
Thermal Diffusivity 0.1 m²/s

Time (s)
Mole Fraction

Graph showing the evolution of concentration of hydrogen with time for different equivalence ratio values.
Parametric Study – Effect of Equivalence Ratio (2)

Evolution of Flame Temperature
Effect of Equivalence Ratio
Initial Temperature 1500K
Thermal Diffusivity 0.1 m²/s

- Phi = 2.0
- Phi = 1.0
- Phi = 0.5
Parametric Study – Effect of Thermal Diffusion

Evolution of Concentration of Hydrogen
Effect of Thermal Diffusivity
Initial Temperature 1500K
Equivalence Ratio 1.0

Mole Fraction

Time (s)

0.00 0.10 0.20 0.30 0.40 0.50 0.60

0.70

0.60

0.50

0.40

0.30

0.20

0.10

0.00

Alpha = 1.0 m²/s
Alpha = 0.1 m²/s
Alpha = 0.01 m²/s
Parametric Study – Effect of Thermal Diffusion (2)

Evolution of Flame Temperature
Effect of Thermal Diffusivity
Initial Temperature 1500K
Equivalence Ratio 1.0

Temperature (K)

Time (s)

- $\alpha = 1.0 \text{ m}^2/\text{s}$
- $\alpha = 0.1 \text{ m}^2/\text{s}$
- $\alpha = 0.01 \text{ m}^2/\text{s}$
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.