Max Plomer

Combustion spring 2011

For Prof Lu

Combustion Project – Unsteady PSR

Step 1: read the notes on stirred reactors posted online. Derive the equations for unsteady PSR for given residence time and initial conditions. Ignore the terms related to surface reactions and heat loss.

Therefore my assumptions are:
Ignore the terms related to surface reactions and heat loss.
Also in class ignoring plasma and charge was mentioned.

<u>Mass conservation (continuity equation):</u>

$$* = \text{in}$$

$$\frac{d(\rho V)}{dt} = \dot{m}^* - \dot{m}$$

$$V\frac{d\rho}{dt} = \frac{\rho V}{\tau} - \dot{m}$$

$$\dot{m} = \frac{\rho V}{\tau} - V\frac{d\rho}{dt}$$

Define terms:

$\dot{m}$ is the outlet mass flow rate

$\dot{m}^*$ is the inlet mass flow rate

ρ is mass density

V is reactor volume

T is gas temperature

<u>Simplified Species equation (surface reactor term dropped):</u>

$$\frac{d(\rho V Y_i)}{dt} = \dot{m}^* Y_i^* - \dot{m} Y_i + \dot{\omega}_i W_i V = \rho V \frac{dY_i}{dt} + Y_i \frac{d(\rho V)}{dt}$$

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \dot{m} Y_i + \dot{\omega}_i W_i V - Y_i \frac{d(\rho V)}{dt}$$

Substitute continuity

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \left[\dot{m}^* - \frac{d(\rho V)}{dt}\right] Y_i + \dot{\omega}_i W_i V - Y_i \frac{d(\rho V)}{dt}$$

Expand terms

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \dot{m}^* Y_i + \frac{d(\rho V)}{dt} Y_i + \dot{\omega}_i W_i V - Y_i \frac{d(\rho V)}{dt}$$

Cancel terms

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \dot{m}^* Y_i + \dot{\omega}_i W_i V$$

Which simplifies to

$$\frac{dY_i}{dt} = \frac{1}{\tau}(Y_i^* - Y_i) + \frac{\dot{\omega}_i W_i}{\rho}$$

Where

$$\tau = \frac{\rho V}{\dot{m}^*}$$

For ρ can use matlab function ckrhoy with input (P, T, Y_i)

<u>Energy Equation:</u>

$$\frac{dH}{dt} = \frac{d(\sum m_i h_i)}{dt}$$

$$\frac{dH}{dt} = \sum m_i \frac{dh_i}{dt} \; + \; \sum h_i \frac{dm_i}{dt}$$

$$\frac{dH}{dt} = \sum \rho V Y_i c_{p_i} \frac{dT}{dt} + \sum h_i \frac{d(\rho V Y_i)}{dt}$$

$$\frac{dH}{dt} = \frac{dT}{dt} \rho V c_{p_{ave}} + \sum h_i \left(Y_i \frac{d(\rho V)}{dt} + \rho V \frac{dY_i}{dt} \right) = \dot{m}^* \sum Y_i^* h_i^* - \dot{m} \sum Y_i h_i$$

$* = \text{in}$

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \dot{m}^* \sum Y_i^* h_i^* - \dot{m} \sum Y_i h_i - \sum h_i \left(Y_i V \frac{d\rho}{dt} + \rho V \frac{dY_i}{dt} \right)$$

Substitute continuity

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \dot{m}^* \sum Y_i^* h_i^* - \left[\frac{\rho V}{\tau} - V \frac{d\rho}{dt} \right] \sum Y_i h_i - \sum h_i \left(Y_i V \frac{d\rho}{dt} + \rho V \frac{dY_i}{dt} \right)$$

Expand terms

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i + V \frac{d\rho}{dt} \sum Y_i h_i - \frac{d\rho}{dt} V \sum h_i Y_i - \rho V \sum h_i \frac{dY_i}{dt}$$

Cancel terms

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i - \rho V \sum h_i \frac{dY_i}{dt}$$

Substitute species equation

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i - \rho V \sum h_i \left[\frac{1}{\tau} (Y_i^* - Y_i) + \frac{\dot{\omega}_i W_i}{\rho} \right]$$

Expand terms

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i - \frac{\rho V}{\tau} \sum h_i Y_i^* + \frac{\rho V}{\tau} \sum h_i Y_i - V \sum h_i \dot{\omega}_i W_i$$

Cancel terms

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum h_i Y_i^* - V \sum h_i \dot{\omega}_i W_i$$

Substitute $\dot{m}^* = \frac{\rho V}{\tau}$

$$\frac{dT}{dt}\rho V c_{p_{ave}} = \frac{\rho V}{\tau} \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum h_i Y_i^* - V \sum h_i \dot{\omega}_i W_i$$

$$\frac{dT}{dt}\rho c_{p_{ave}} = \frac{\rho}{\tau} \sum Y_i^* [h_i^* - h_i] - \sum h_i \dot{\omega}_i W_i$$

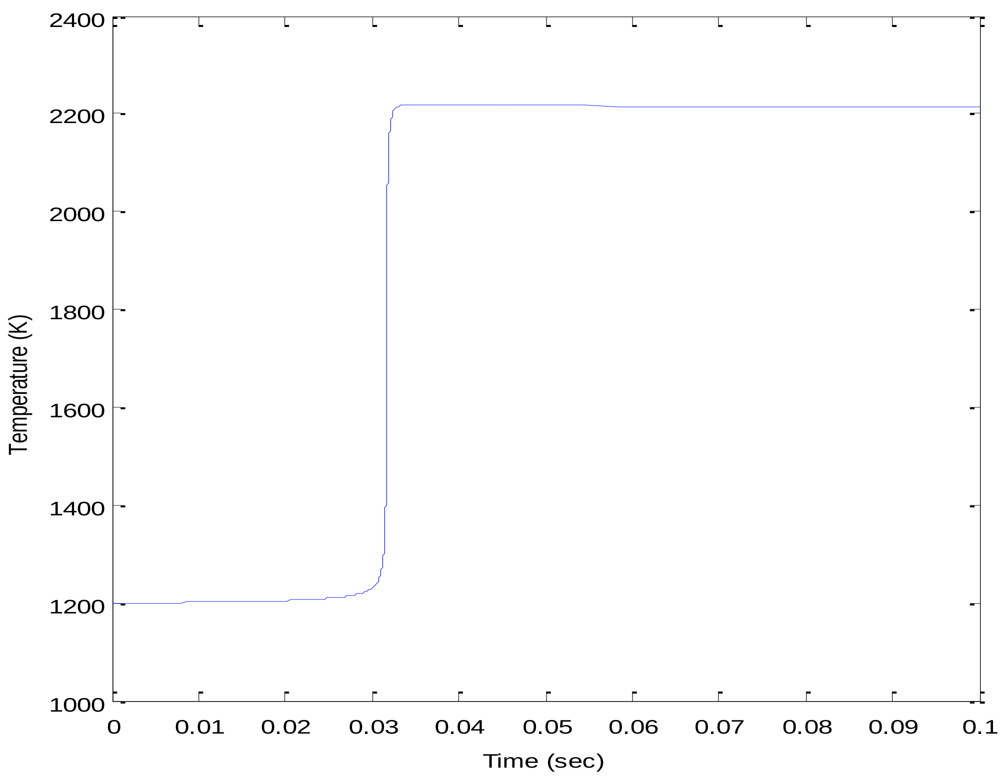
$$\frac{dT}{dt} = \frac{1}{\tau c_{p_{ave}}} \sum Y_i^* [h_i^* - h_i] - \frac{1}{\rho c_{p_{ave}}} \sum h_i \dot{\omega}_i W_i$$

Results:

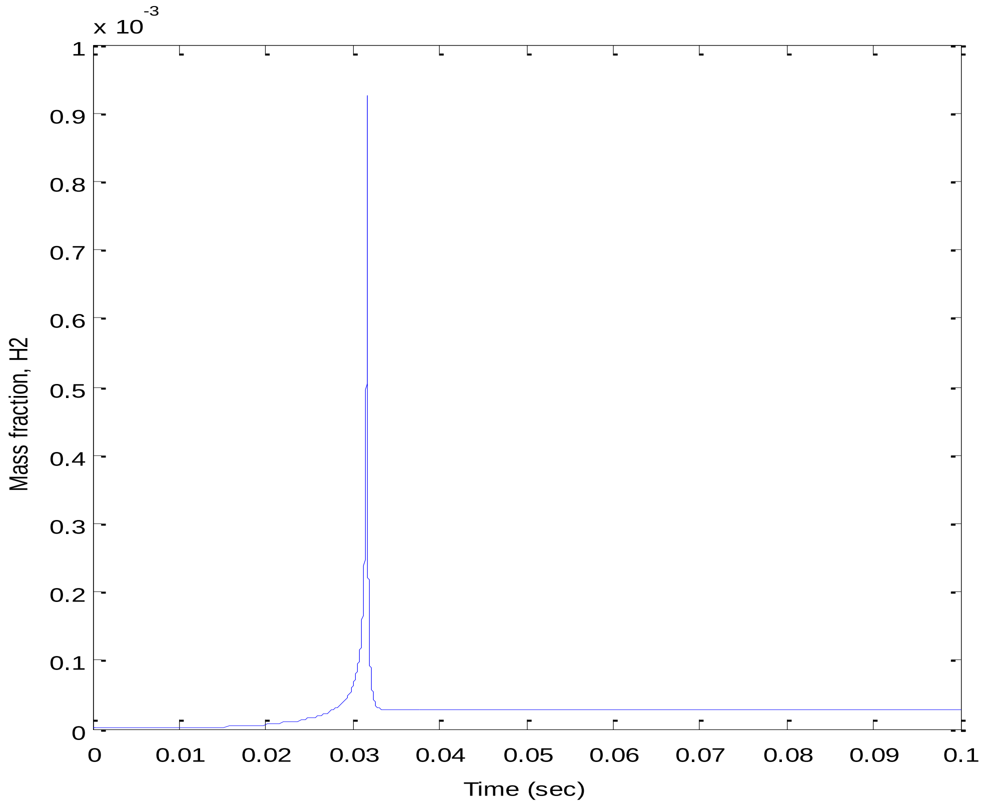
1. Starting from fuel-air mixture at Tin = Tout= 1200K, p=1 atm, and phi=0.5 solve the temperature and species concentrations for different resident times, tau= 1 millionth of a second, 1 millisecond and 1 second. Make sure you get a solution on the upper branch for the long residence time.

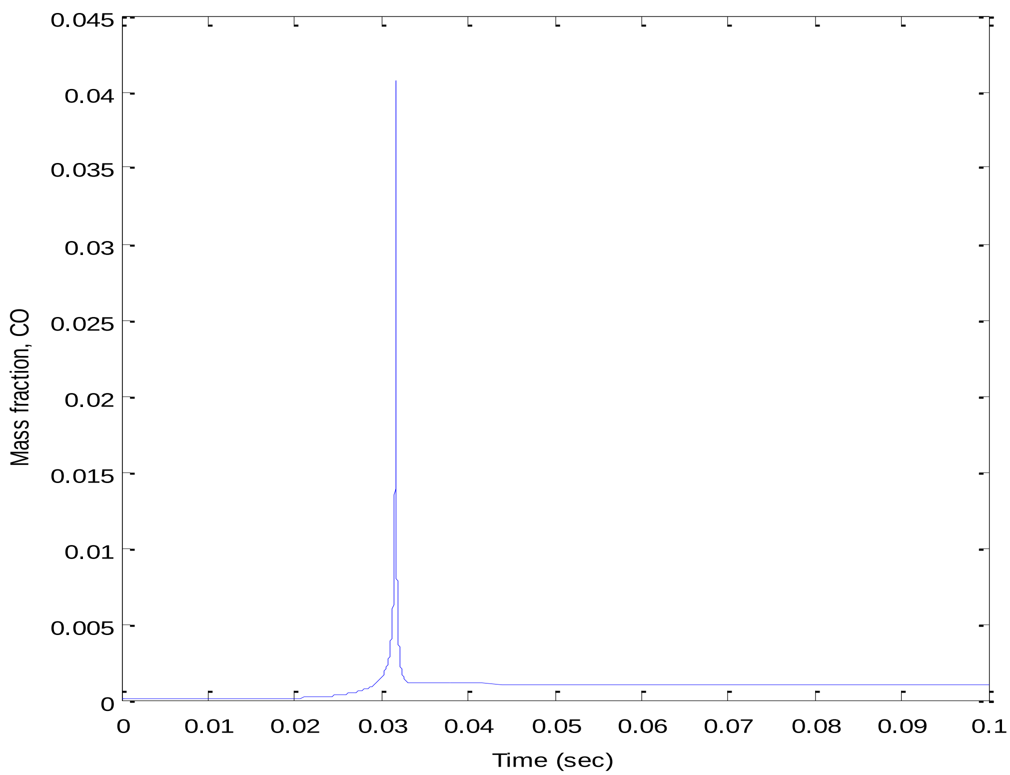
For tau = 1 second

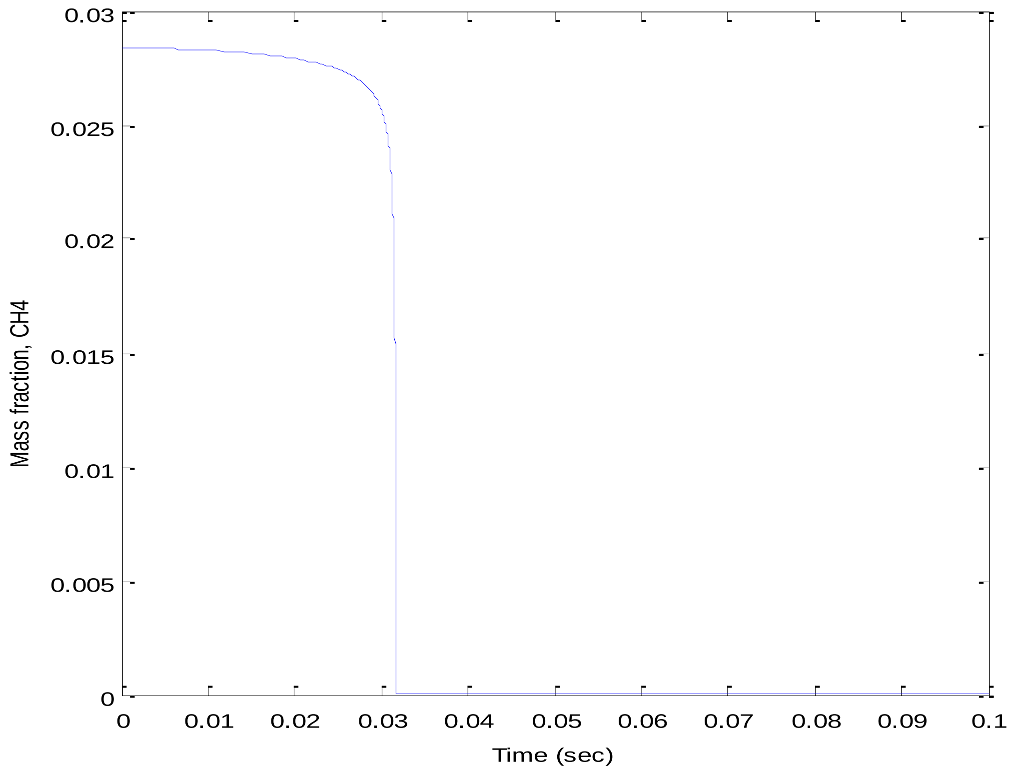
Temperature



Mass fractions of H2, CO, CH4


× 10^-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Mass fraction, H2
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
Time (sec)

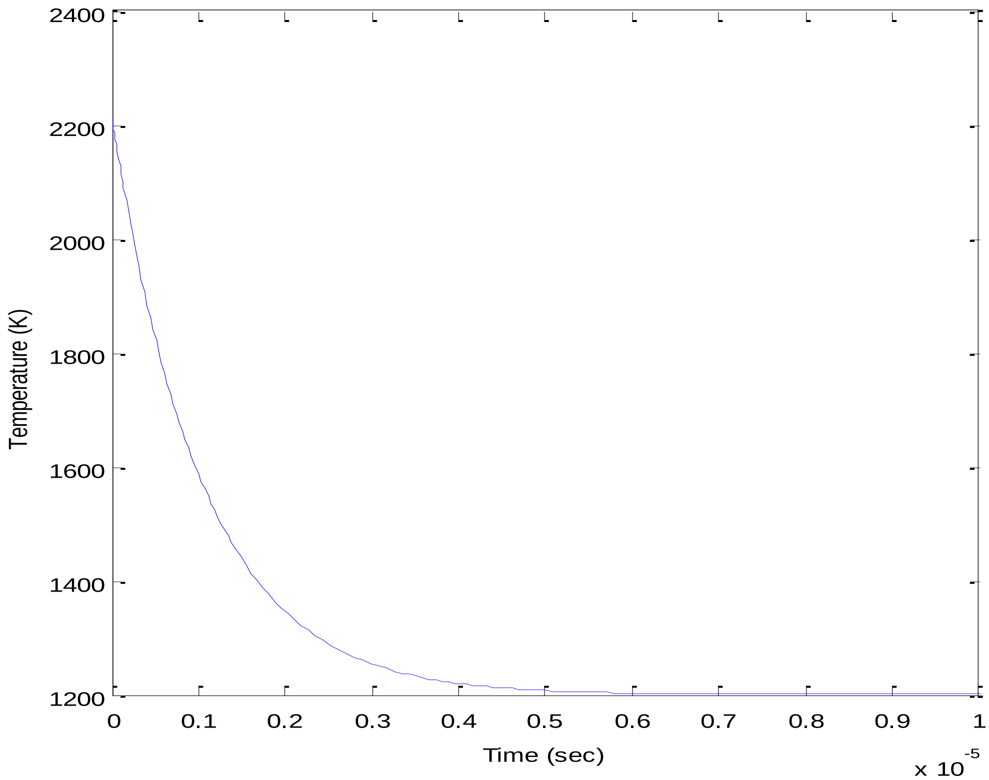

0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
Mass fraction, CO
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
Time (sec)



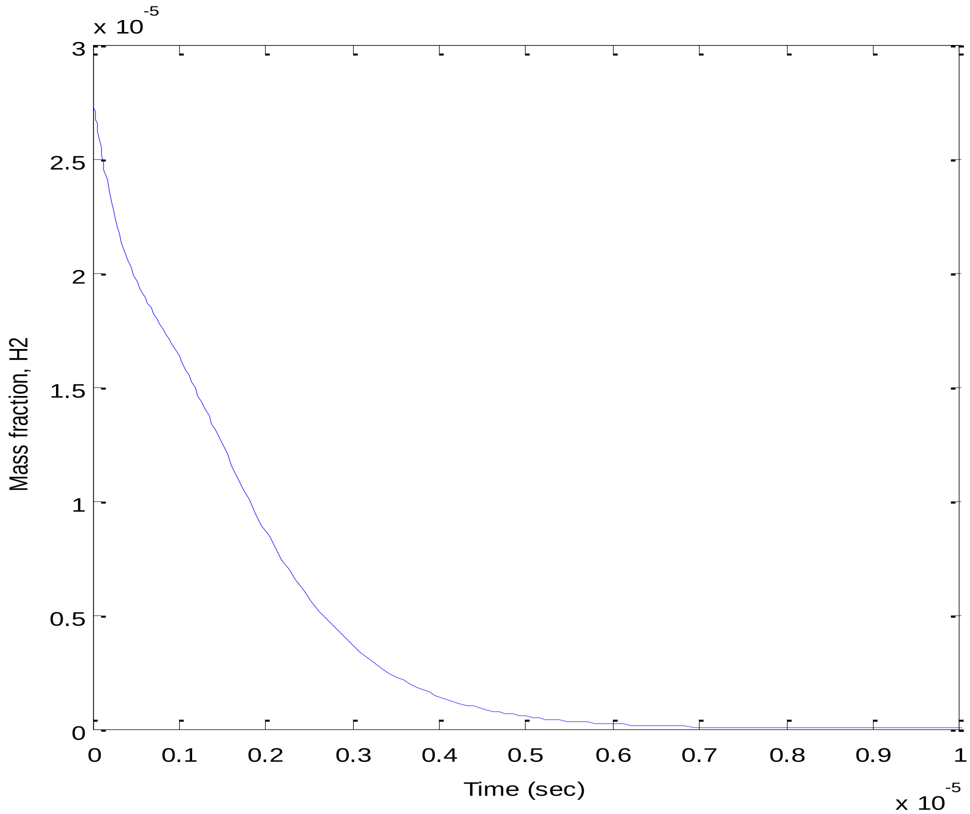
For tau = 1 millisecond and 1 millionth of a second did not receive any ignition.

2. Use the solution on the upper branch as the initial condition, solve the temperature and species profiles for tau = 1 millionth of a second, make sure extinction occurs.

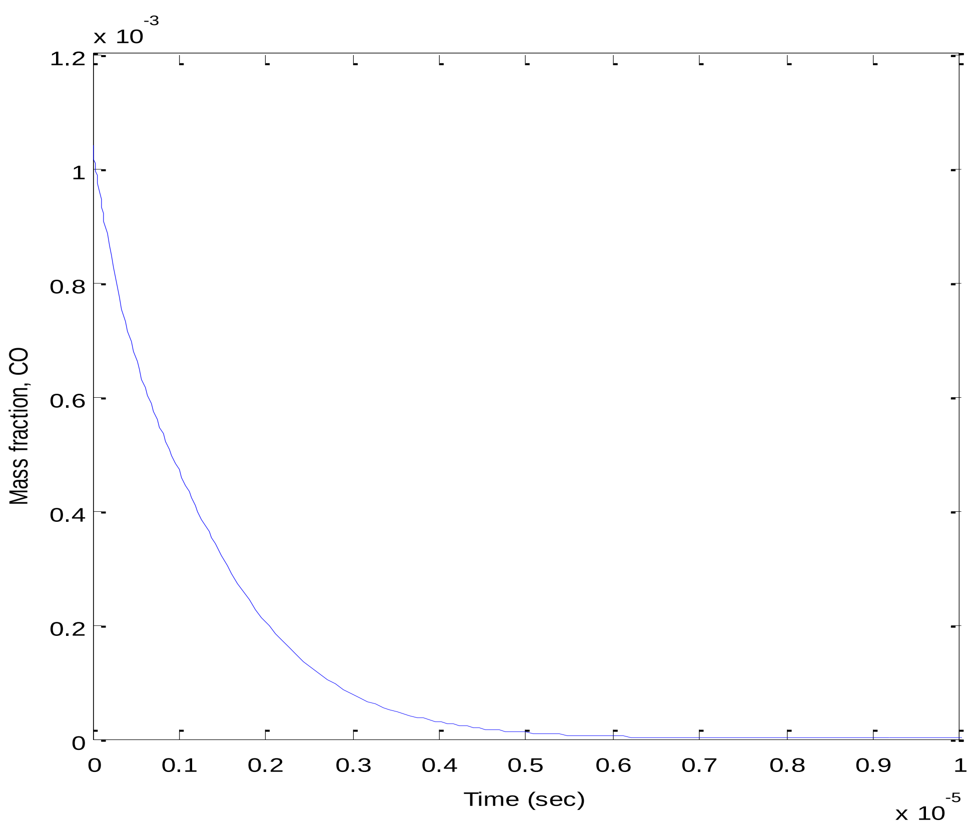
Temperature



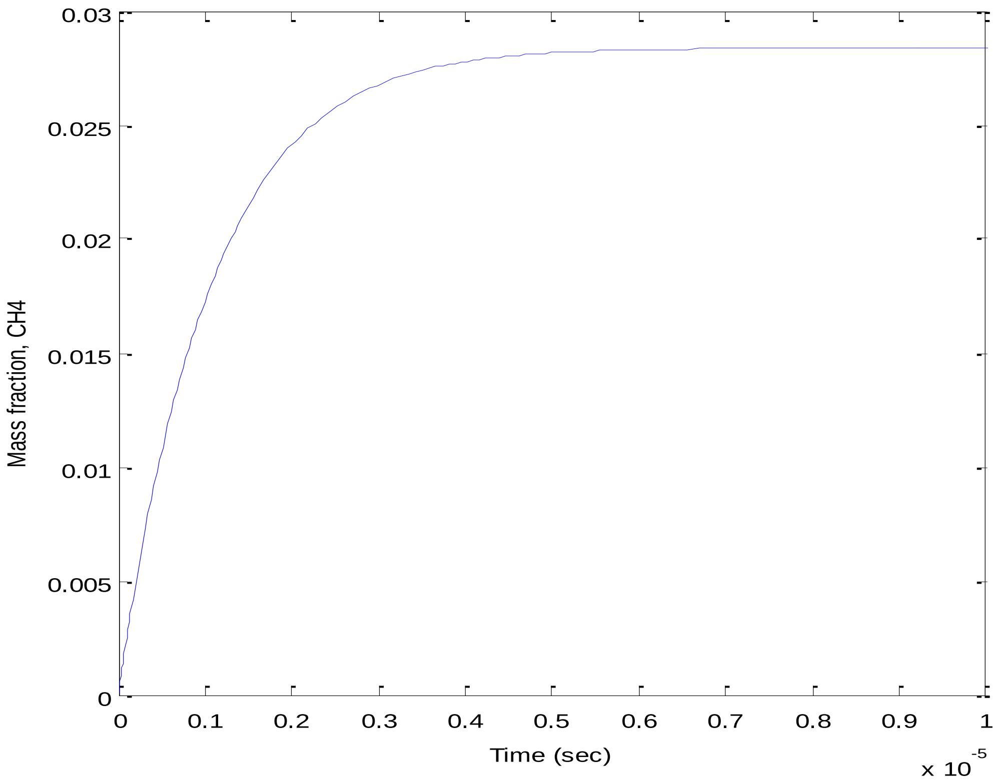
Mass fractions of H2, CO, CH4



x 10^-5
3
2.5
2
1.5
1
0.5
0
Mass fraction, H2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time (sec)
x 10^-5



x 10^-3
1.2
1
0.8
0.6
0.4
0.2
0
Mass fraction, CO
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time (sec)
x 10^-5



Mass fraction, CH4
0.03
0.025
0.02
0.015
0.01
0.005
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time (sec)
x 10^-5