Modeling Pyrolyzing Ablative Materials with COMSOL Multiphysics®

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Outline

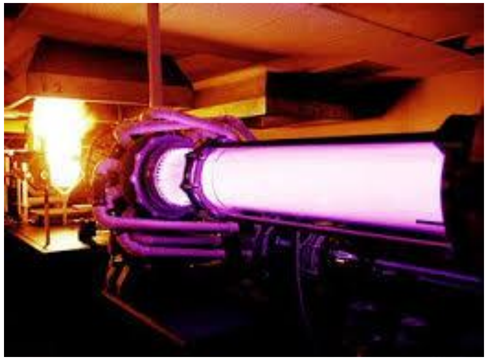
- Definition and Applications
- General Pyrolyzing Ablator Problem
- Solution Example Using Finite Element Model
- Summary and Conclusions

Definitions

- **Ablation** is removal of material from the surface of an object by melting, vaporization, chipping, or other erosive processes.
- **Pyrolysis** is the decomposition of a material brought about by high temperatures
- **Pyrolyzing Ablator** is a material that undergoes sub-surface decomposition when heated and when becomes sufficiently hot, loses surface mass loss through melting or vaporization

Applications of Pyrolyzing Ablator Modeling

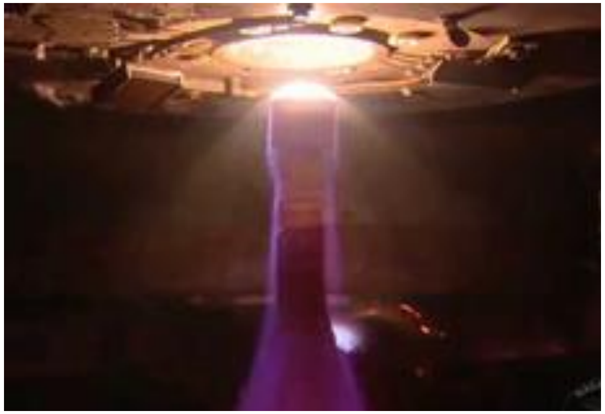
Reentry Heat Shields



Laser Machining

Wood Combustion

Rocket Nozzles

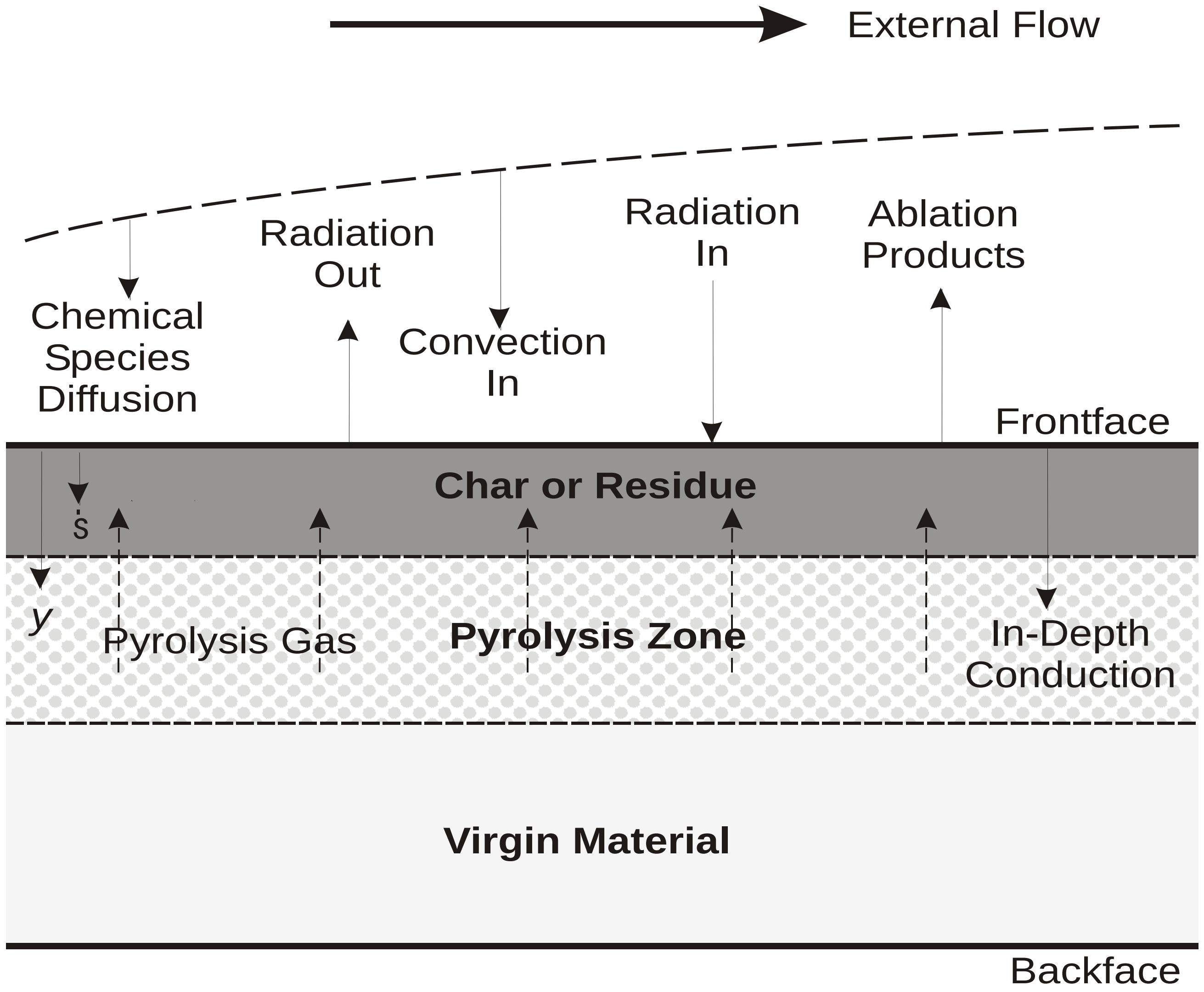


Plasma Heating

Heated Pyrolyzing Ablator

From Başkaya, A. O. “CFD Analysis of The Cork-Phenolic Heat Shield Of A Reentry Cubesat In Arc-Jet Conditions Including Ablation And Pyrolysis”, 15th International Planetary Probe Workshop

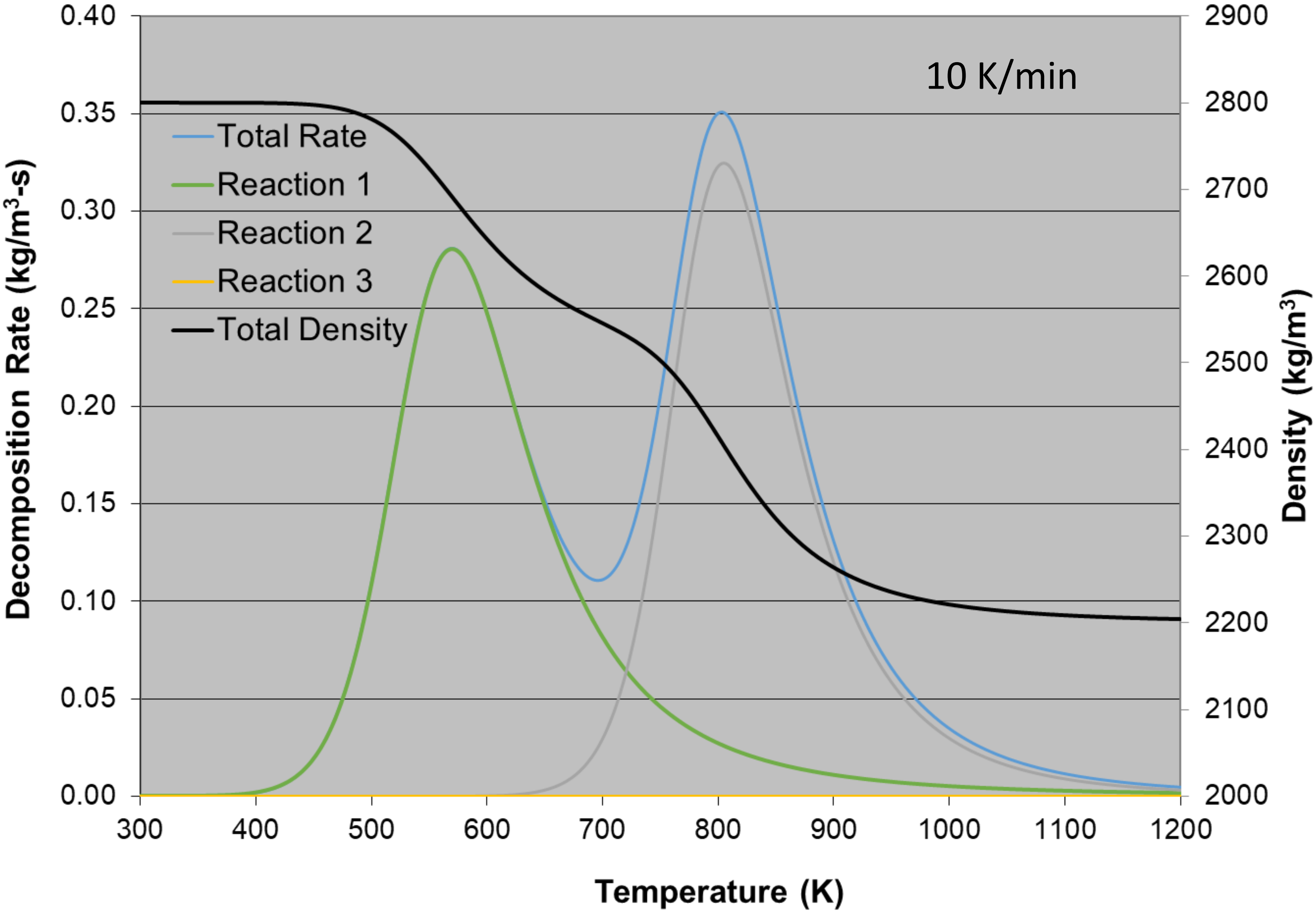
General Problem Illustration



Modeling Requirements for Pyrolyzing Ablators

- Non-linear heat conduction in solids
- Non-linear, thermal boundary conditions
- Moving boundaries
- Non-linear, time-dependent quasi-solid in-depth reactions
- Transport and thermal properties as a function of material state as well as temperature
- Inclusion of the thermal effects of gas flow within the solid material
- In-depth pore pressure due to pyrolysis gas transport (not always employed)

Material Pyrolysis



Decomposition Model

- Material consists of three constituents (although the number could be increased)

$$\rho = \Gamma(\rho_A + \rho_B) + (1 - \Gamma)\rho_C$$

- Components A and B decompose according to:

$$\left(\frac{\partial \rho_i}{\partial t}\right)_y = -A_i \exp\left(-\frac{E_i}{RT}\right)\rho_{o,i}\left(\frac{\rho_i - \rho_{r,i}}{\rho_{o,i}}\right)^{\psi_i}$$

- Material properties are a function not only of temperature, but also material state

In-Depth Temperature History

- In-depth temperature time history can come from:
  - Thermogravimetric Analysis (TGA)

$$T = \beta t + T_0$$

  - Steady-State energy balance (1-D transformed coordinate)

$$\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \left(\frac{\partial \dot{m}_g h_g}{\partial y}\right) + \dot{s}\left(\frac{\partial \rho h_s}{\partial y}\right) = 0$$

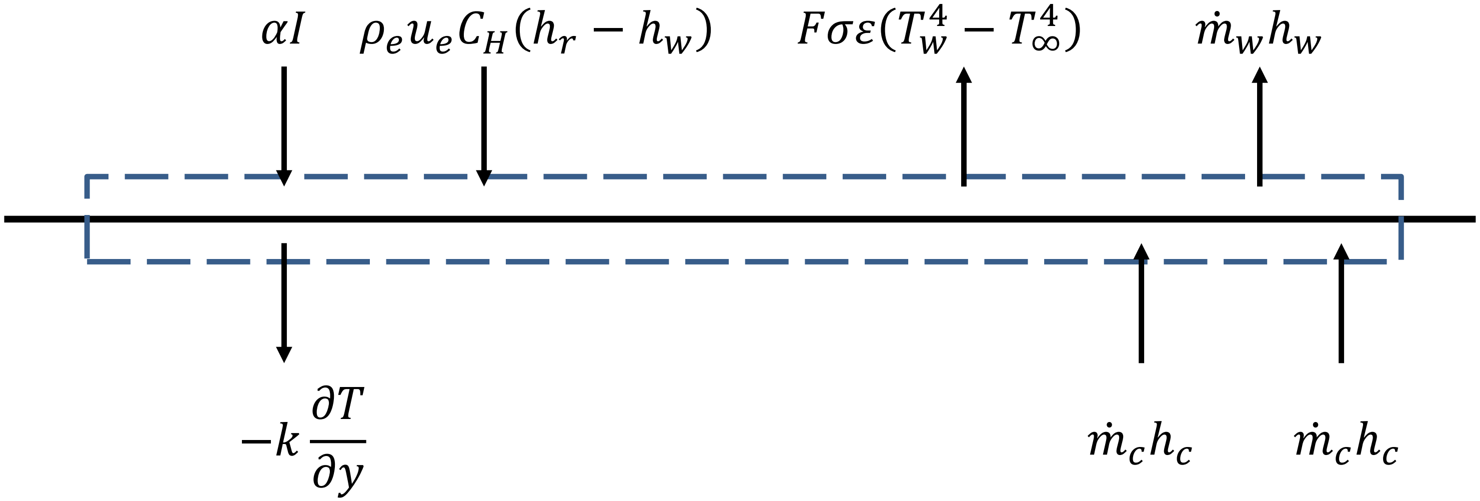
  - Transient energy balance (1-D transformed coordinate)

$$\rho C_p\left(\frac{\partial T}{\partial t}\right)_y = \frac{1}{A}\frac{\partial}{\partial y}\left(kA\frac{\partial T}{\partial y}\right)_t - \bar{h}(T)\left(\frac{\partial \rho}{\partial t}\right)_y + \dot{s}\rho C_p\left(\frac{\partial T}{\partial y}\right)_t + \frac{1}{A}\left(\frac{\partial \dot{m}_g h_g A}{\partial y}\right)_t$$

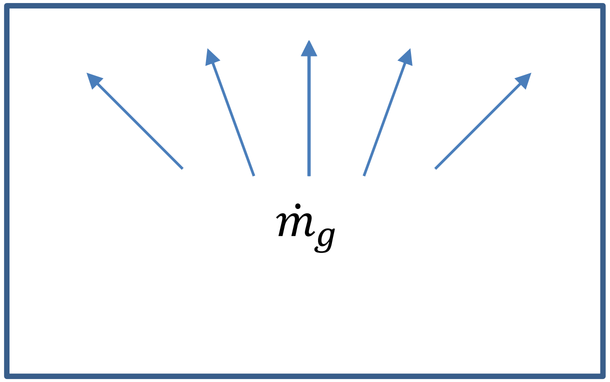
  - Transient Energy Balance (1- and 2-D fixed coordinate)

$$\rho C_p\left(\frac{\partial T}{\partial t}\right) = \frac{1}{A}\nabla(kA\nabla T) - \bar{h}(T)\left(\frac{\partial \rho}{\partial t}\right) + \frac{1}{A}\nabla\cdot\left(\dot{\boldsymbol{m}}_{\boldsymbol{g}} h_g A\right)$$

Surface Energy Balance and Pyrolysis Gas Flow



$$\alpha I + \rho_e\, u_e C_H (h_r - h_w) + k\frac{\partial T}{\partial y} - F\sigma\varepsilon(T_w^4 - T_\infty^4) - \left(\dot{m}_w h_w - \dot{m}_c h_c - \dot{m}_g h_g\right) = 0$$



$$\nabla^2\Phi = \frac{\partial\rho}{\partial t}$$

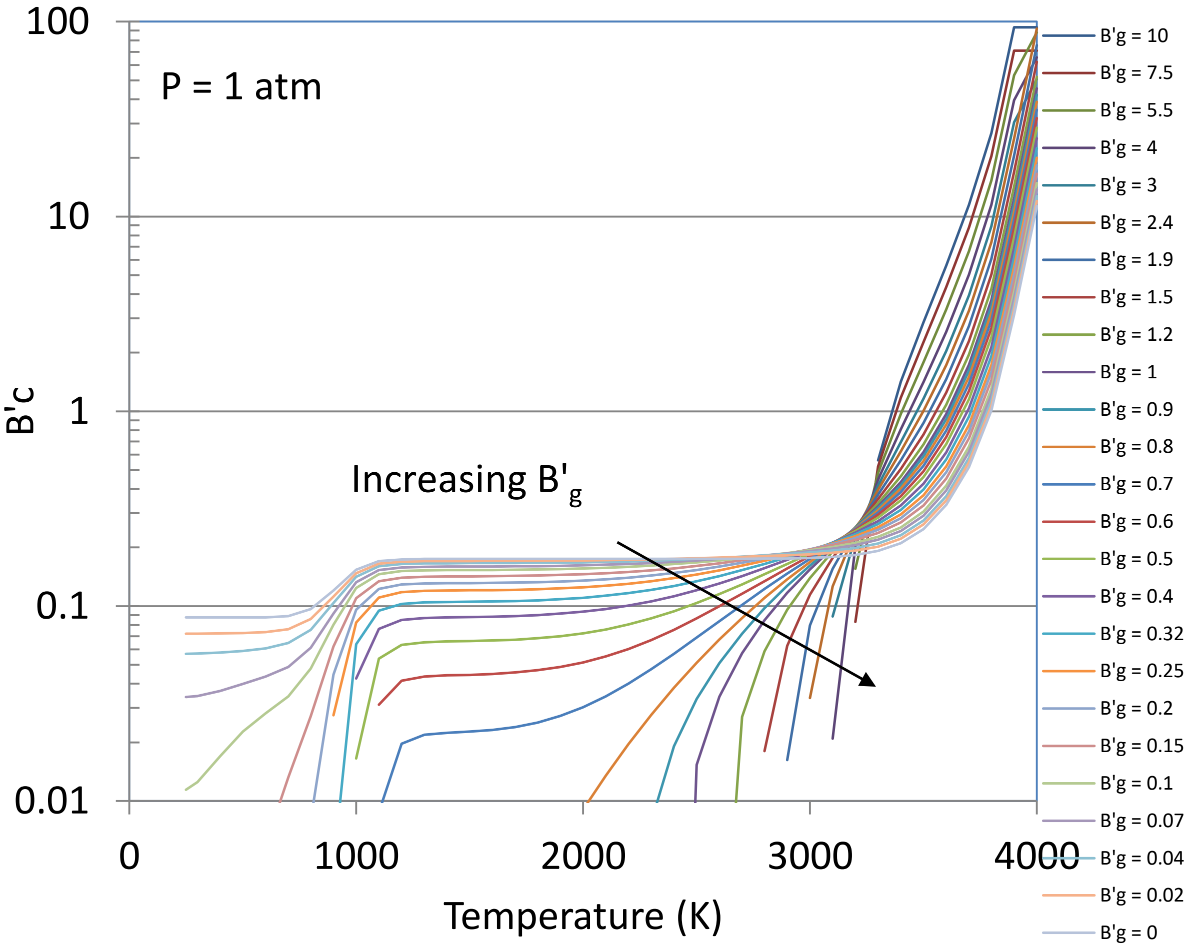
$$\boldsymbol{\dot{m}_g} = \nabla\Phi$$

Surface Thermochemistry – Normalized Mass Loss

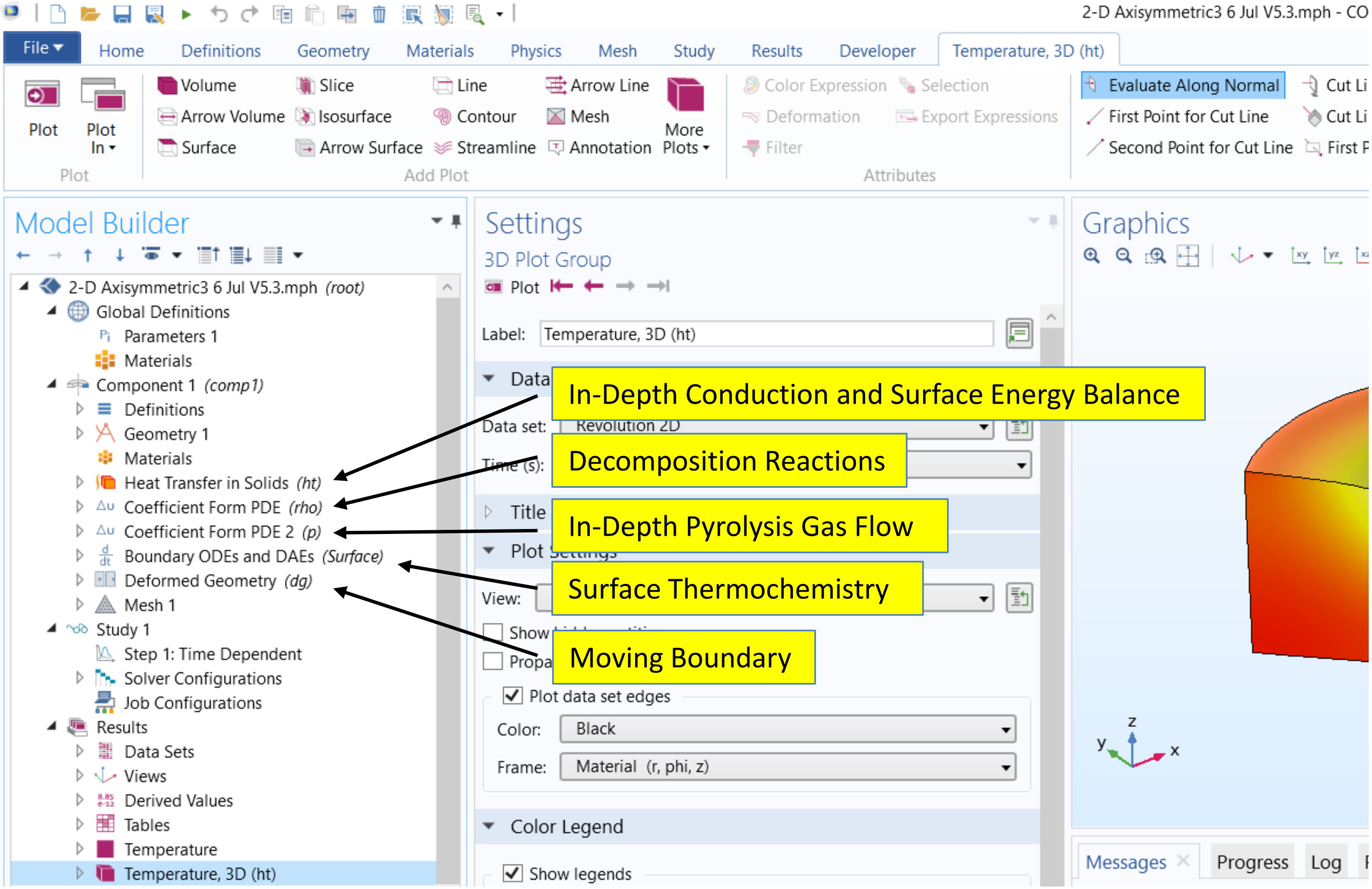
Surface thermochemistry conditions computed from equilibrium thermochemistry in terms of normalized mass fluxes.

$$B'_c = \dot{m}_c / \rho_e u_e C_M$$
$$B'_g = \dot{m}_g / \rho_e u_e C_M$$

$$B'_c = B'_c(p, B'_g\,, T_s)$$



Implementation



2-D Axisymmetric3 6 Jul V5.3.mph *(root)*
- Global Definitions
  - Parameters 1
  - Materials
- Component 1 *(comp1)*
  - Definitions
  - Geometry 1
  - Materials
  - Heat Transfer in Solids *(ht)*
  - Coefficient Form PDE *(rho)*
  - Coefficient Form PDE 2 *(p)*
  - Boundary ODEs and DAEs *(Surface)*
  - Deformed Geometry *(dg)*
  - Mesh 1
- Study 1
  - Step 1: Time Dependent
  - Solver Configurations
  - Job Configurations
- Results
  - Data Sets
  - Views
  - Derived Values
  - Tables
  - Temperature
  - Temperature, 3D (ht)

Settings

3D Plot Group

Plot

Label: Temperature, 3D (ht)

Data

Data set: Revolution 2D

Time (s):

Title

Plot Settings

View:

☐ Show

☐ Propa

☑ Plot data set edges

Color: Black

Frame: Material (r, phi, z)

Color Legend

☑ Show legends

In-Depth Conduction and Surface Energy Balance

Decomposition Reactions

In-Depth Pyrolysis Gas Flow

Surface Thermochemistry

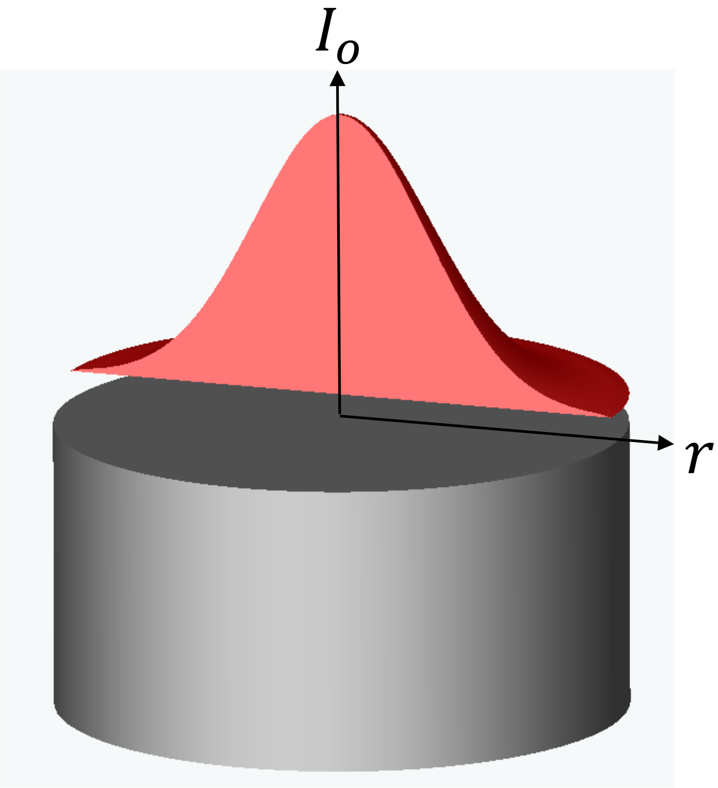
Moving Boundary

Two-Dimensional Transient Example

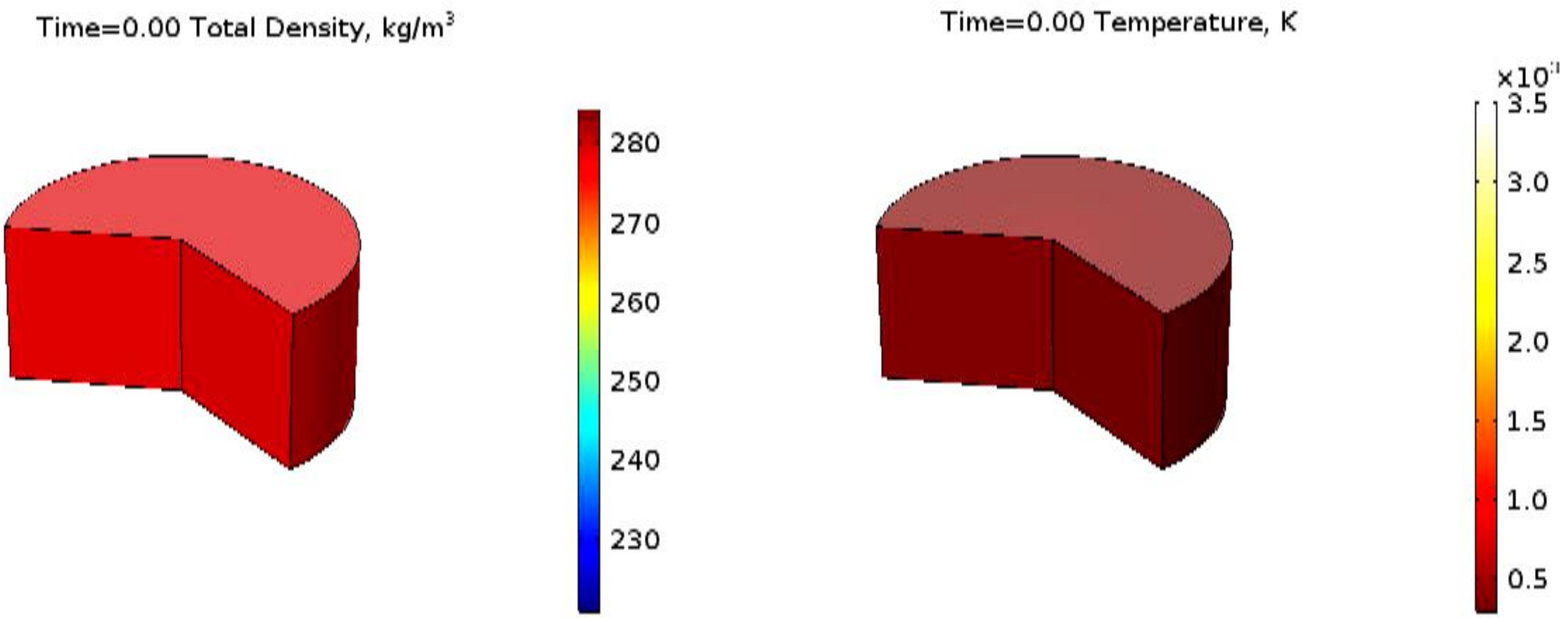
- Problem is for a two-dimensional, axisymmetric puck
- Top of puck heated with Gaussian flux profile
- Pyrolysis gas flow calculated from potential flow
- Full surface thermochemistry with recession
- 2-D COMSOL Multiphysics® results compared to a series of 1-D results

$$I = I_o \cdot \exp(-C\ (r/r_0)^2)$$

$$I_o = 1 \times 10^7\ \mathrm{W/m^2} : C = 5$$

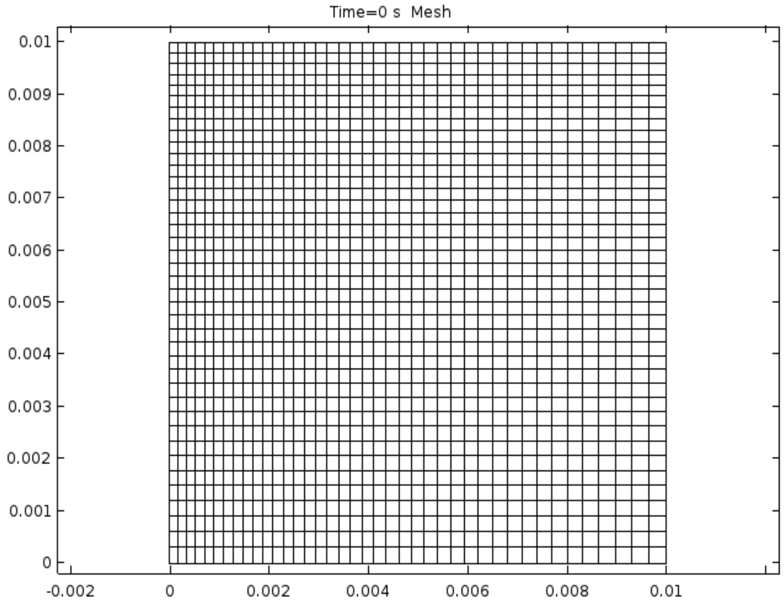


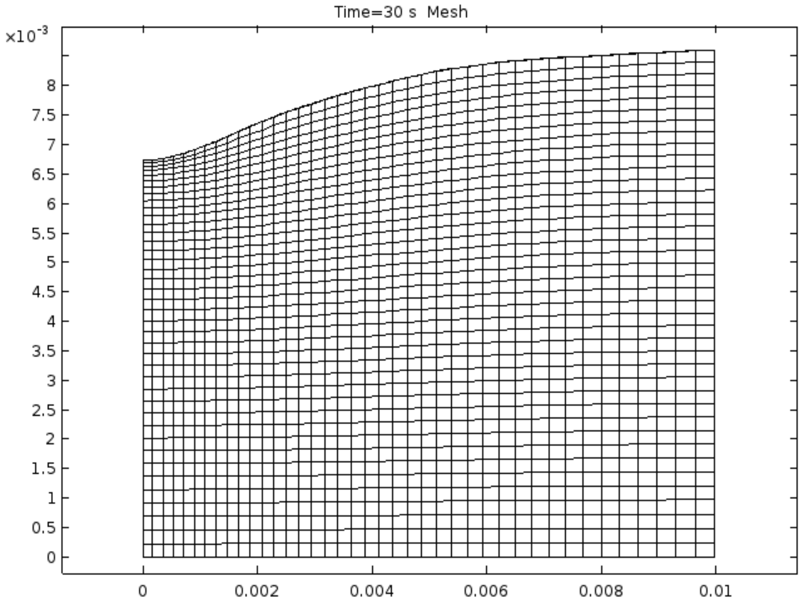
2-D Problem Animation



Animation is twice actual speed

Original and Deformed Mesh





Summary

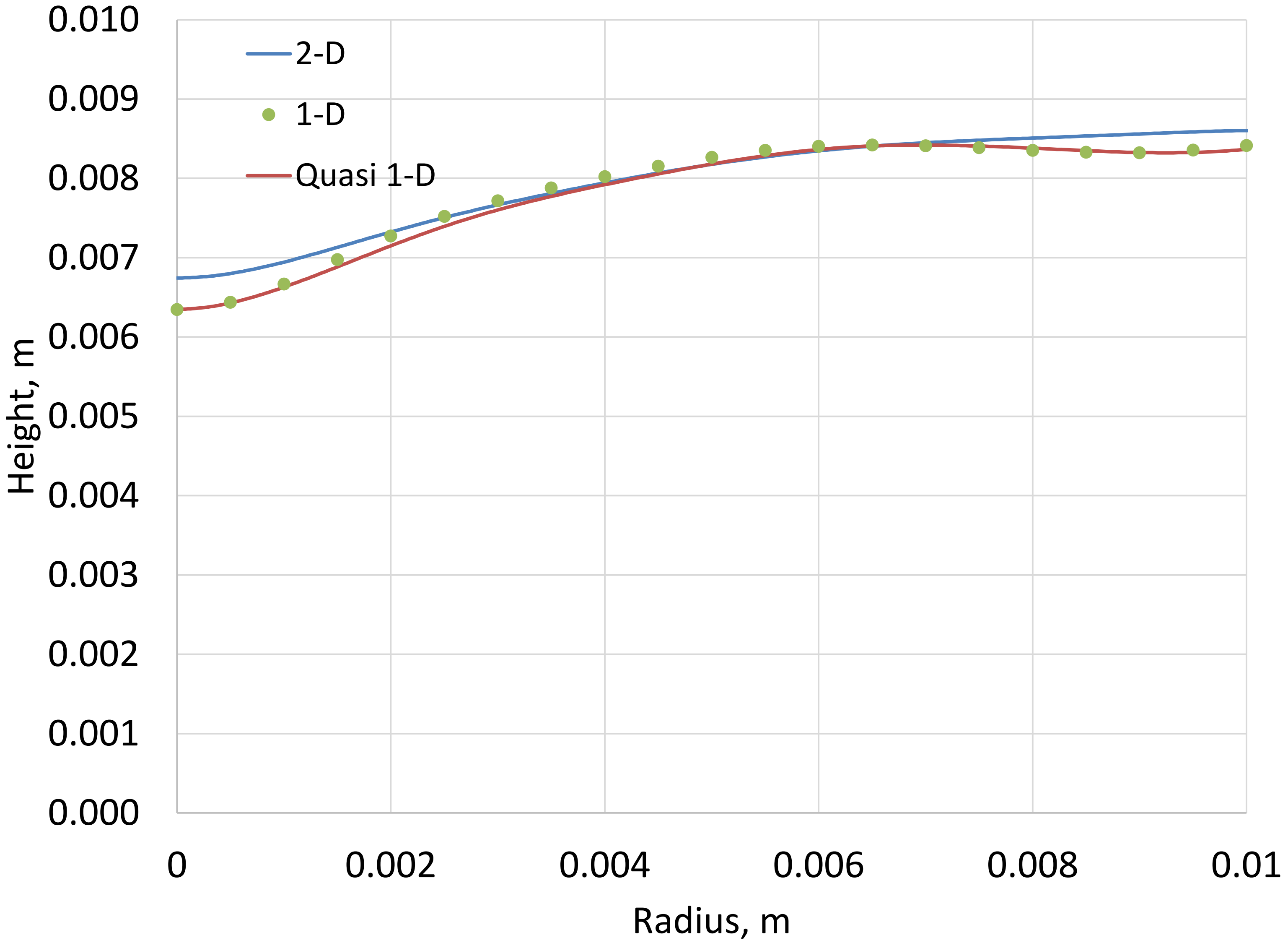
- COMSOL is a suitable tool for modeling pyrolyzing ablative materials
- General capabilities of COMSOL Multiphysics® allow for a wide variety of geometries and problems to modeled
- COMSOL allows for modifications to model to be made quickly and easily
- Solution algorithms are efficient and stable
- Integrated environment provides a very user friendly and powerful system for modeling
- Multiphysical modeling capability allows for structural and external flow to be incorporated into analysis (in progress)

For Additional Information

Risch, T., “Verification of a Finite-Element Model for Pyrolyzing Ablative Materials”, presented at the AIAA 47th AIAA Thermophysics Conference, Denver CO, June 5-9, 2017.

QUESTIONS?

Final Recession Profile at 30 s



Example Problems

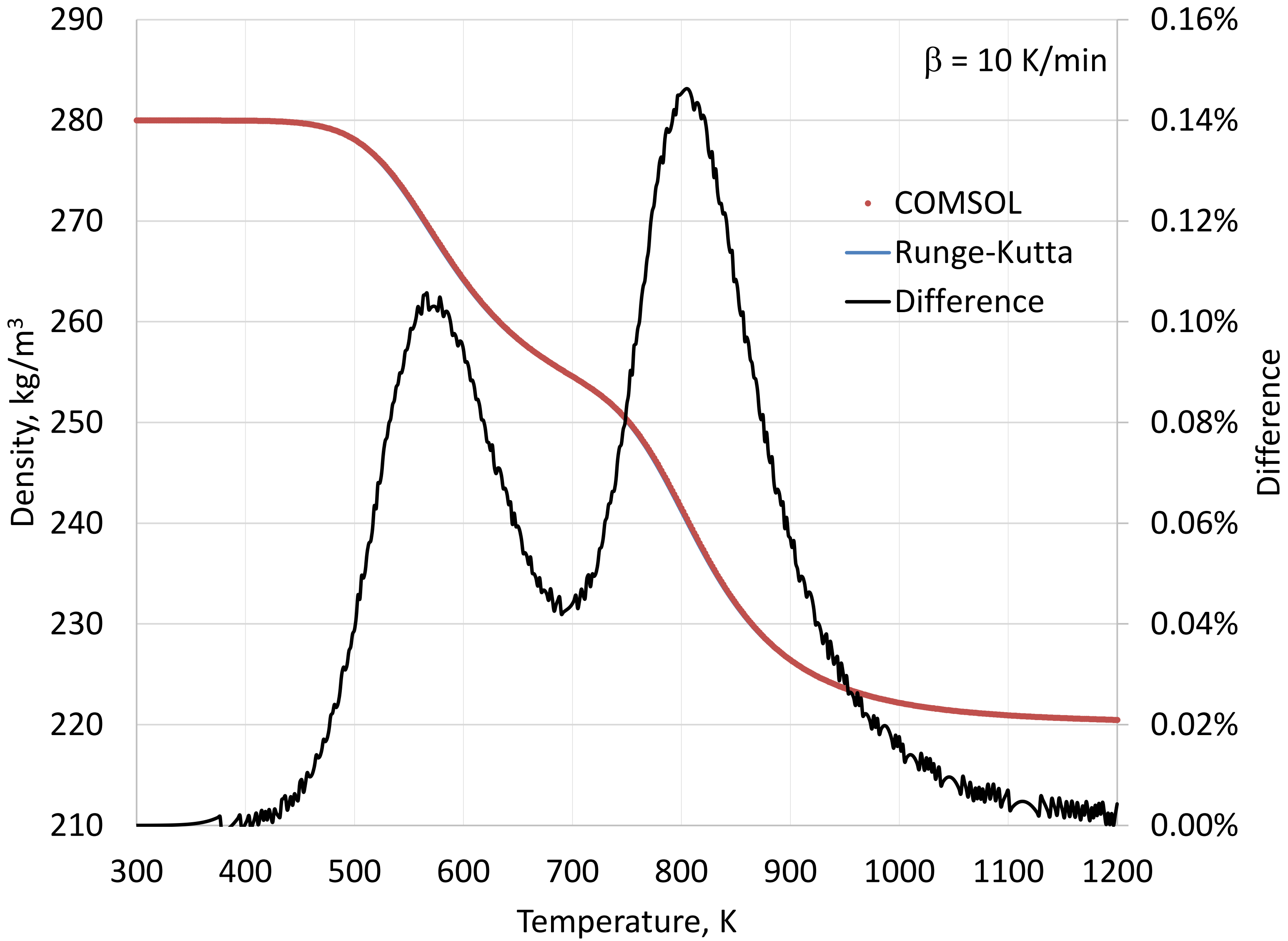
- Look at four examples solved with COMSOL
    - Thermogravimetric Analysis (TGA)
    - Steady-state one-dimensional thermal and density profile
    - One-dimensional transient temperature and recession history
    - Two-dimensional transient temperature and recession history

Thermogravimetric Analysis (TGA) Example

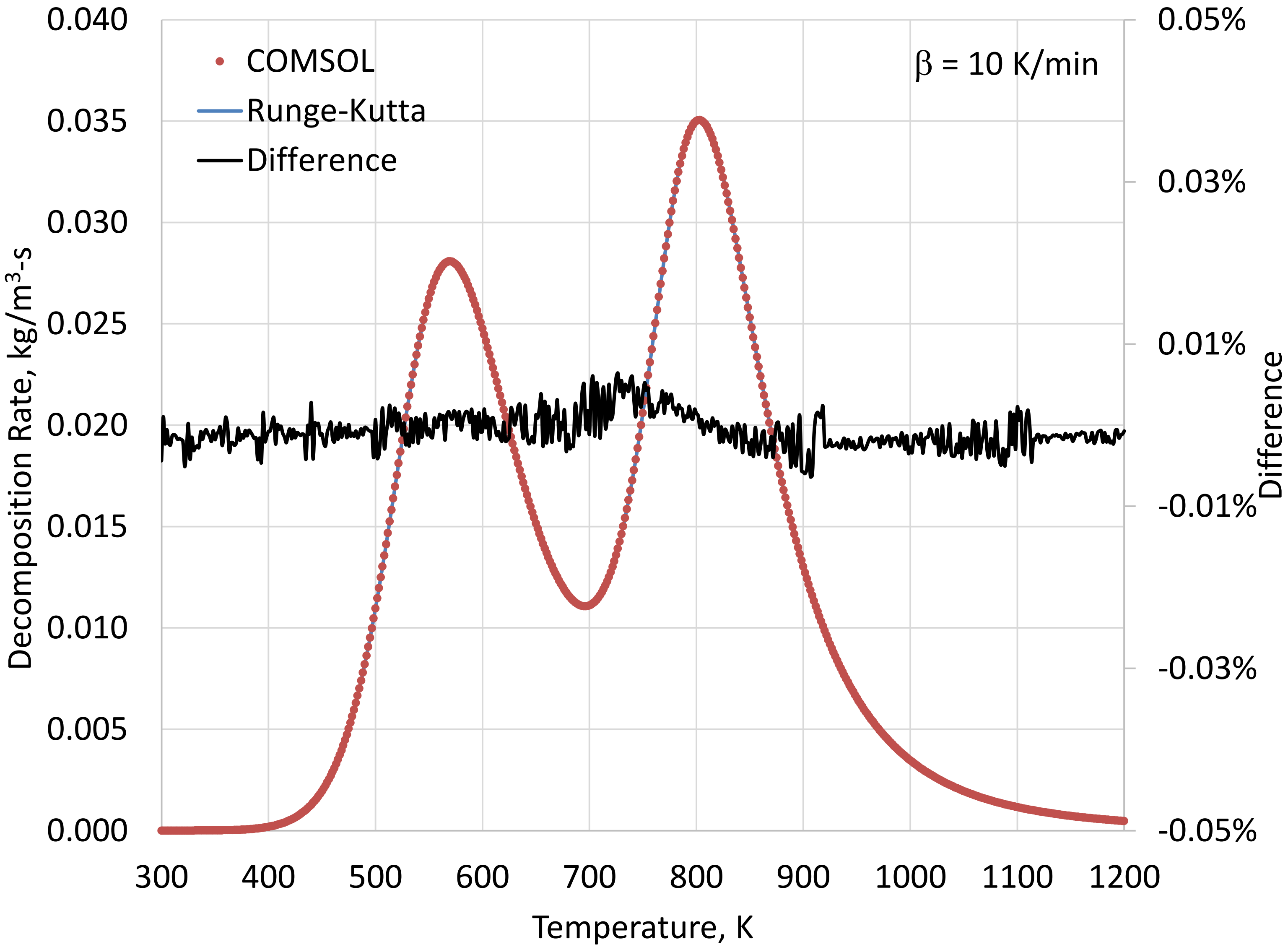
Thermogravimetric Analysis (TGA) Example

- Three component TACOT model
- Linear ramp increase in temperature at 10 K/min
- First-order time integration, not a spatial problem
- Results provide density and reaction rate for three components as a function of time
- COMSOL Multiphysics® results compared to independent fourth-order Runge-Kutta calculation

TGA Results - I



TGA Results - II

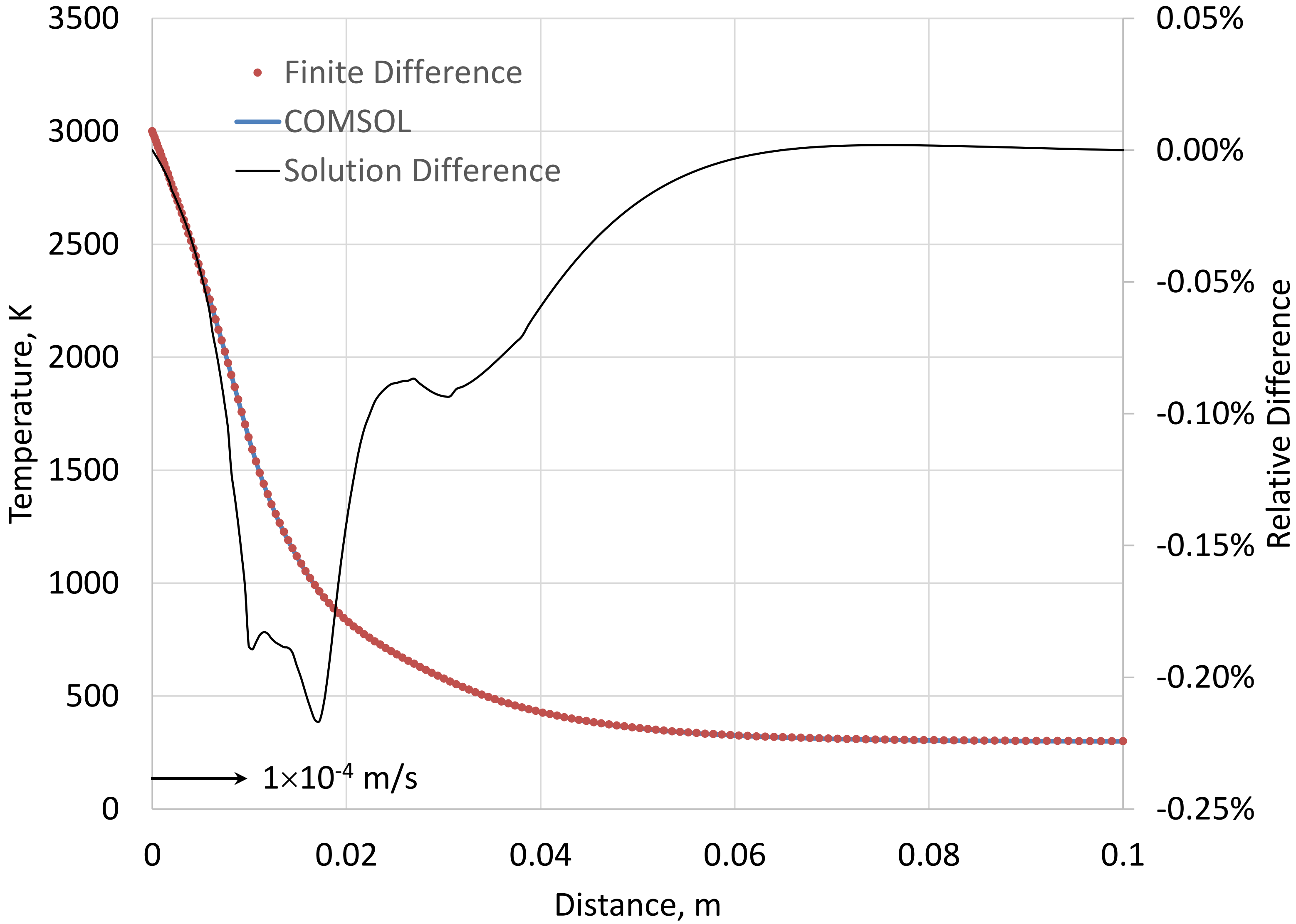


Steady-State Profile Example

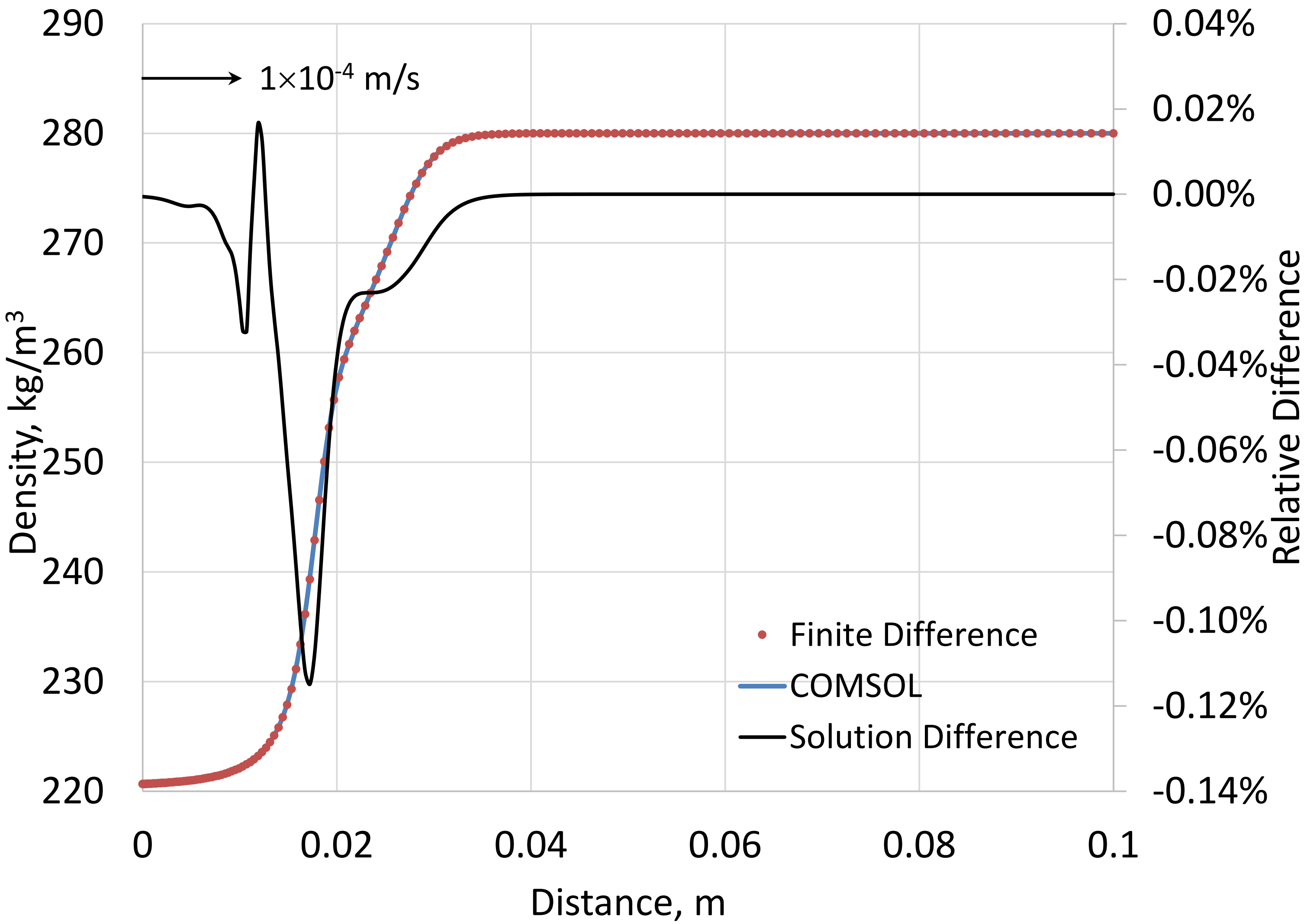
Steady-State Profile Example

- After long times in an infinite sample with a fixed surface temperature and recession, temperature and density profile will reach a steady state
- Problem solution becomes independent of time
- Specified surface temperature (3000 K) and steady recession rate (1×10^{-4} m/s)
- COMSOL Multiphysics® results compared to independent second order finite difference calculation and results from the Fully Implicit Ablation and Thermal Analysis Program (FIAT)

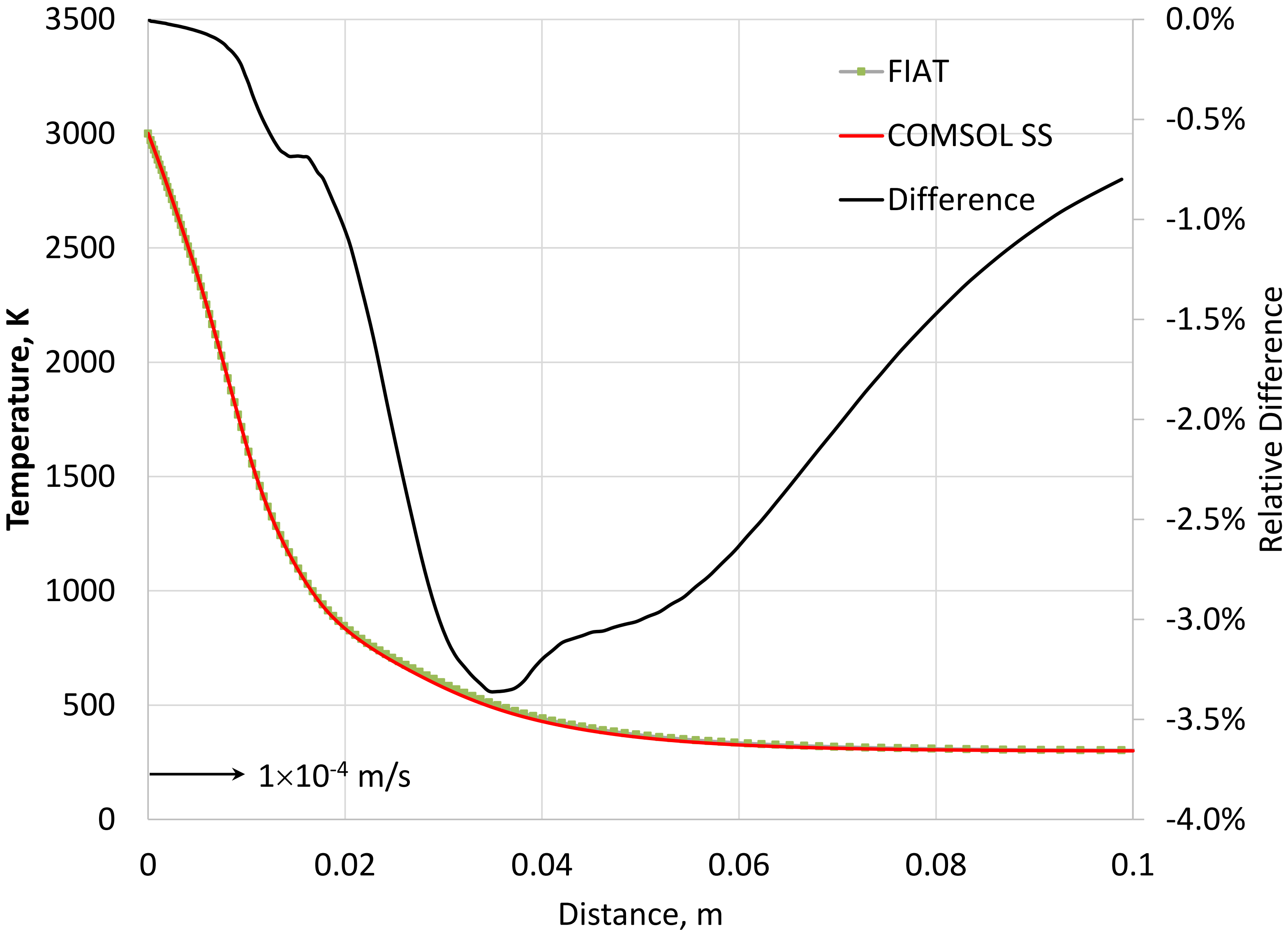
Finite Difference Temperature Profile Comparison



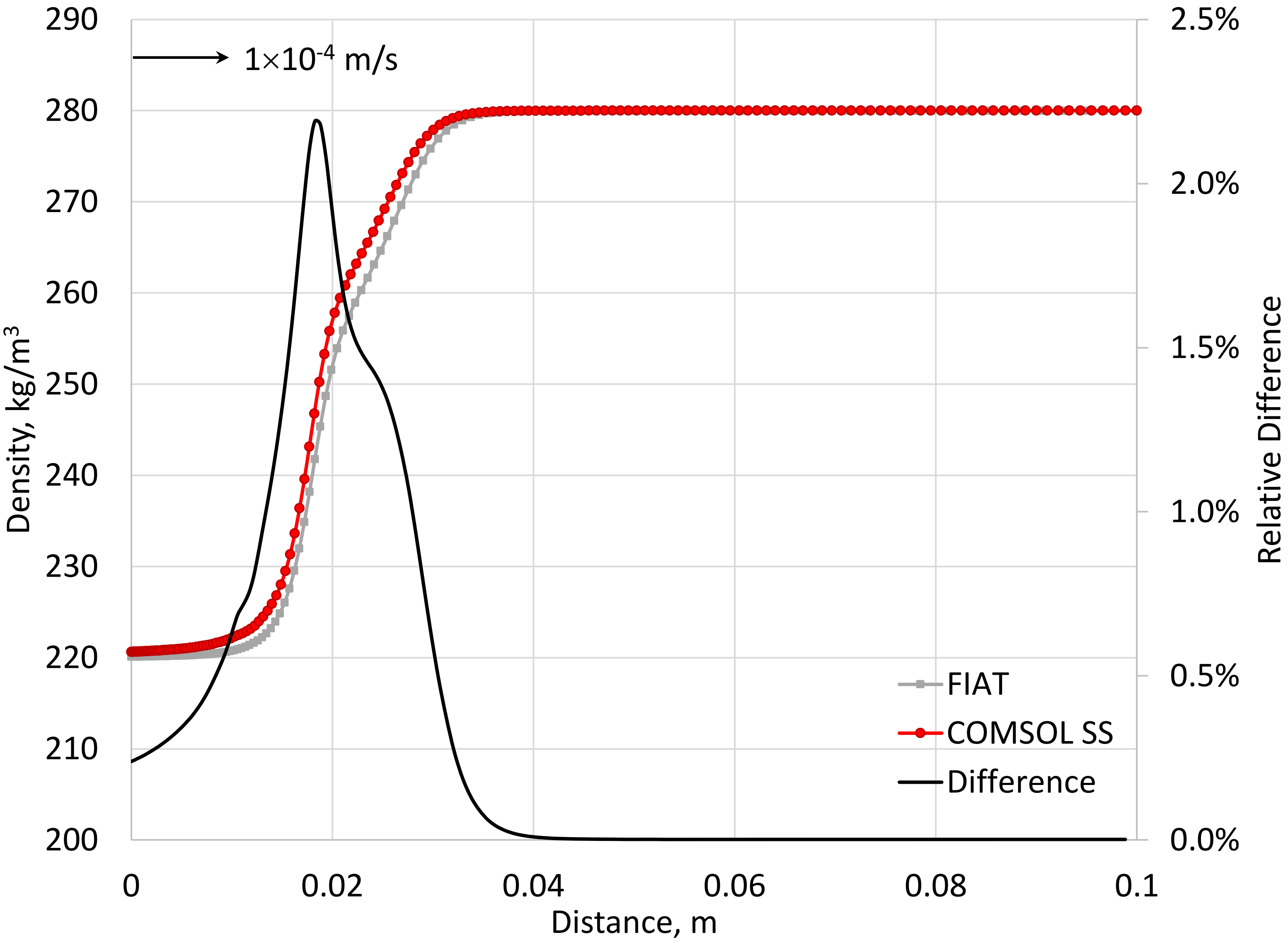
Finite Difference Density Profile Comparison



FIAT Temperature Profile Comparison



FIAT Density Profile Comparison

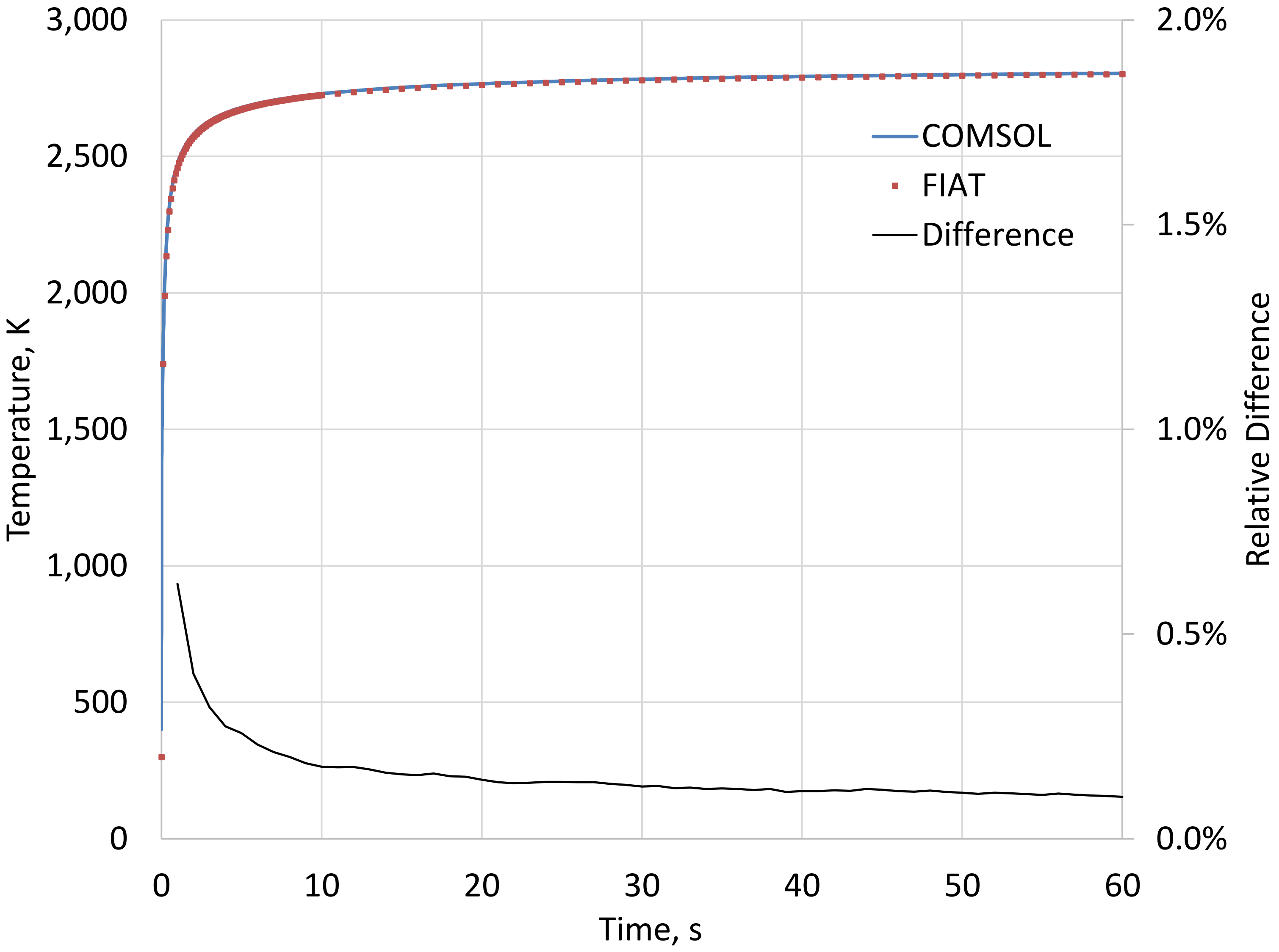


One-Dimensional Transient Example

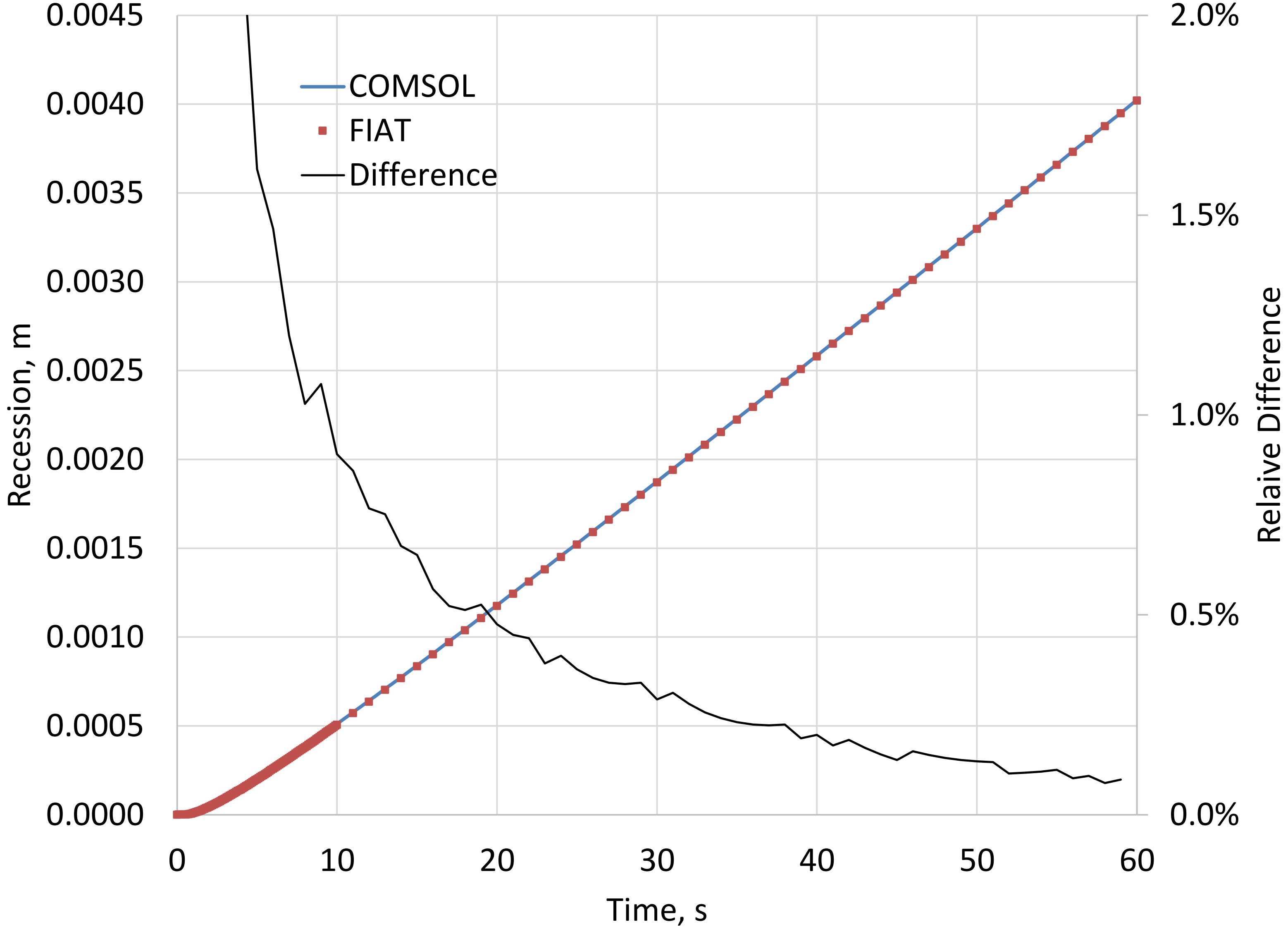
One-Dimensional Transient Example

- Problem is for a planar, finite width slab heated on one surface
- Frontface free stream enthalpy of 40 MJ/kg, a heat transfer coefficient of 0.1 kg/m^2-s, and reradiation
- Backface is adiabatic
- Full surface thermochemistry
- Thermocouples located at 0.001, 0.002, 0.004, 0.008, 0.016, 0.024, and 0.050 m
- COMSOL Multiphysics® results compared to FIAT results

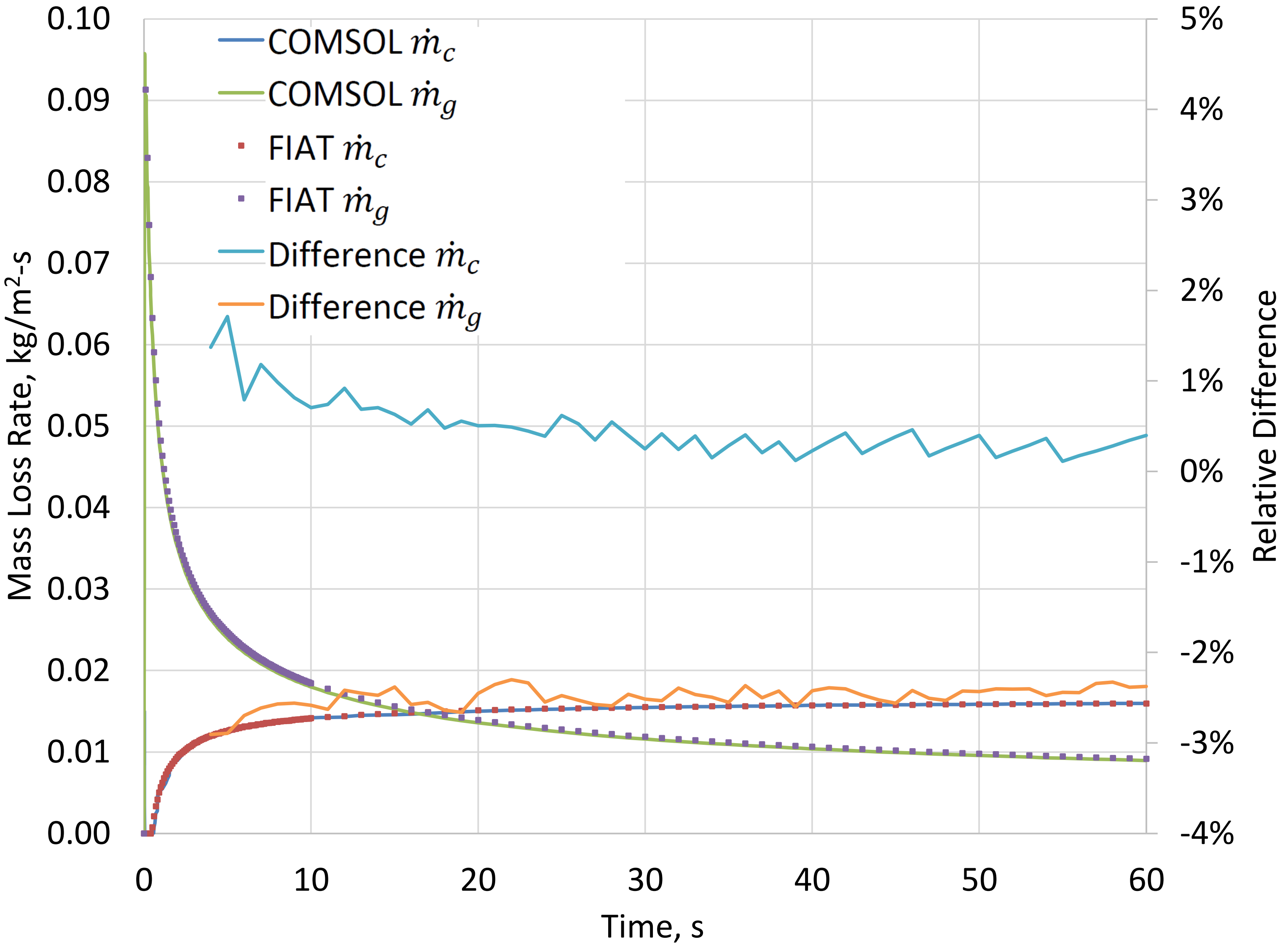
FIAT Surface Temperature Comparison



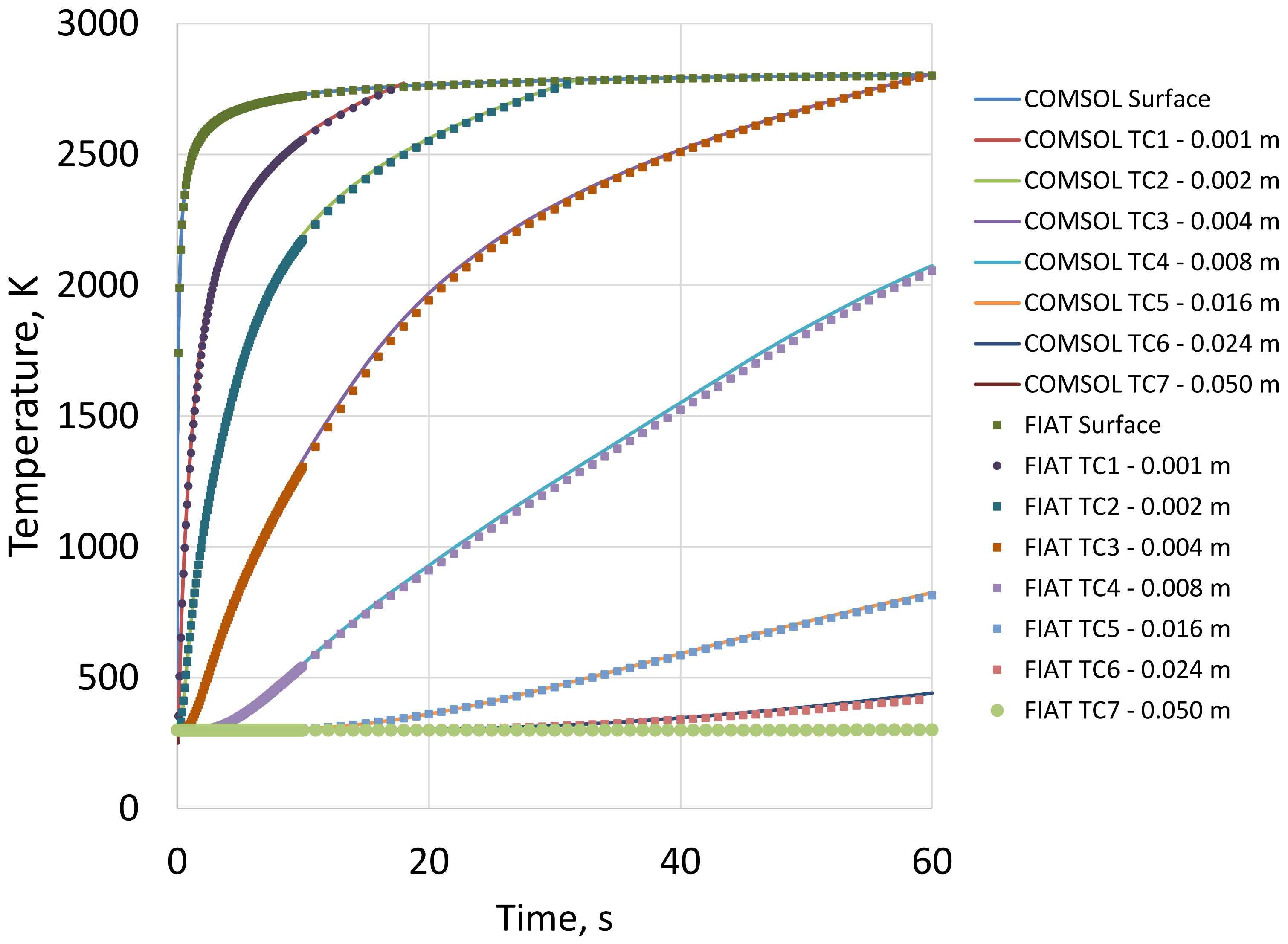
FIAT Recession Comparison



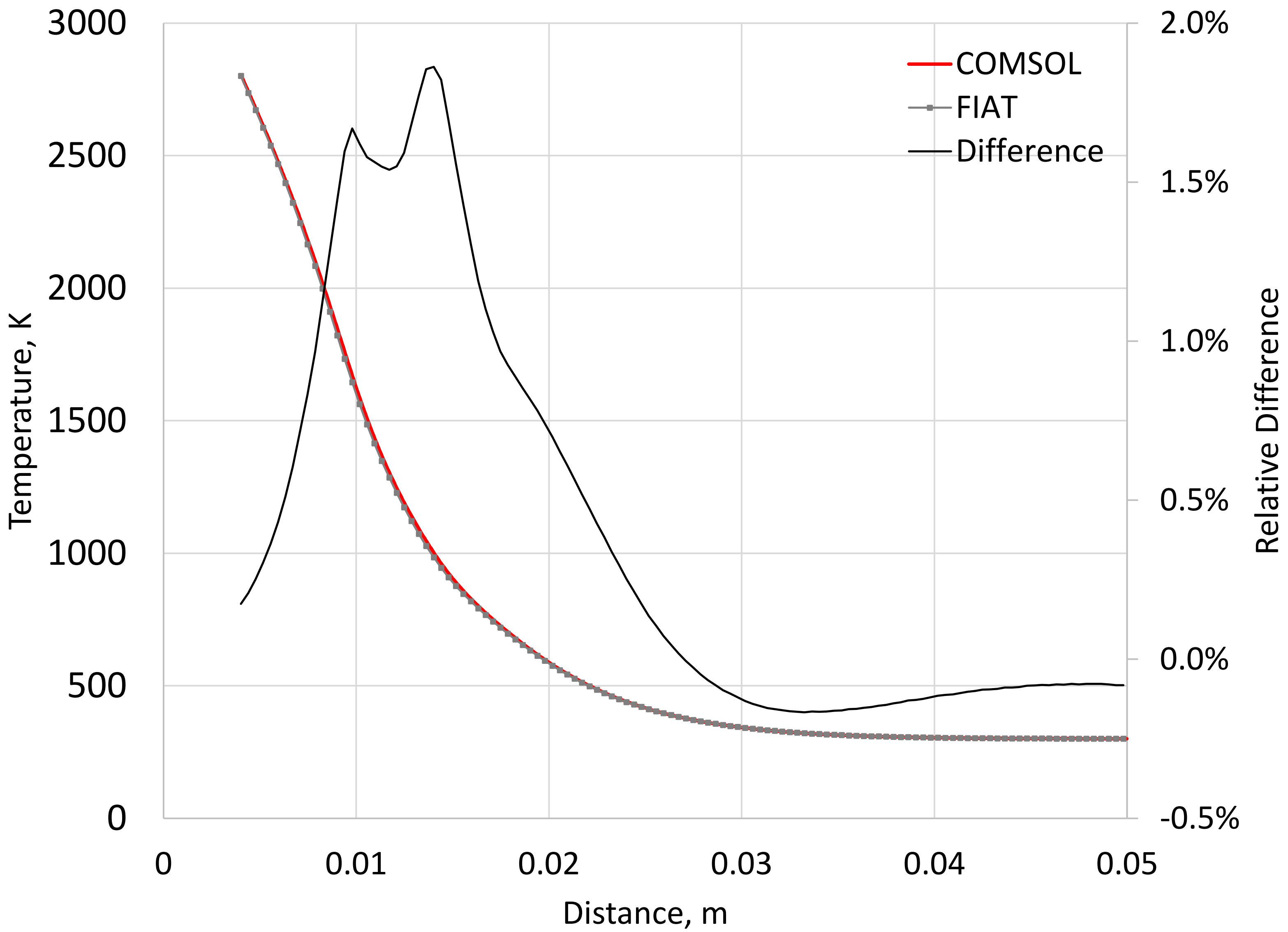
Char and Pyrolysis Surface Mass Loss Rates



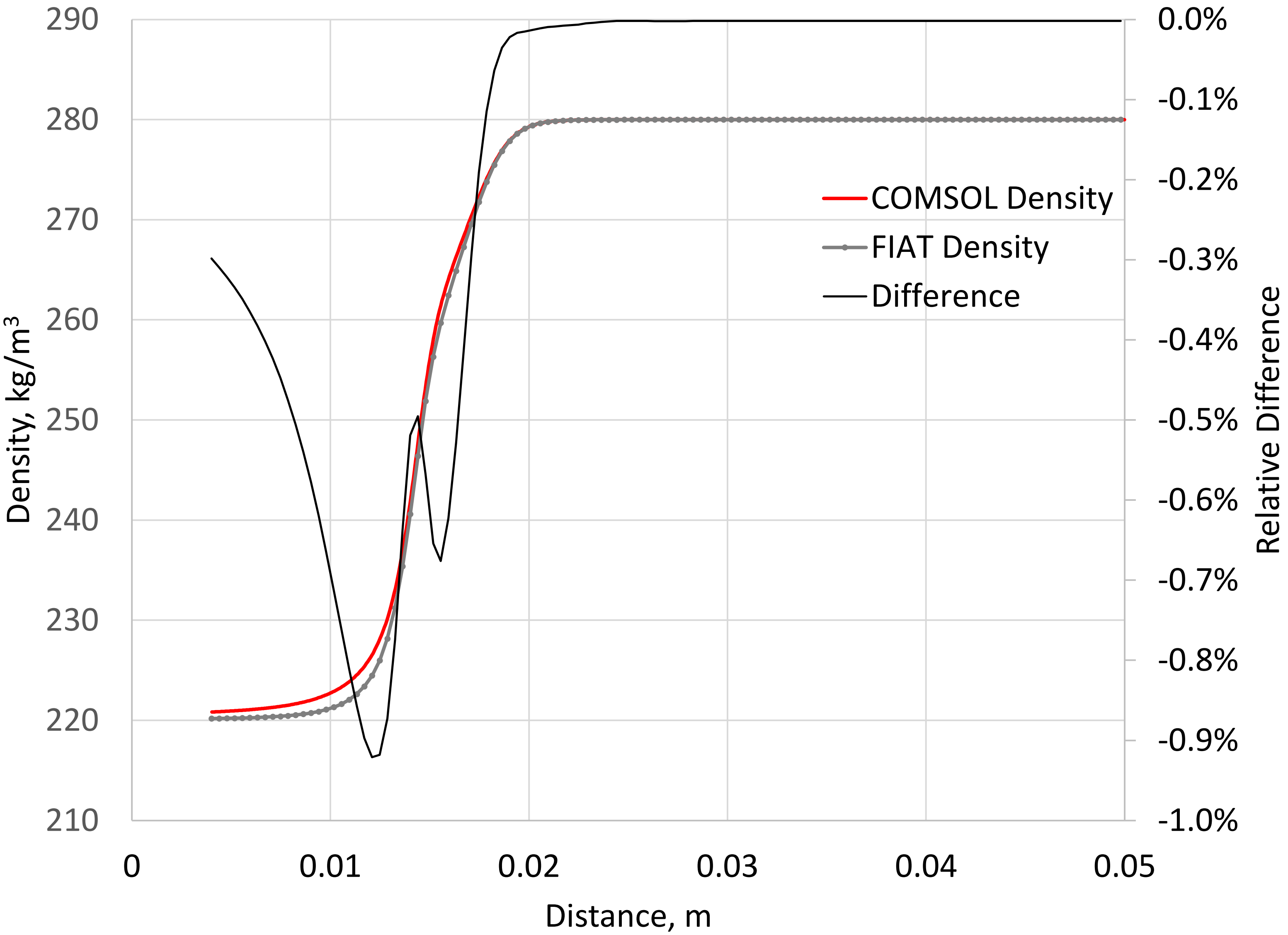
FIAT In-Depth Temperature Comparison



FIAT Temperature Profile Comparison after 60 s



FIAT Density Profile Comparison after 60 s



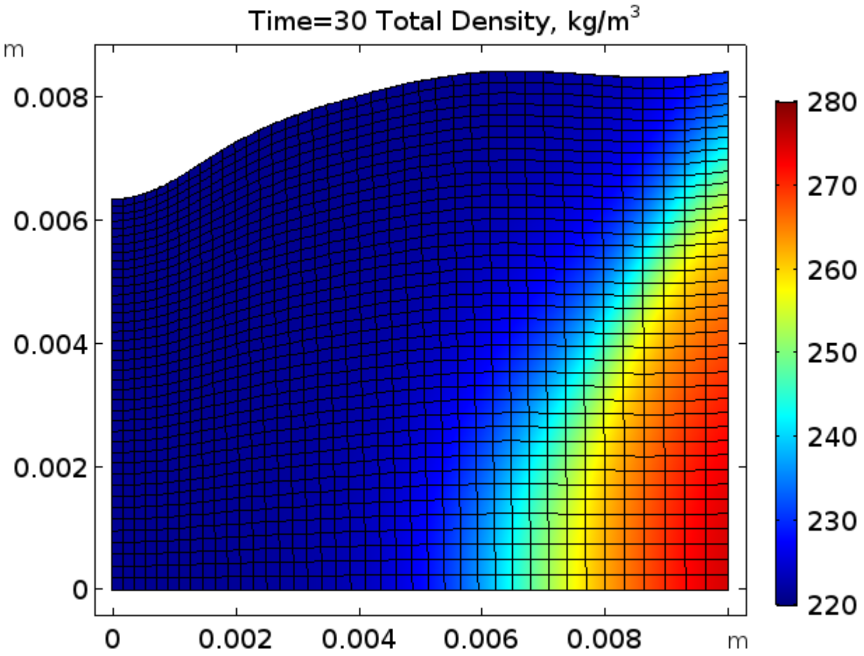
Two-Dimensional Transient Example

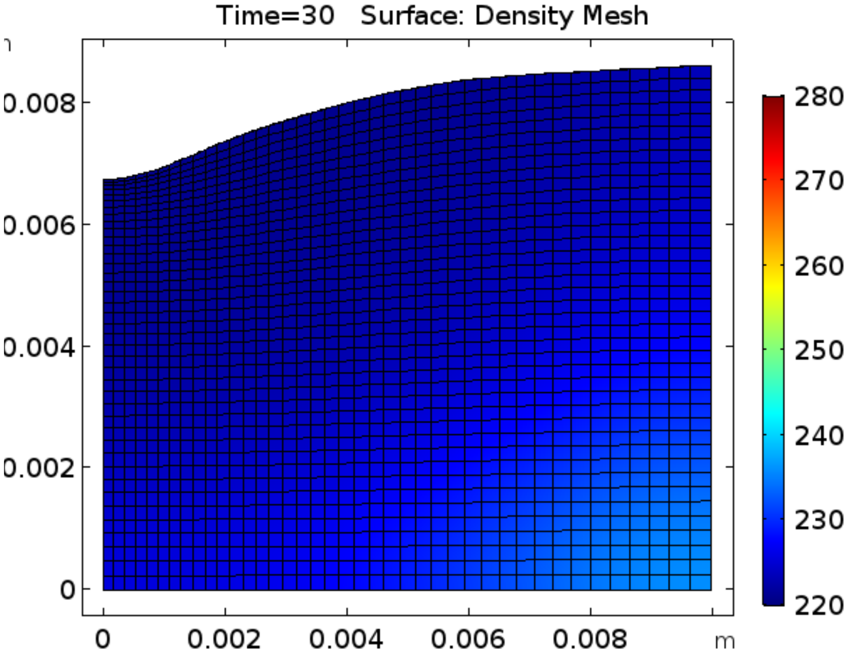
BACKUP

Density Comparison 1-D vs 2-D

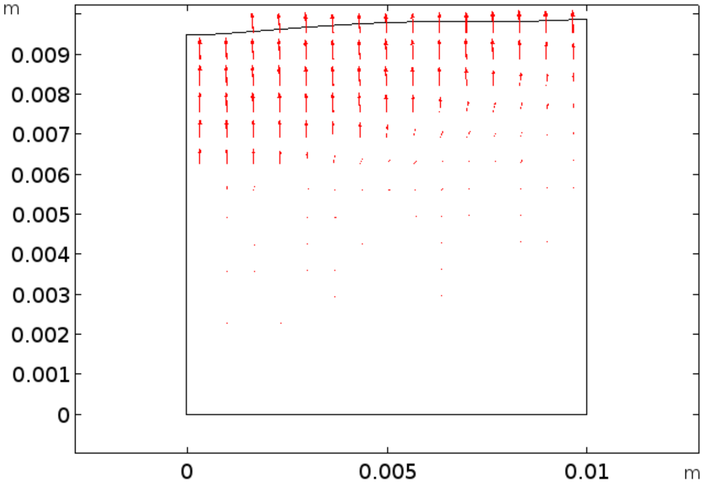
1-D

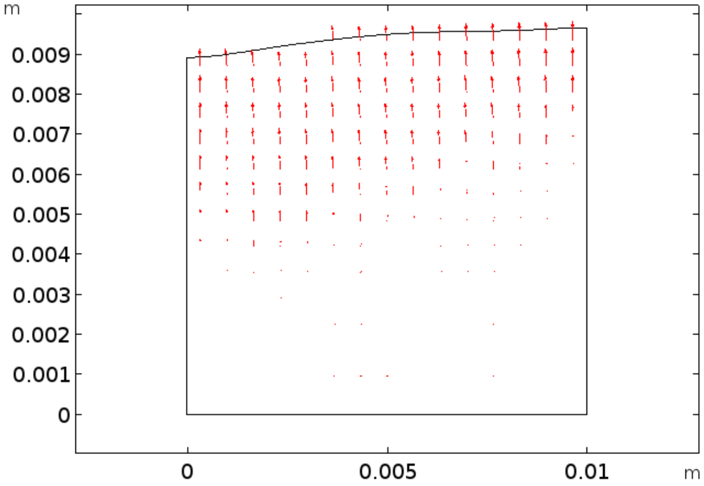
2-D

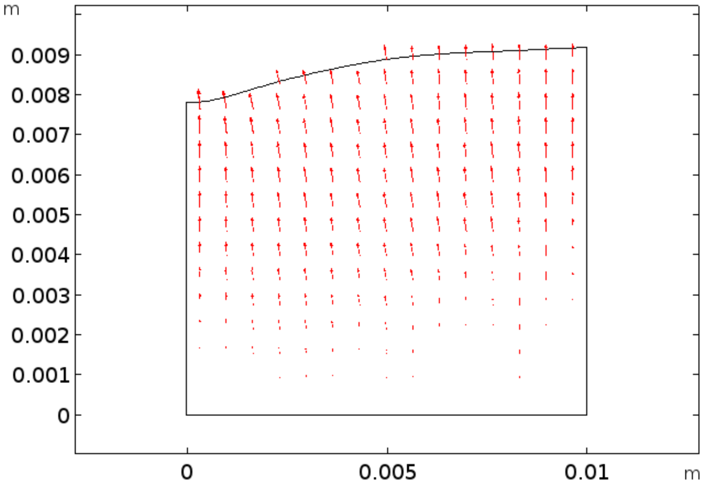


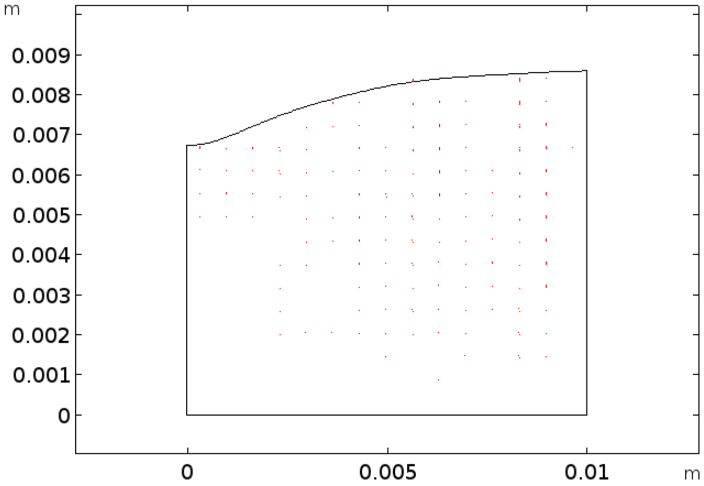


Pyrolysis Gas Flowrate


Time=5.0 Pyrolysis Gas Flow, kg/m^2-s


Time=10 Pyrolysis Gas Flow, kg/m^2-s


Time=20 Pyrolysis Gas Flow, kg/m^2-s


Time=30 Pyrolysis Gas Flow, kg/m^2-s

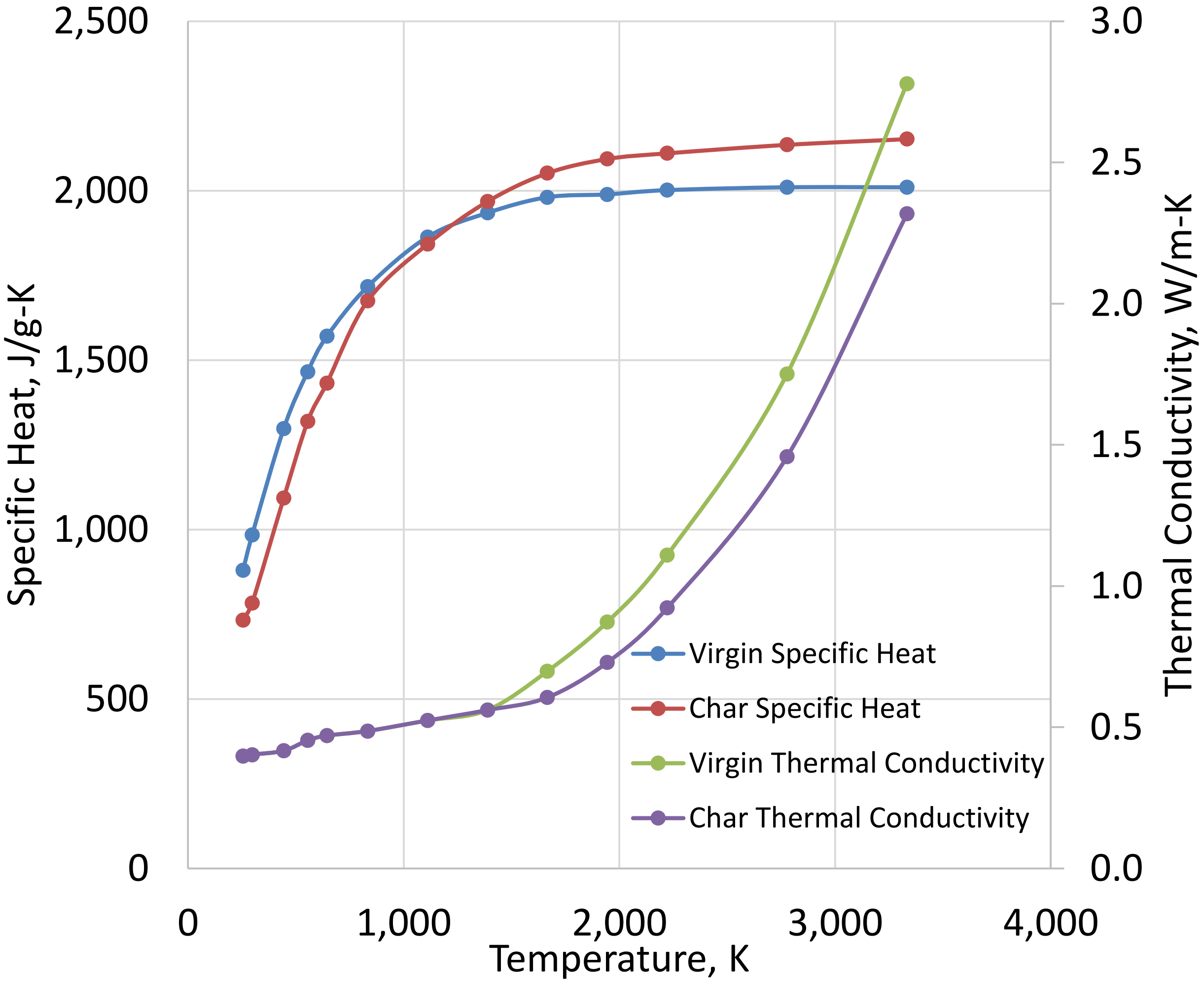
Thermophysical Properties

Thermophysical properties defined separately for virgin and char constituents. Composite properties determined by mixing rule based on mass.

$$k = x k_v + (1 - x) k_c$$

$$C_p = x C_{p,v} + (1 - x) C_{p,c}$$

$$x = \frac{\rho_v}{\rho_v - \rho_c}\left(1 - \frac{\rho_c}{\rho}\right)$$

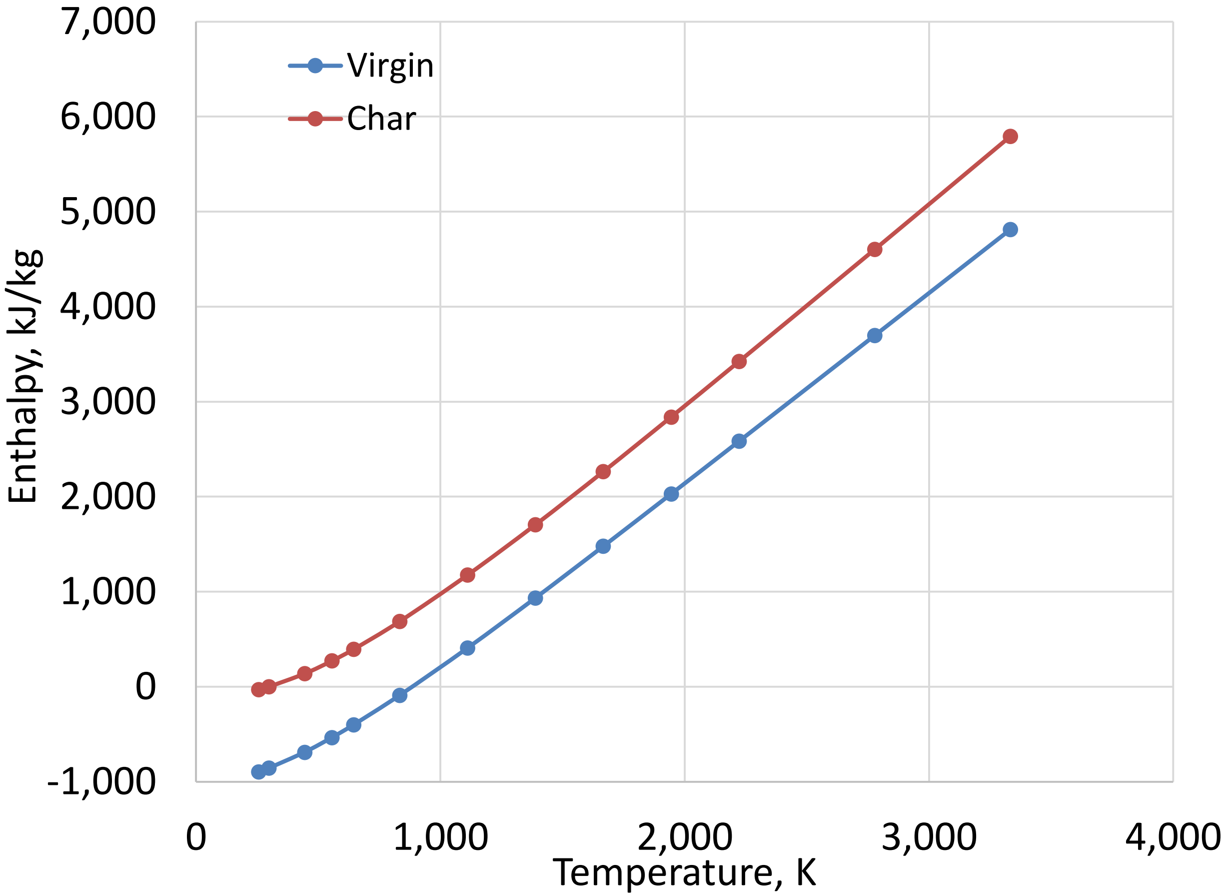


Material Enthalpy

Virgin and char enthalpies computed from integration of specific heats.

$$h = \int_{T_0}^{T} C_p dT + h_0$$

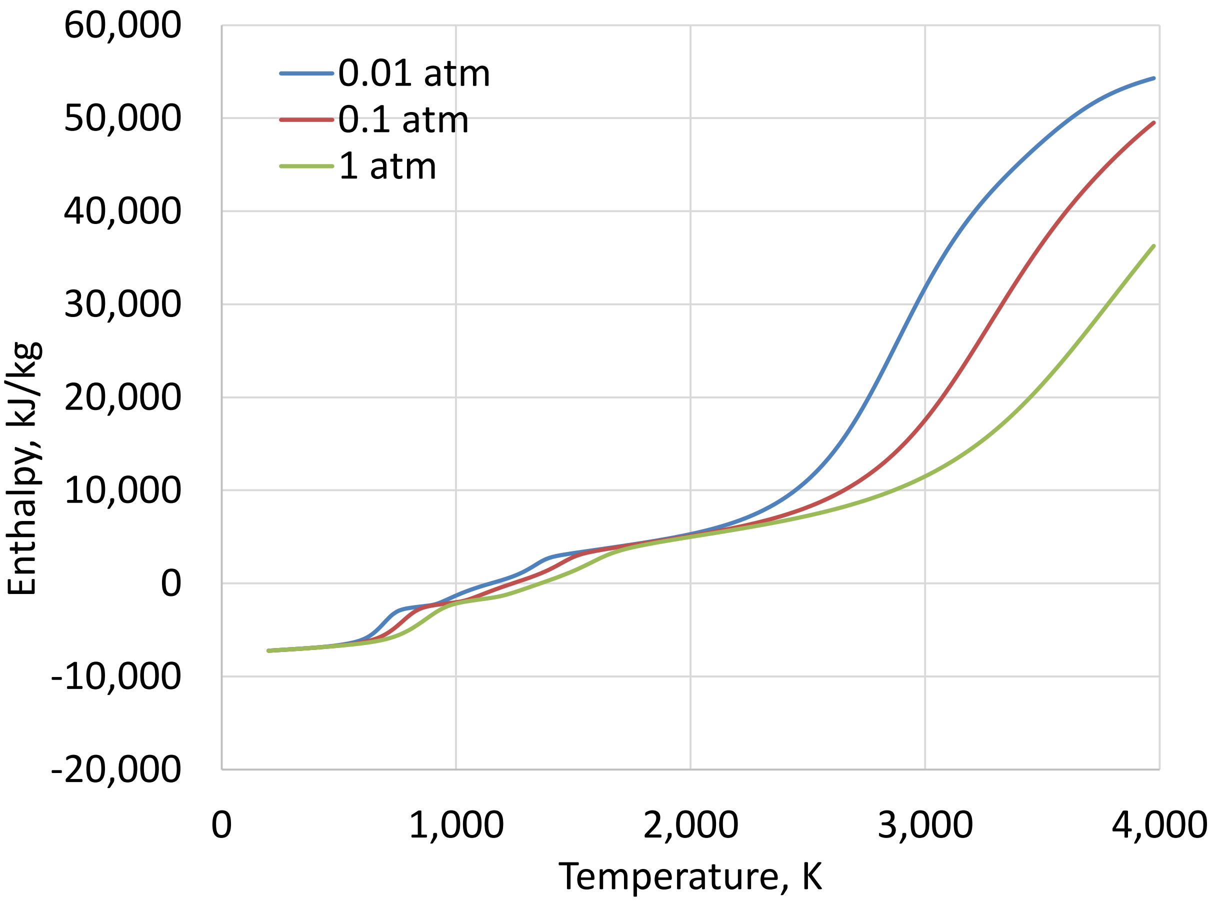
$$h = xh_v + (1 - x)h_c$$



Pyrolysis Gas Enthalpy

Pyrolysis gas enthalpy computed from equilibrium thermochemistry as a function of temperature and pressure.

$$h_{pg} = h_{pg}(p, T)$$

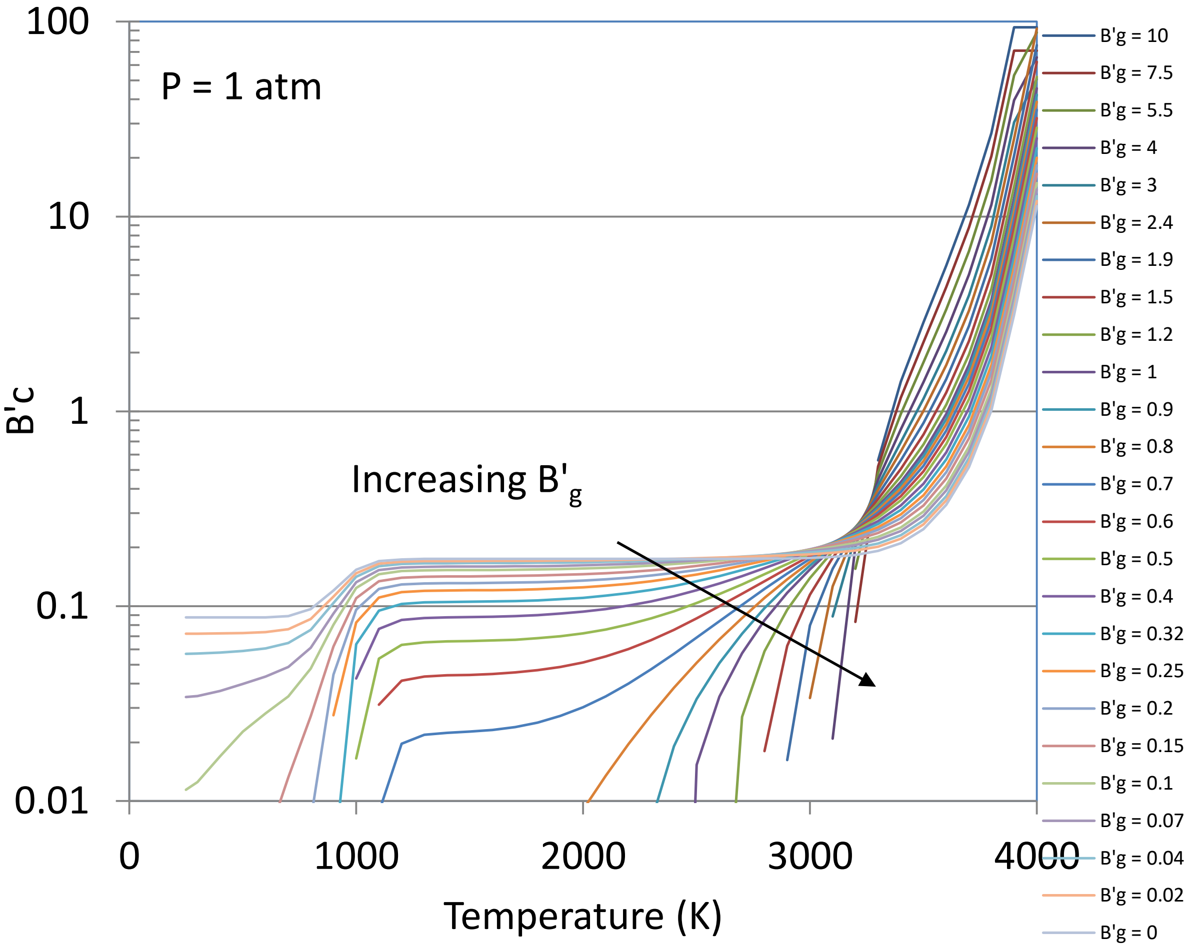


Surface Thermochemistry – Normalized Mass Loss

Surface thermochemistry conditions computed from equilibrium thermochemistry in terms of normalized mass fluxes.

$$B'_c = \dot{m}_c / \rho_e u_e C_M$$
$$B'_g = \dot{m}_g / \rho_e u_e C_M$$

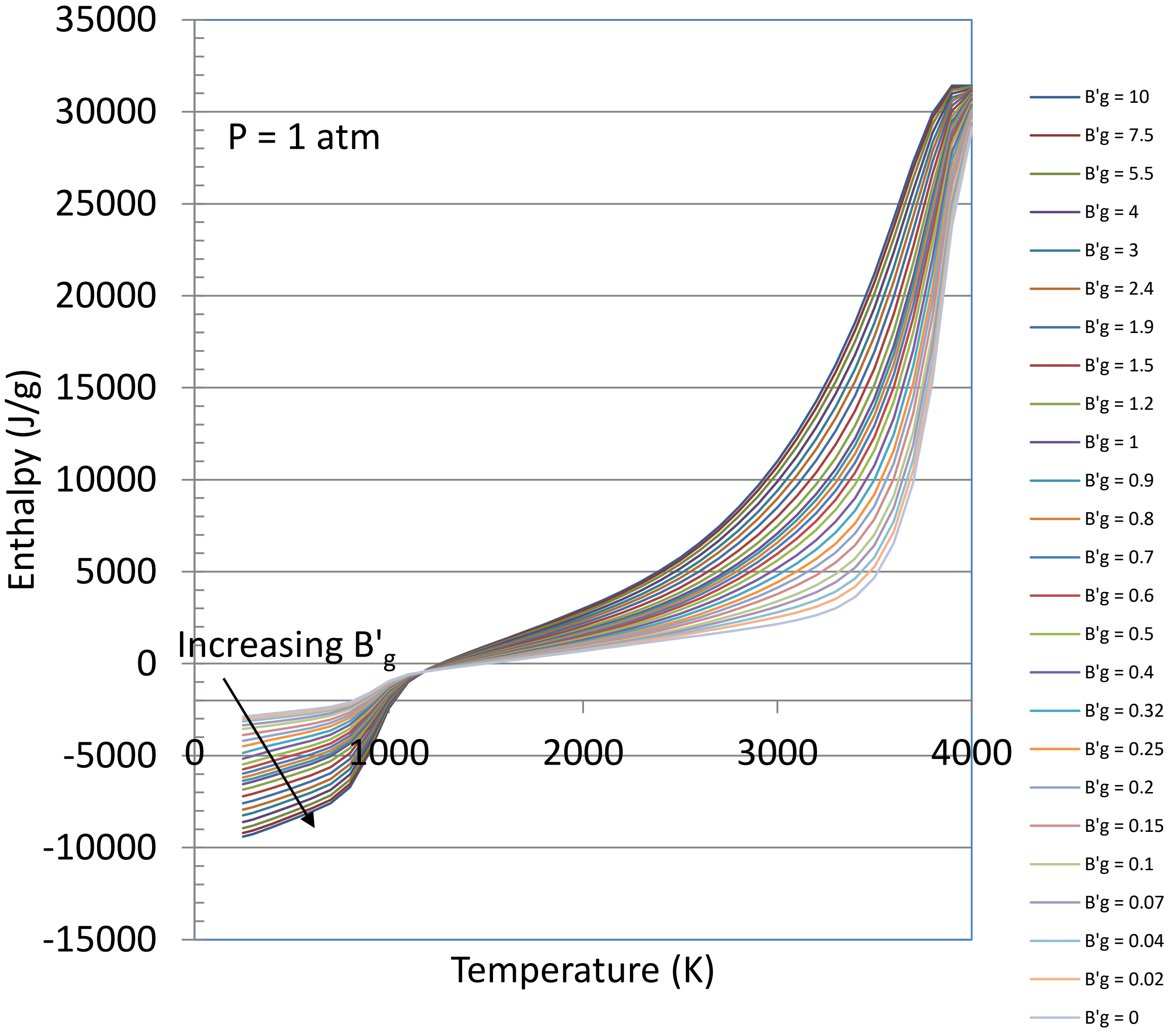
$$B'_c = B'_c(p, B'_g, T_s)$$



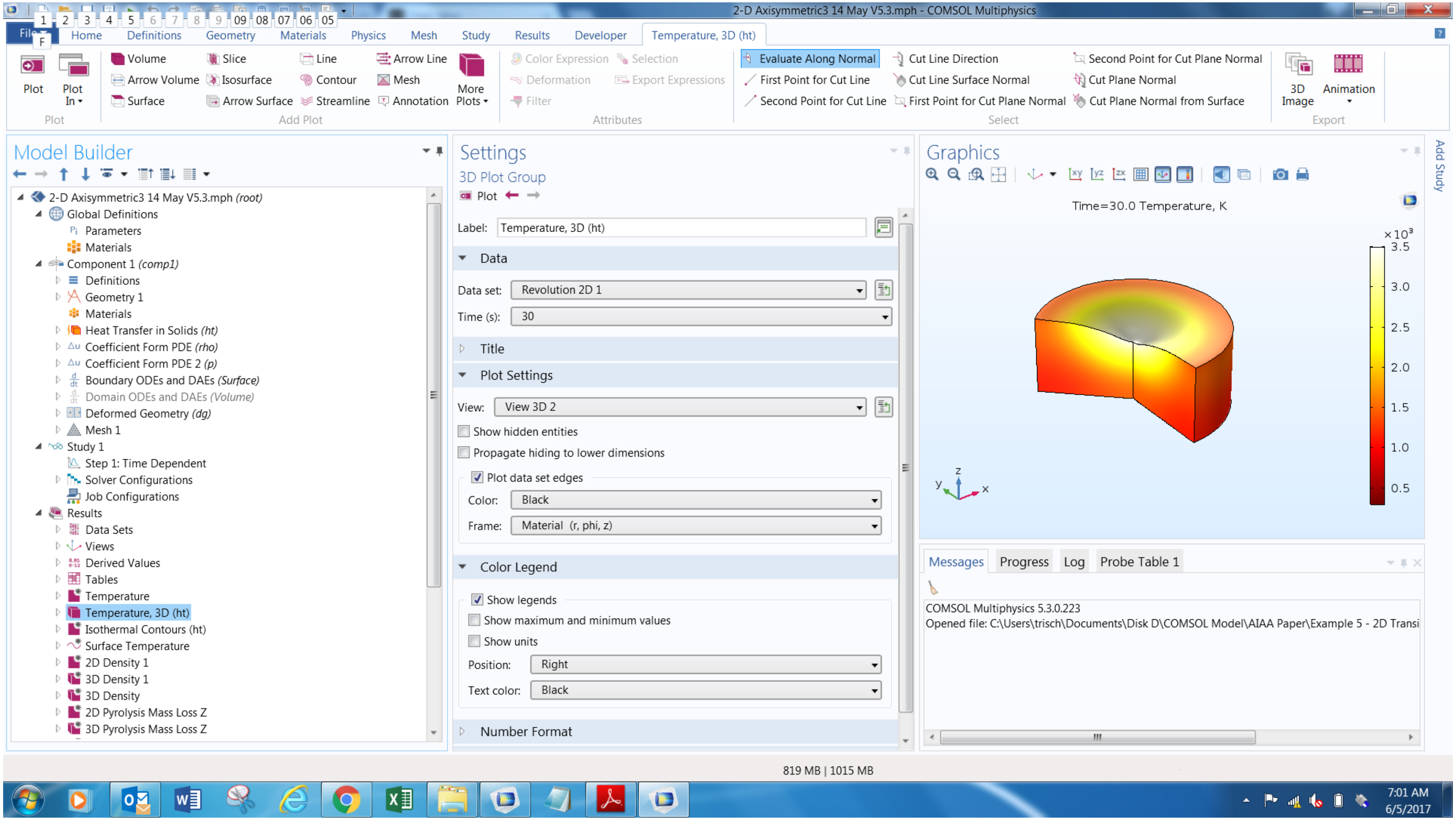
Surface Thermochemistry –Gas Phase Enthalpy

Enthalpy of gases at the wall computed similarly from equilibrium thermochemistry.

$$h_w = h_w(p, B_g', T_s)$$



COMSOL Multiphysics® User Interface



Settings

3D Plot Group

Plot

Label: Temperature, 3D (ht)

Data

Data set: Revolution 2D 1

Time (s): 30

Title

Plot Settings

View: View 3D 2

☐ Show hidden entities

☐ Propagate hiding to lower dimensions

☑ Plot data set edges

Color: Black

Frame: Material (r, phi, z)

Color Legend

☑ Show legends

☐ Show maximum and minimum values

☐ Show units

Position: Right

Text color: Black

Number Format

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COMSOL Multiphysics 5.3.0.223
Opened file: C:\Users\trisch\Documents\Disk D\COMSOL Model\AIAA Paper\Example 5 - 2D Transi
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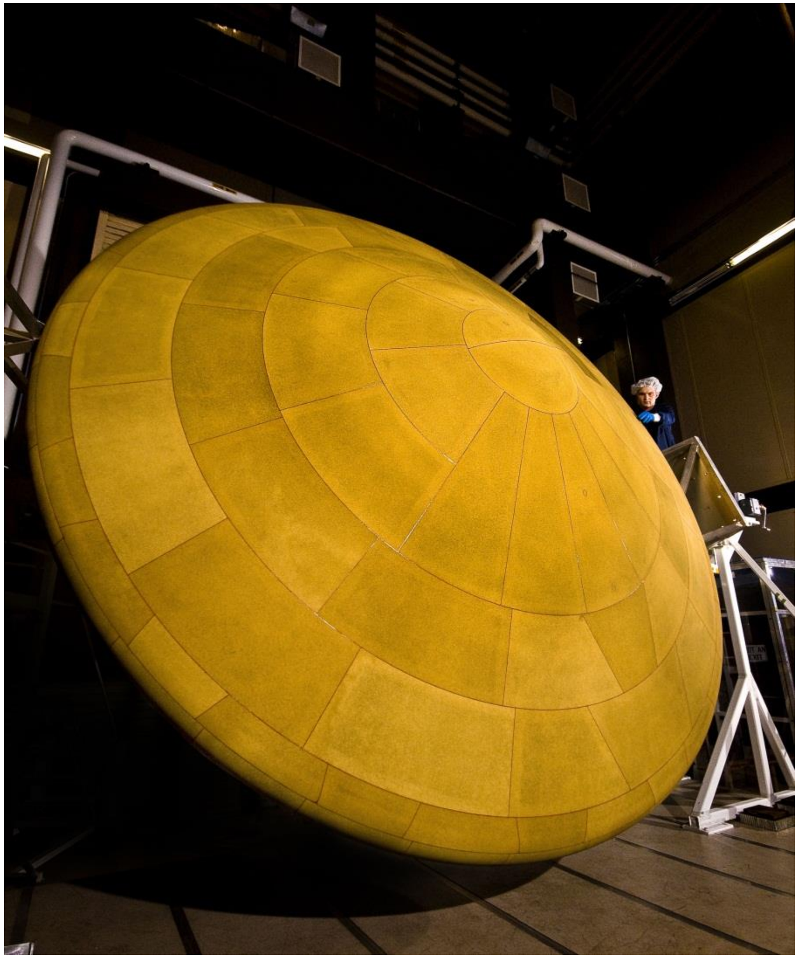
Example Uses of Pyrolyzing Ablator



Objective

- NASA primarily relies on custom written codes to analyze ablation and design TPS systems
- The basic modeling methodology was developed 50 years ago
- Through the years, CFD, thermal, and structural mechanics calculations have migrated from custom, user-written programs to commercial software packages
- Objective is to determine that a commercial finite element code can accurately and efficiently solve pyrolyzing ablation problems

Advantages of Commercial Codes

- Usability (e.g. GUI)
- Built–in pre- and post-processing
- Built-in grid generation
- Efficient solution algorithms
- Multi-dimensional capability (planar, cylindrical, 1-D, 2-D, & 3-D)
- Built in function capability (predefined, analytic, and tabular)
- Validated by a wide user base
- Reduced life cycle cost
- Regular upgrades and maintenance
- Modeling flexibility
- Better documentation

Material Selection

- For comparisons, utilize Theoretical Ablative Composite for Open Testing (TACOT) Material Properties
- Open, simulated pyrolyzing ablator that has been used a baseline test case for modeling ablation and comparing various predictive models
- Properties Required
  - Solid virgin and char specific heat, enthalpy, thermal conductivity, absorptivity and emissivity
  - Pyrolysis gas enthalpy
  - Surface thermochemistry mass loss and gas phase enthalpy