

Modeling a Catalytic Converter in Comsol Multiphysics

By Jacob Harding
December 10th, 2007
Chem E 499

Problem

The goal of this project was to develop a model of a catalytic converter in Comsol Multiphysics. The catalytic converter was first modeled in two dimensions with a circular cross-section then in three dimensions with a square cross-section. It is expected that the model should provide a large temperature change in fluid temperature as a result of the reaction between catalyst and fluid. Also, a hysteresis effect should be observed illustrating ignition and extinction temperatures.

Shapes and Boundary Conditions

The shape of the two dimensional model is of a pipe with circular cross-section. The model itself is only a rectangle for the fluid to flow through with a catalytic layer on the outer edge. The model is only half of the pipe with the left boundary being axially symmetric; this boundary is the middle of the pipe. See Figure 1 and Table 1 for a description of the boundary conditions and a visual representation of the model in two dimensions. The pink section in Figure 1 is the catalytic layer. The units at the bottom of the figure are millimeters.

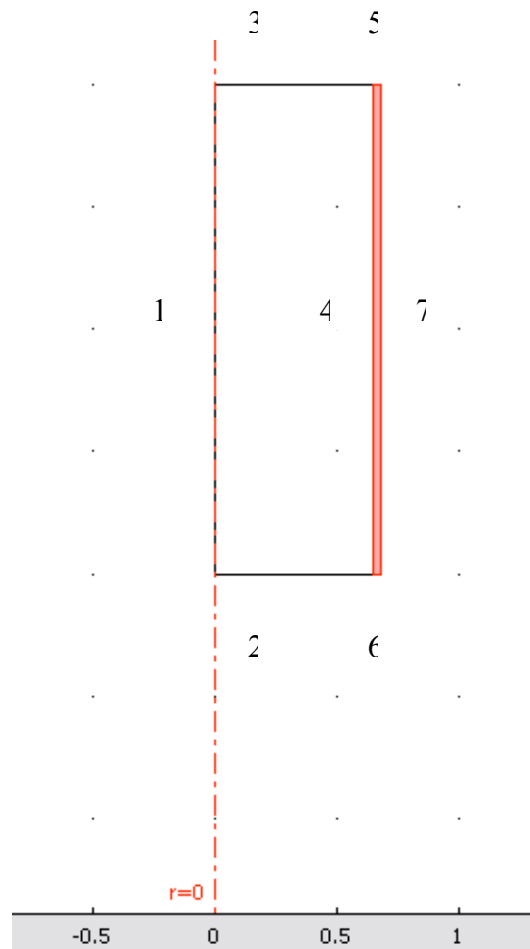


Figure 1: Two dimensional model of catalytic converter with the boundaries labeled

Table 1: Description of the boundary conditions for the two dimensional model

Boundary	Fluid Flow	Diffusion	Conduction
1	Axial Symmetry	Insulation/Symmetry	Axial Symmetry
2	Velocity	Concentration	Temperature
3	Normal Flow	Convective Flux	Convective Flux
4	No Slip	Continuity	Continuity
5	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation
6	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation
7	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation

The shape of the three dimensional model is of a pipe with a square cross section. The model itself is a square with the catalytic layer on two sides of it and the other two sides being symmetric. See Figure 2 for the two dimensional model and the extruded version of this can be seen in Figure 3. This section is one quarter of the total pipe with the center of the pipe being the front line in Figure 3. The numbers in Figure 3 refer to boundary faces not just boundary lines. The units at the bottom of Figure 2 are in millimeters and the units in Figure 3 are in meters.

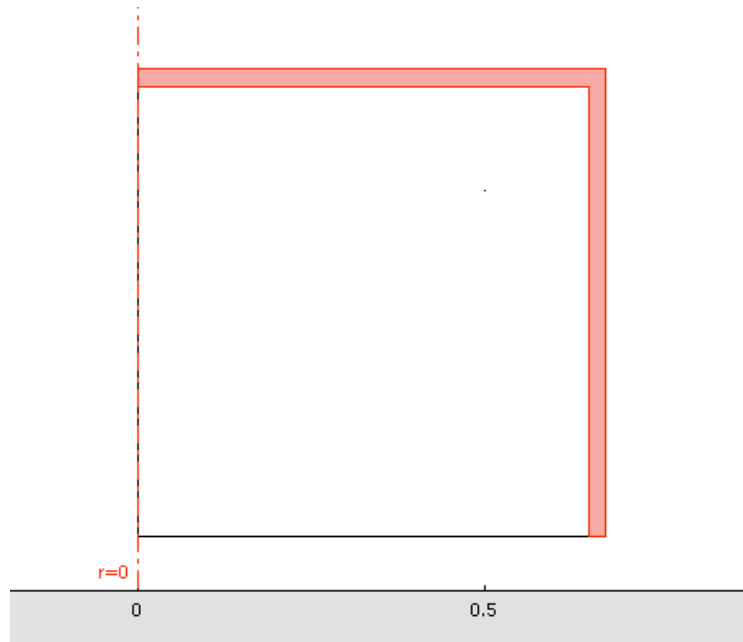


Figure 2: Three dimensional model before extrusion



Figure 3: Three dimensional model after extrusion with boundary faces labeled

Table 2: Description of boundaries and boundary conditions for three dimensional model

Boundary	Fluid Flow	Diffusion	Conduction	Description
1	Symmetry	Insulation/Symmetry	Thermal Insulation	Nearest fluid face on the left
2	Symmetry	Insulation/Symmetry	Thermal Insulation	Nearest fluid face on the right
3	Laminar Inflow	Concentration	Temperature	Bottom of the pipe fluid face
4	Normal Flow	Convective Flux	Convective Flux	Top of the pipe fluid face
5	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation	Nearest catalyst face on the left
6	No Slip	Continuity	Continuity	Catalyst face on inside of pipe on left
7	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation	Bottom of the pipe catalyst face
8	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation	Top of the pipe catalyst face
9	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation	Catalyst face on outside of pipe on left
10	No Slip	Continuity	Continuity	Catalyst face on inside of pipe on right
11	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation	Nearest catalyst face on the right
12	Not Active in this Domain	Insulation/Symmetry	Thermal Insulation	Catalyst face on outside of pipe on right

The two dimensional model was solved with 3,940 elements created from meshing. This created 30,128 degrees of freedom. For the three dimensional model, it had to be meshed on a coarse setting because memory errors were thrown when solved with normal meshing. This led to the three dimensional model having 4,976 elements and 32,172 degrees of freedom.

Multiphysics and Parameters

To solve this problem three sets of physics were used; the same sets of physics were used for both the two dimensional model and the three dimensional model. The physics to model the fluid flow was Incompressible Navier-Stokes under mass transport and laminar flow. The equation solving this physics model was

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} \quad \text{where } \rho = 1.18 \frac{\text{kg}}{\text{m}^3}, \eta = 1.74 \times 10^{-6} \text{ Pa.s}, \mathbf{F} = 0$$

The physics to model the reaction taking place was the Convection and Diffusion under mass transport. The equation for this model was $\nabla \cdot (-D \nabla c) = R - \mathbf{u} \cdot \nabla c$ where

$$D = 1 \times 10^{-5} \frac{\text{m}^2}{\text{s}}, R = -\text{rate} \left(\frac{1}{T} \right) (1000) \frac{\text{mol}}{\text{m}^3 \text{s}}, \text{rate} = \frac{\left(\frac{4.67 \times 10^{16}}{T} \right) \exp \left(\frac{-12256}{T} \right) y_{O_2} y_{CO}}{\left(1 + y_{CO} 65.5 \exp \left(\frac{961}{T} \right) \right)^2} \frac{\text{kmol K}}{\text{m}^3 \text{s}}$$

and $y_{O_2} = \frac{2}{3}(0.03 + y_{CO})$, $y_{CO} = c$, $c = \text{mole fraction}$.. The physics to model the temperature change in the catalytic converter due to the reaction taking place was the Convection and Conduction under energy transport. The equation solving this physics was $\nabla \cdot (-k \nabla T + \sum_j h_j N_{D,j}) = Q - \rho C_p \mathbf{u} \cdot \nabla T$, $k = 0.625 \frac{W}{m K}$, $\rho_{fluid} = 1.205 \frac{kg}{m^3}$, $\rho_{catalysst} = 1000 \frac{kg}{m^3}$, $C_p = 900 \frac{J}{kg K}$, $Q = \Delta H_{rx} \cdot rate \left(\frac{1}{T} \right) \frac{W}{m^3}$, $\Delta H_{rx} = 3.31 \times 10^8 \frac{J}{kmol}$.

Results

To solve this problem, the fluid flow was solved first in Comsol. It was solved separately from the other two physics models because it has no dependence on the other physics. For both two and three dimensional models, once the fluid flow was solved for it was checked to see if it was fully developed and plug flow by looking at the stream lines and the cross-section plot of velocity field. These fully developed plug flow profiles can be seen in Figures 4 and 5. Since the stream lines in Figure 4 are straight at the entrance of the pipe and continue on straight to the exit, this shows that the fluid flow is fully developed. To see that it is plug flow, you can see the velocity profile in Figure 5 shows the maximum velocity is at the center of the pipe and that maximum is twice the defined average velocity. Also, because there is a no slip condition at the catalyst wall, there is no fluid velocity at the wall.

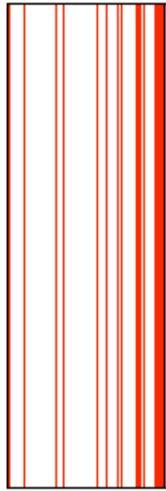


Figure 4: Stream lines for the two dimensional model

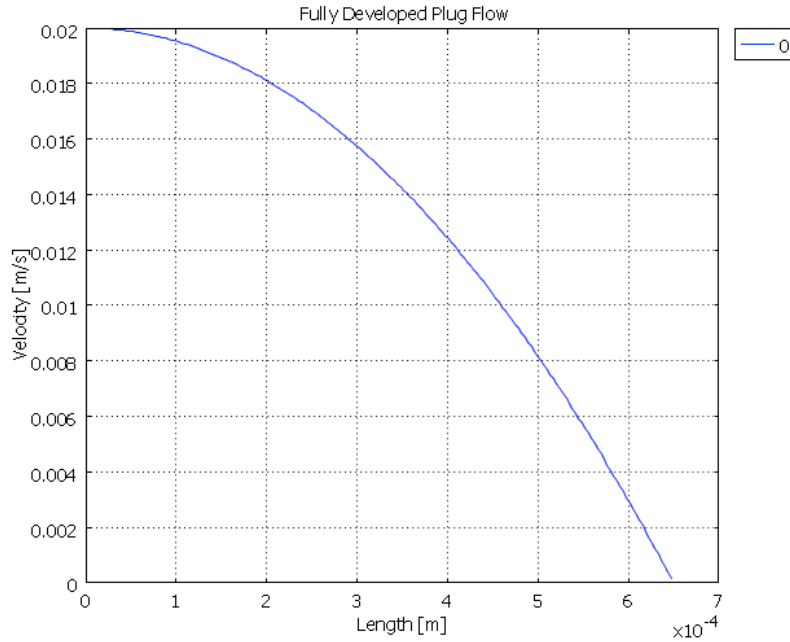


Figure 5: Two dimensional model displays plug flow for fluid flow

For the three dimensional model, fully developed velocity profile of the fluid was once again checked by looking at the domain plot of the inlet face. This plot is displayed in Figure 6. Here one can see that the maximum velocity is at the center of the pipe and once again it is twice the defined average velocity. In addition, there is no fluid velocity at the catalyst walls because there is a no slip condition defined here.

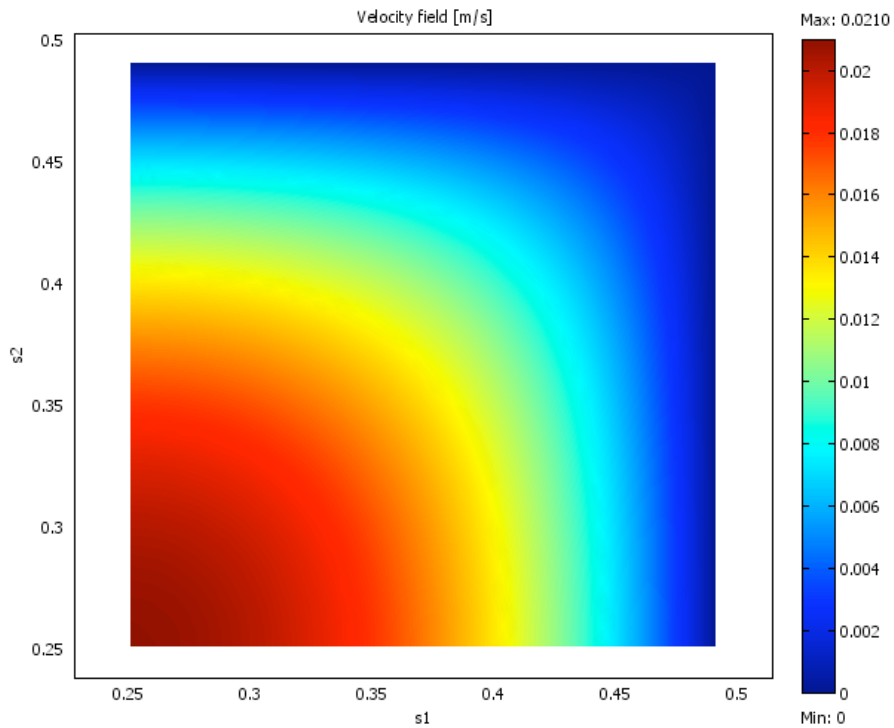


Figure 6: Three dimensional model displays fully developed plug flow for fluid flow

The diffusion due to reaction and temperature change due to reaction were solved simultaneously due to their dependence on each other. It is expected that the reaction between the fluid and the catalyst will create a large temperature change on the order of magnitude of 400K to 700K. The results obtained in this project however were much different. The current findings are of a temperature change of only 0.01K to 3K. Though the trend of temperature change is correct, the magnitude of this change is incorrect and that fact is also affecting the values obtained for the change in Carbon Monoxide concentration in the fluid. Once again, the trends of concentration vs. temperature are correct but the exact values are currently incorrect due to the small temperature change.

The trends of concentration vs. temperature for the two dimensional and three dimensional models can be seen in Figure 7 and 8 respectively. Notice that in both cases, as the temperature increases, the amount of Carbon Monoxide in the fluid decreases at a greater rate. This is expected from looking at the implemented rate law. To check that the rate law is working correctly, calculations were done by hand to check that the value of the rate law that Comsol was solving for was indeed the value of the rate law at that temperature and concentration. This calculation can be seen in the sample calculations in the appendix.

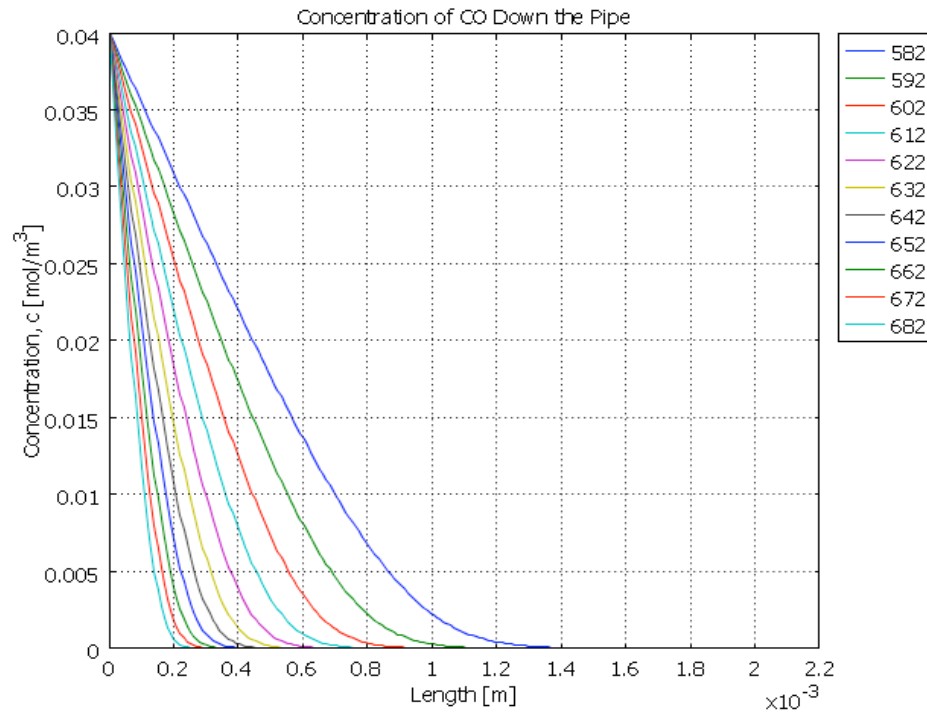


Figure 7: Two dimensional model concentration profile at various temperatures

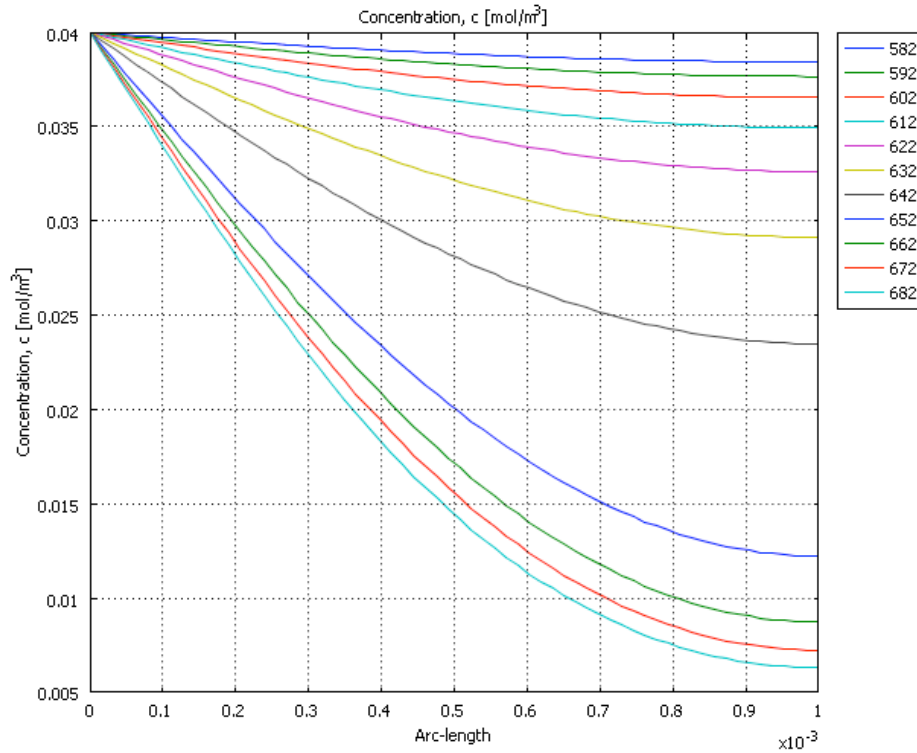


Figure 8: Three dimensional model concentration profile at various temperatures

As stated earlier, a too small temperature change is currently being observed but the correct trend of temperature is also being seen. The temperature is increasing down the length of the pipe due to the reaction taking place between the fluid and the catalyst, illustrated in Figures 9 and 10. In addition, the maximum temperature is taking place at the catalyst wall right where the reaction is taking place, exemplified in Figure 11.

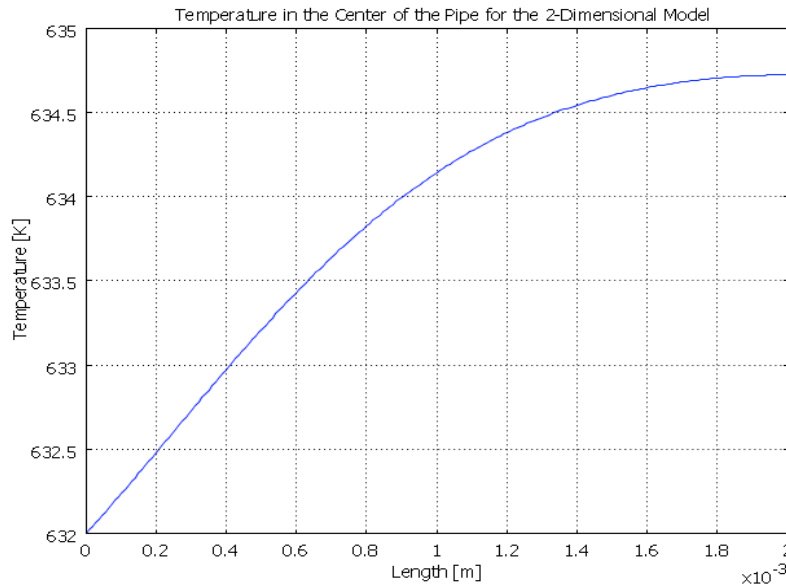


Figure 9: Temperature in the center, down the length of the pipe, for the two dimensional model

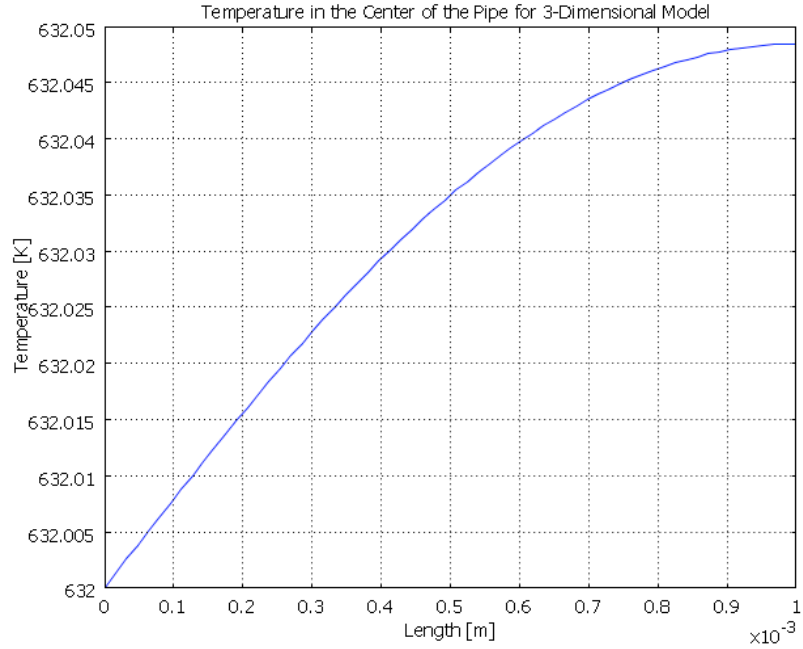


Figure 10: Temperature in the center, down the length of the pipe, for the three dimensional model

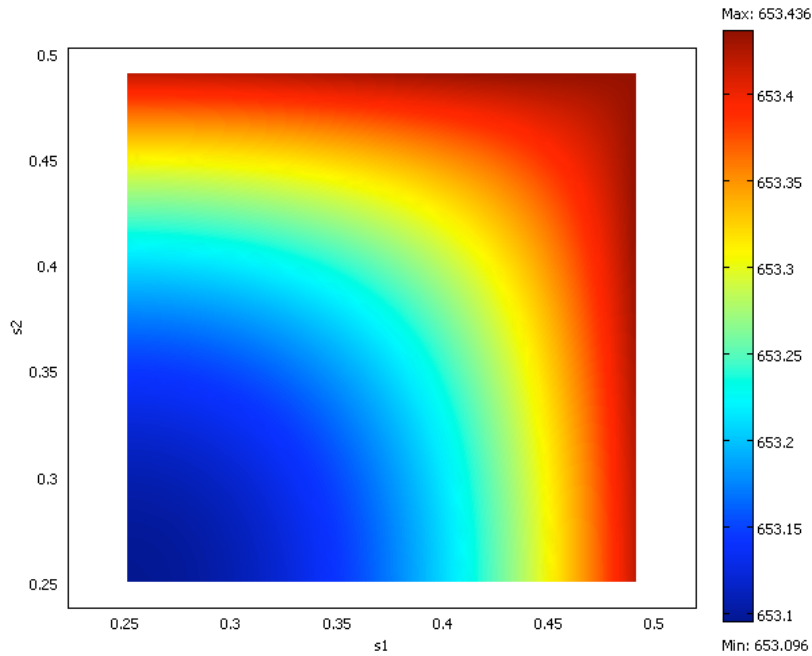


Figure 11: Temperature profile at pipe exit for three dimensional model with inlet temperature $T_{in}=582K$

Since the temperature change is not large enough, and is known to be incorrect, the evaluation of the hysteresis effect was not done for this experiment. It would not have made sense to do analysis to find ignition and extinction temperatures for a system that is not solving correctly with regards to temperature. However, included in the sample calculations is the work done by hand to try and find the error for why the temperature change is so small.

Appendix

Rate Law Check:

$$rate = \frac{\left(\frac{4.67 \times 10^{16}}{T}\right) \exp\left(\frac{-12256}{T}\right) y_{O_2} y_{CO}}{\left(1 + y_{CO} 65.5 \exp\left(\frac{961}{T}\right)\right)^2} \frac{kmol K}{m^3 s}$$

From point evaluator tool in Comsol:

$$T = 684.22 K, c = 2.14 \times 10^{-5} \frac{mol}{m^3 s}, rate = 0.481 \frac{mol}{m^3 s}$$

Calculated by hand:

$$rate = \frac{\left(\frac{4.67 \times 10^{16}}{684.22}\right) \exp\left(\frac{-12256}{684.22}\right) \left(\frac{2}{3} (0.03 + 2.14 \times 10^{-5})\right) (2.14 \times 10^{-5})}{\left(1 + y_{CO} 65.5 \exp\left(\frac{961}{684.22}\right)\right)^2} = 0.4807$$

The difference is simply a rounding error when solving by hand.

Temperature difference work:

$$\rho C_p \frac{\partial T}{\partial z} = Q$$

$$\rho C_p \frac{\partial T}{\partial z} = \Delta H_{rx}(rate) \left(\frac{1}{T}\right)$$

$$\Delta T = \frac{\Delta H_{rx}(rate) \left(\frac{1}{T}\right)}{\rho C_p}$$

Unit analysis on ΔT gives:

$$\Delta T = \frac{\left(\frac{J}{kmol}\right) \left(\frac{kmol K}{m^3 s}\right) \left(\frac{1}{K}\right)}{\left(\frac{kg}{m^3}\right) \left(\frac{J}{kg K}\right)} = \frac{K}{s}$$

It should not be per time. There is still an error somewhere.