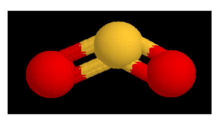
Development of a User Interface for Design of SO_2 Oxidation Fixed-Bed Reactors

COMSOL Conference 2015
Boston, MA October 7-9

SO_2



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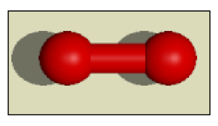
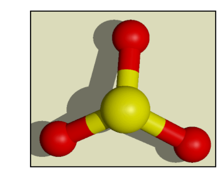
O_2





SO_3

SO_2 Oxidation Catalysts

SO_2 Oxidation Convertor

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Introduction

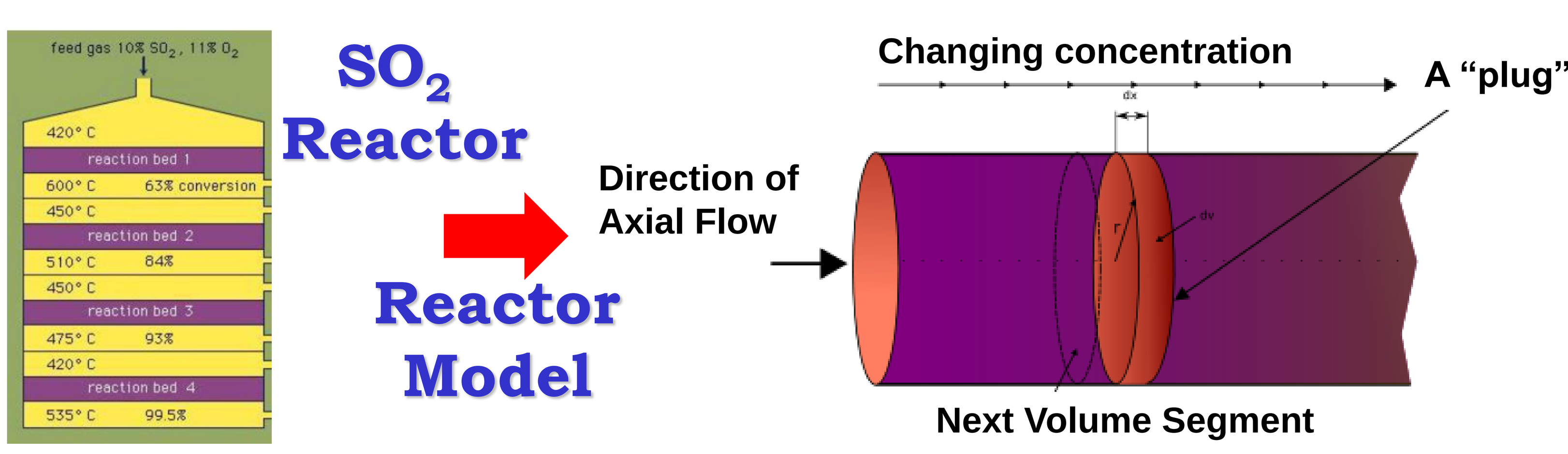
Sulfuric acid (H_2SO_4) is a very important commodity chemical since a nation's sulfuric acid production is a good indicator of its industrial strength. A key reaction used to manufacture H_2SO_4 involves the gas phase oxidation of SO_2 to SO_3 over solid catalysts. Development of improved catalysts with higher activities at lower temperatures that can convert future industrial process gas streams containing SO_2 to SO_3 at higher efficiencies is a challenge of increasing importance from both an environmental and practical process perspective. Typical SO_2 converter consists of four catalyst beds operated adiabatically with intercooling between beds. The staged operation is needed due to the equilibrium limitation of the reaction.

Development of a plug-flow reactor (PFR) model is important for SO_2 oxidation because the PFR is an ideal reactor and thus it produces the maximum adiabatic temperature rise and conversion. The temperature and conversion values from a PFR model can be used as a reference for a non-ideal fixed-bed catalytic model.

Objectives

- Develop a 1-D adiabatic plug flow reactor model for SO_2 oxidation reaction for all four passes for typical operating conditions using COMSOL Reaction Engineering Lab 3.5a.
- Develop a graphical user interface that allows end-users to study the effect of various design parameters on reactor performance.
- Illustrate how COMSOL can be used to minimize the effort on setting up the problem so that more time can be allocated on understanding the interaction of various multiphysics.

1-D Adiabatic Plug Flow Reactor



Transport - Kinetics Model

Mass Balance*:

$$\frac{\partial X_{SO_2}}{\partial z} = \eta \frac{r_{SO_2} \rho_b M_t}{G Y_{0,SO_2}}$$

Energy Balance*:

$$\frac{\partial T}{\partial z} = \eta \frac{r_{SO_2} (-\Delta H_{SO_2}) \rho_b}{G C_{Pmix}}$$

Momentum Balance*:

$$\frac{\partial P}{\partial z} = \frac{1-\varepsilon_b}{\varepsilon_b^3} \frac{G^2}{d_p \rho_g g_c} \left(1.75 + \frac{150(1-\varepsilon_b)}{Re_p} \right)$$

Reference: Azizollah Nodehi, Mohammad Ali Mousavian.Chemical Engineering Technology, 2006. 29(1): p. 84-90.

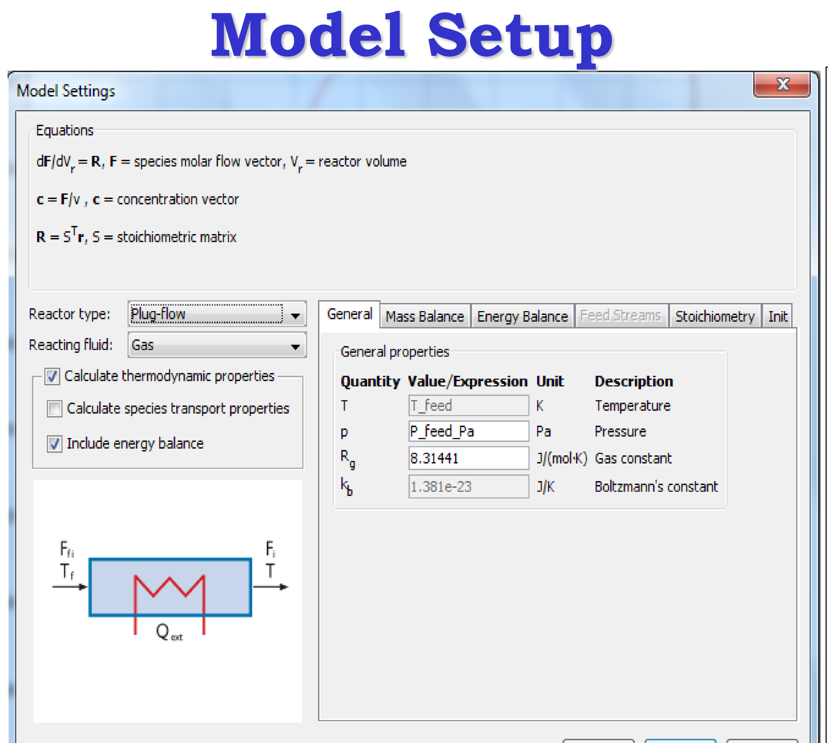
SO_2 Oxidation Kinetics:

$$r = \frac{k_1 p_{O2} p_{SO2} \left(1 - \frac{p_{SO3}}{p_{SO2} \sqrt{p_{O2}} K_p} \right)}{22.414 (1 + K_2 p_{SO2} + K_3 p_{SO3})^2}$$

(Collina *et al*, 1971) T = 420 to 590°C

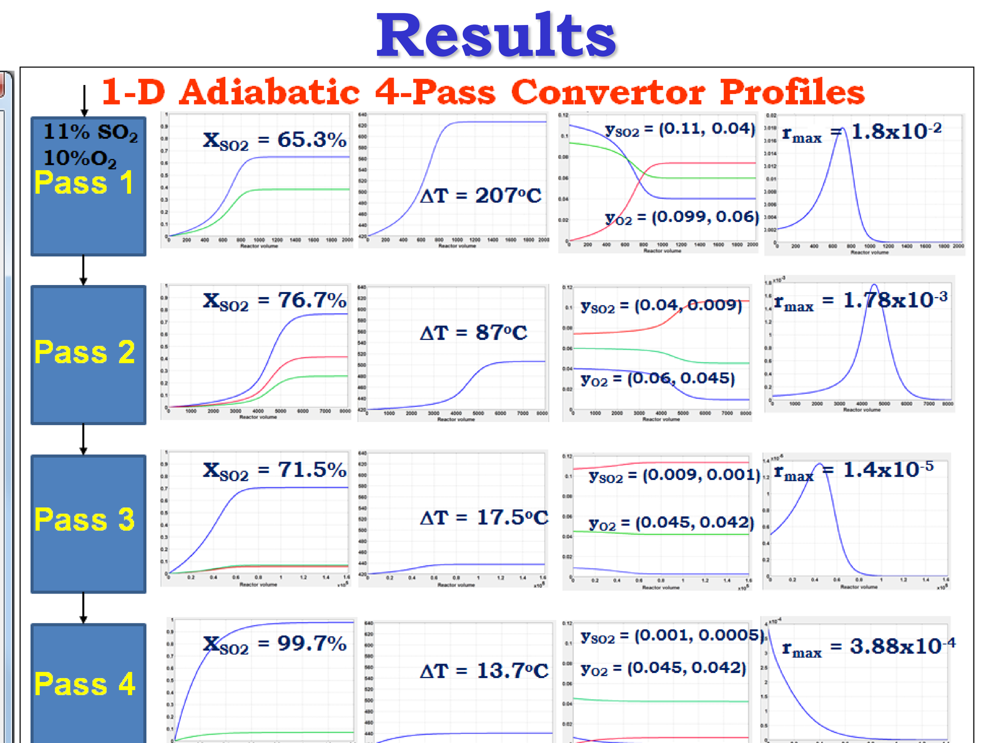
Reaction Engineering Lab Model

Model Setup



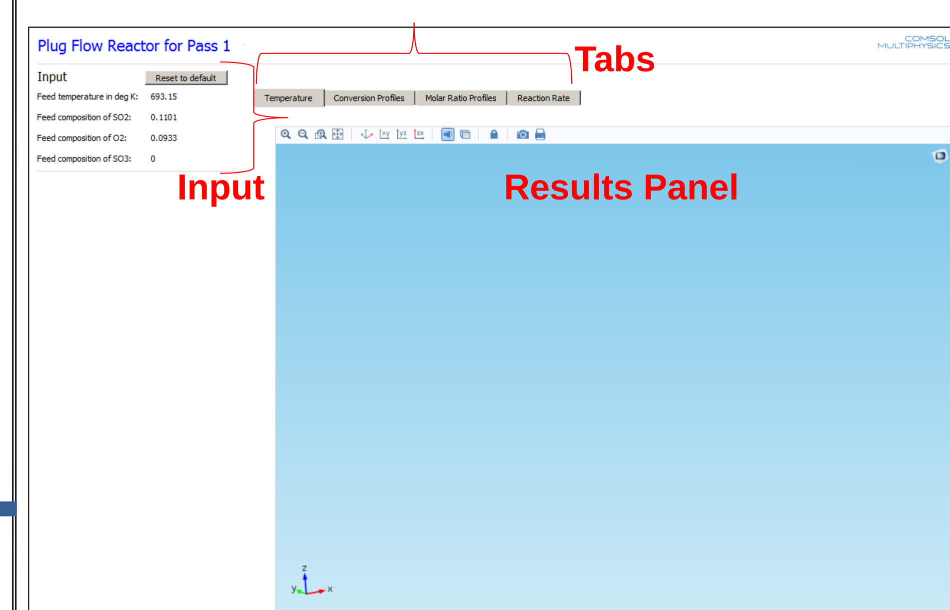
Results

1-D Adiabatic 4-Pass Convertor Profiles

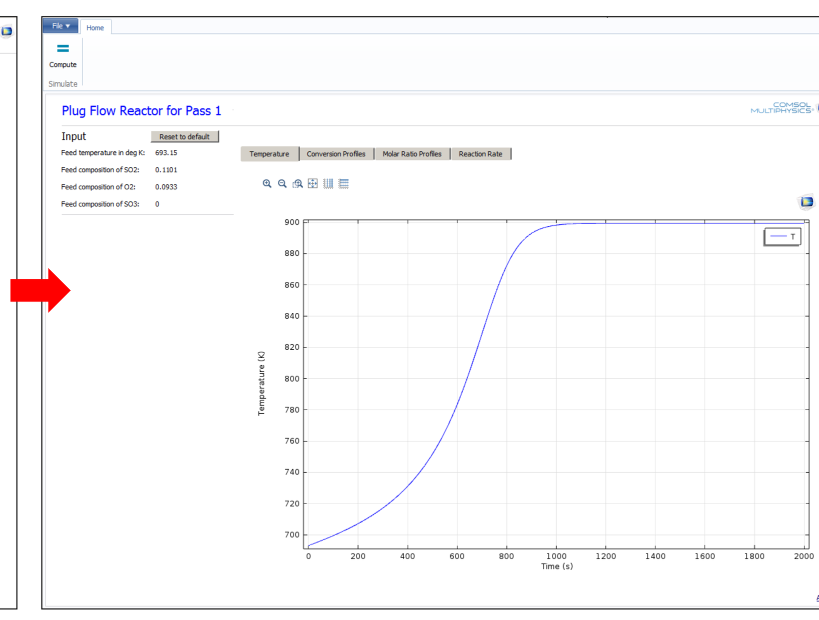


COMSOL Application Results

User Interface

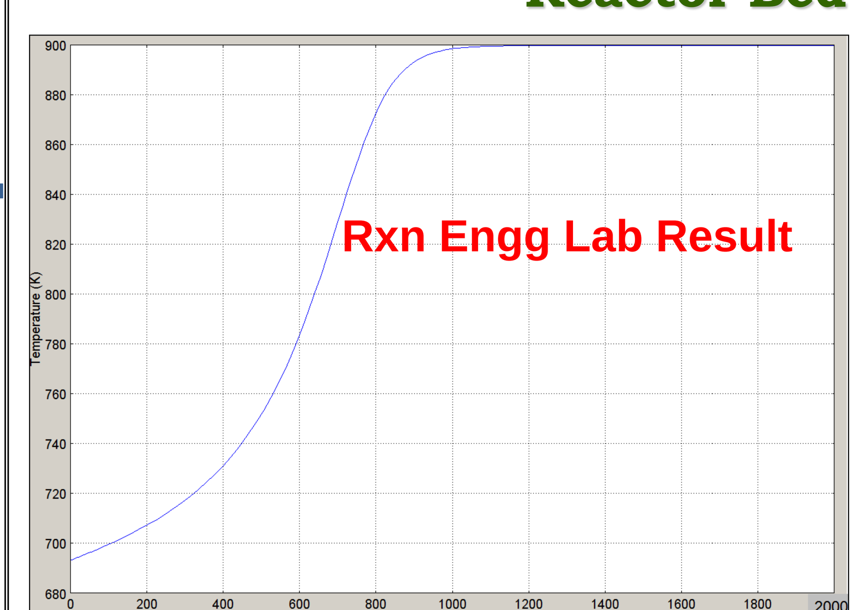


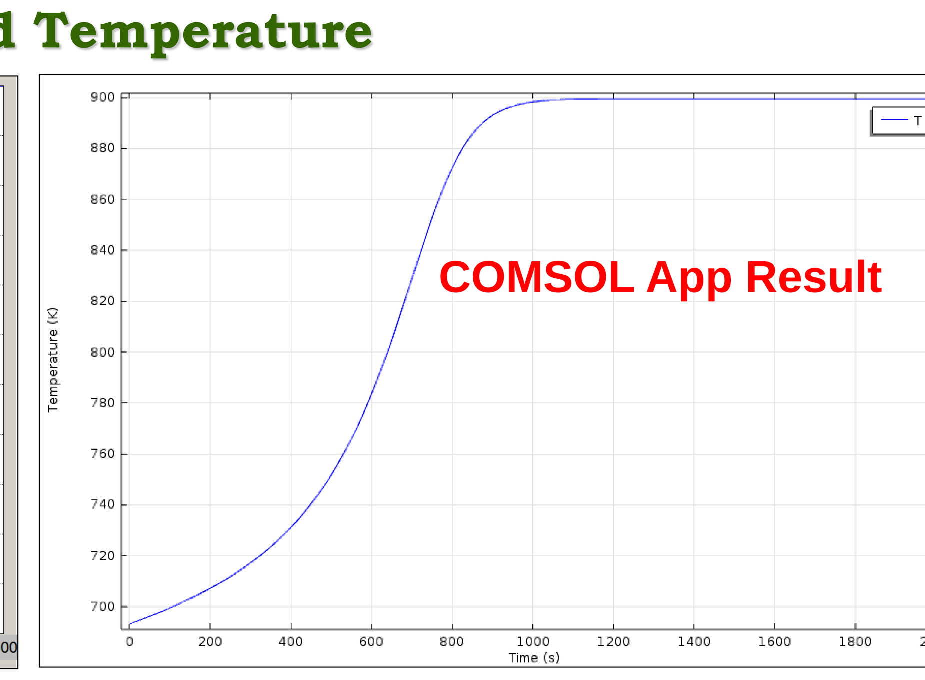
Model Application



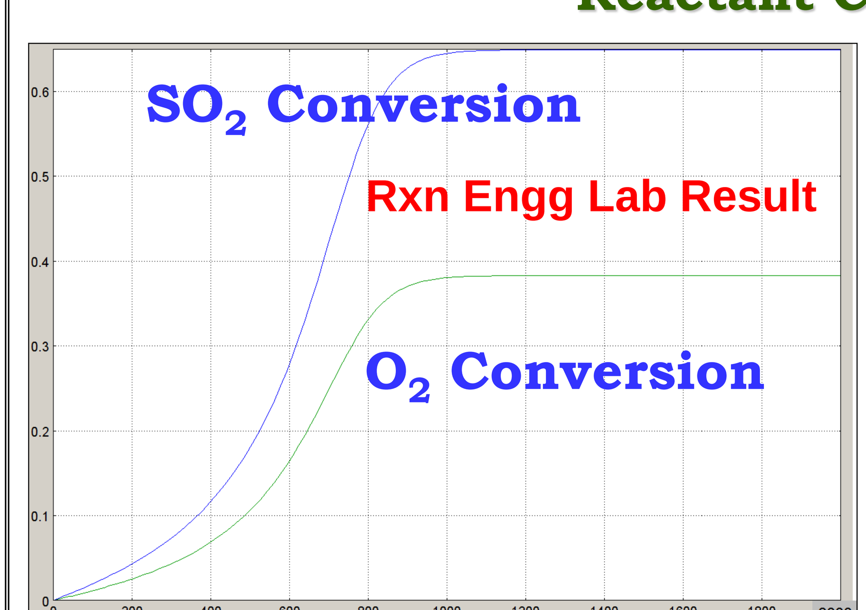
Gas Temperature, SO_2 Conversion, Species Molar Ratio and Reaction Rate Profiles

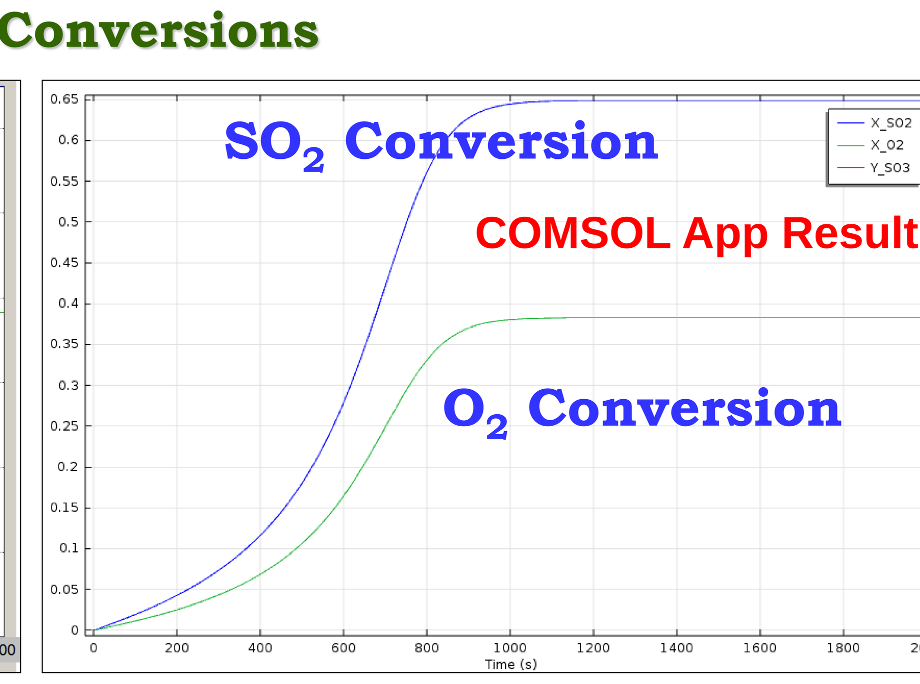
Reactor Bed Temperature



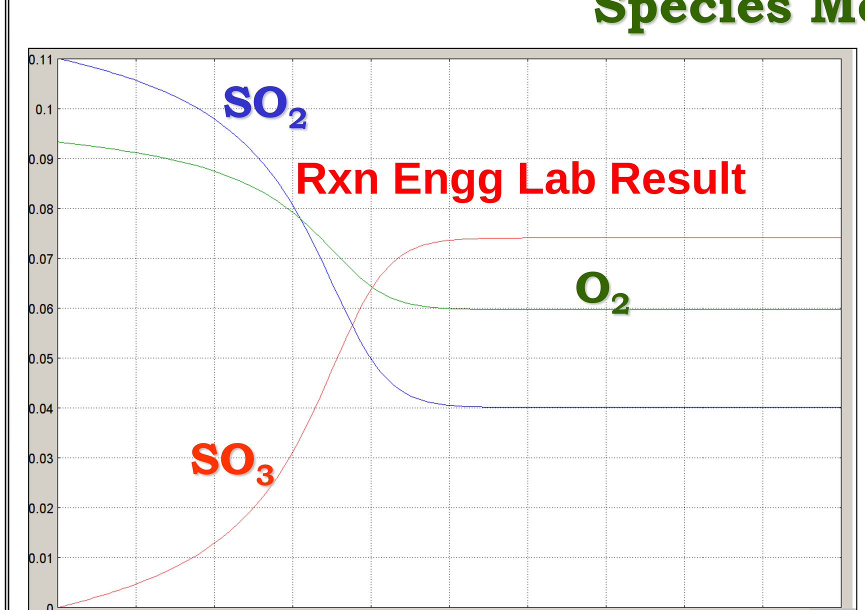


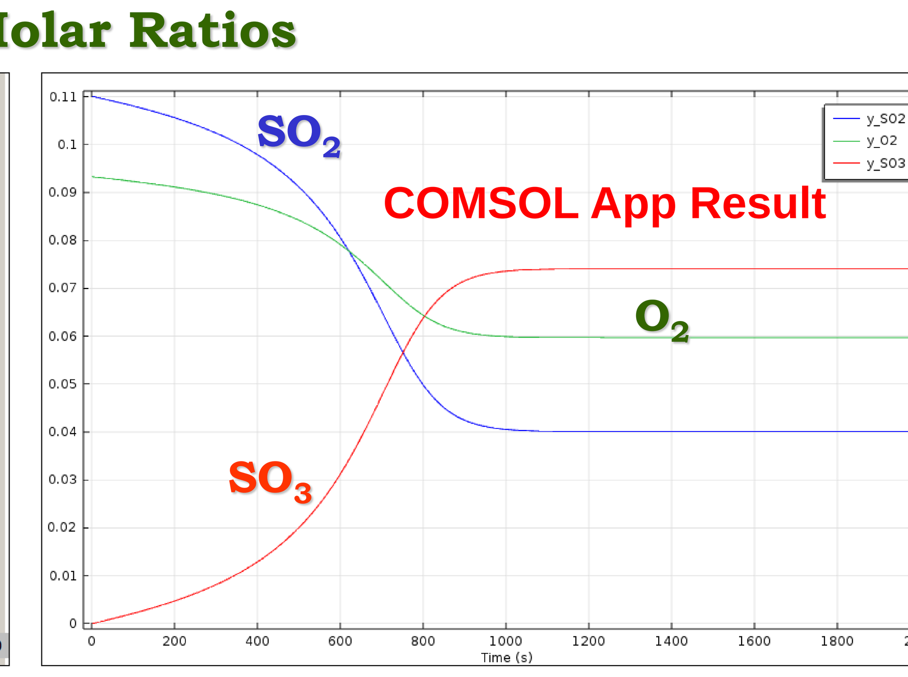
Reactant Conversions



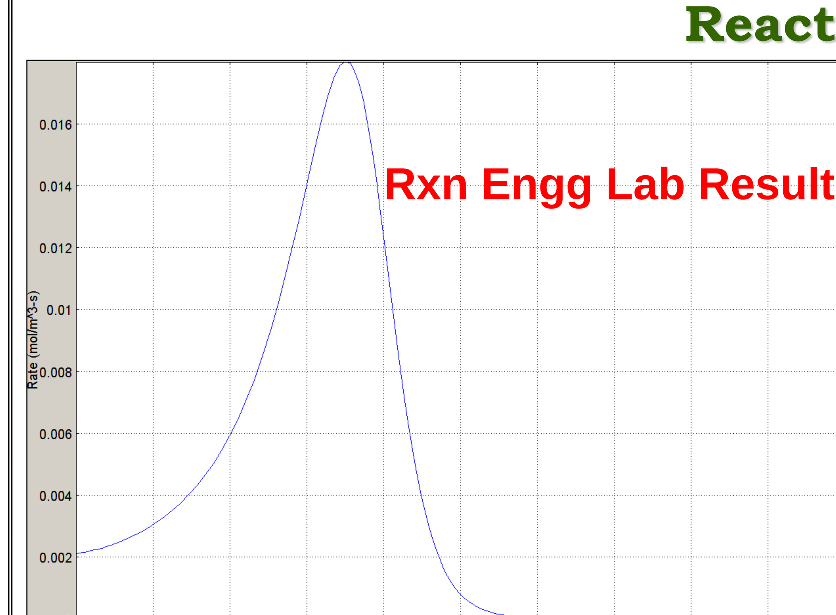


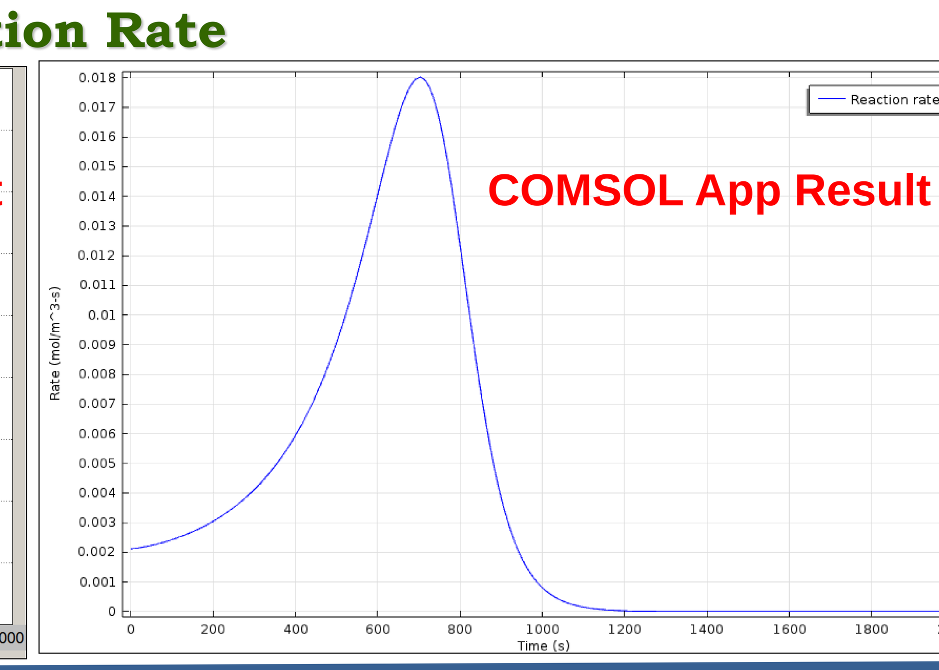
Species Molar Ratios





Reaction Rate





Conclusions

- The 1-D adiabatic plug flow reactor model originally simulated using COMSOL Reaction Engineering Lab 3.5a was successfully recreated using *COMSOL Application Builder*. This allows end-users of the model simulation to study the effect of various system parameters on reactor performance as part of reactor design analysis.
- This application reduces the complexity involved in the COMSOL reactor model setup by end-users while also allowing flexibility in adding additional advanced features to the App as these are developed.