Reactor technology, TKP 4145, project 1

In the manufacture of sulfuric acid from sulfur, the first step is the burning of sulfur in a furnace to form sulfur dioxide:

$$S + O_2 \rightarrow SO_2$$

Following this step, the sulfur dioxide is converted to sulfur trioxide, using a catalyst:

$$SO_2 + \frac{1}{2}O_2 \rightarrow SO_3$$

A multi-tube reactor might be applied for the latter step. You are going to simulate this reactor. It is here sufficient to simulate only one tube. Plug-flow can be assumed, since the tubes are long and thin. Effects like temperature change and pressure drop in the reactor should be included, and all necessary data for doing the calculations are given.

You should develop stationary differential equations for how the <u>total pressure</u>, <u>temperature</u> and <u>gas velocity</u> as well as <u>partial pressures</u> of the components change in the axial direction of the reactor. Then implement the equations in Matlab. The respective variable values are found by integration along the in-dependable variable which is the reactor length.

First, formulate the necessary differential- and algebraic equations. Then implement the equations in Matlab. An example of how these equations are solved in Matlab are given in chapter 6.1 in the "Fixed Bed Reactors" compendium.

The paper should include a complete set of equations, print-outs of the Matlab implementation and results of the simulation.

Information

$$
\begin{aligned}
\text{Feed} &= 995.38\,\text{mol/s} \\
\text{Feed per tube} &= 995.38/4631\,\text{mol/s} = 0.2149\,\text{mol/s} \\
L &= 6.096\,\text{m} \\
T^{\text{out}} &= 702.6\,\text{K (temperature outside in cooling media)} \\
\epsilon &= 0.45 \\
\rho_0 &= 0.865\,\text{kg/m}^3 \\
P_0 &= 2\,\text{atm} = 202650\,\text{Pa} \\
D_p &= 0.004572\,\text{m} \\
R_0 &= 0.0353\,\text{m} \\
\mu &= 3.7204 \cdot 10^{-5}\,\text{kg/(m} \cdot \text{s)} \\
U &= 56.783\,\text{J/(m}^2 \cdot \text{s} \cdot \text{K)} \\
A_c &= 0.00392\,\text{m}^2 \\
T_0 &= 777.78\,\text{K} \\
&\text{and} \quad 666.67\,\text{K} \\
\rho_c^{\text{bulk}} &= 541.42\,\text{kg}/\,m^3 \\
P_{\text{SO}_2,0} &= P_0 \cdot 0.11 = 22291.5\,\text{Pa} \\
P_{\text{O}_2,0} &= P_0 \cdot 0.1 = 20265\,\text{Pa} \\
P_{\text{SO}_3,0} &= 0 \text{ should be set to f.ex } \ 10^{-10} \text{ to avoid division by 0 in the reaction rate.}
\end{aligned}
$$

Equilibrium constant is

$$K_p\left[\mathrm{Pa}^{-1/2}\right] = 3.142\cdot 10^{-3}\exp\left(\frac{98325}{RT}-11.24\right) \qquad T \text{ i K}$$

The reaction rate “constant” is given as

$$k\left[\frac{\mathrm{mol}\,(\mathrm{SO_2})}{\mathrm{kg}(cat)\mathrm{s}\cdot\mathrm{Pa}}\right] = 9.8692\cdot 10^{-3}\exp\left(\frac{-97782}{T}-(110.1\ln T)+848.1\right) \qquad T \text{ i K}$$

The reaction rate

$$r=-r_{\mathrm{SO_2}}=k\sqrt{\frac{P_{\mathrm{SO_2}}}{P_{\mathrm{SO_3}}}}\left[P_{\mathrm{O_2}}-\left(\frac{P_{\mathrm{SO_3}}}{K_pP_{\mathrm{SO_2}}}\right)^2\right]$$

Heat capacity

$$\begin{aligned}
C_{p\mathrm{SO_2}} &= 30.178+42.452\cdot 10^{-3}T-18.218\cdot 10^{-6}T^2\\
C_{p\mathrm{O_2}} &= 23.995+17.507\cdot 10^{-3}T-6.628\cdot 10^{-6}T^2\\
C_{p\mathrm{SO_3}} &= 35.634+71.722\cdot 10^{-3}T-31.539\cdot 10^{-6}T^2\\
C_{p\mathrm{N_2}} &= 26.159+6.615\cdot 10^{-3}T-2.889\cdot 10^{-7}T^2
\end{aligned}$$

med C_p i J/(mol $\cdot$ K) and T i K.
Reaction energy

$$\Delta H_R(699.8\mathrm{K}) = -98787.5\,\mathrm{J/(mol\,SO_2)}$$

The reaction energy at a specific temperature can be calculated from

$$\Delta H_R(T)=\Delta H_R^\circ(T_R)+\Delta\alpha(T-T_R)+\frac{\beta}{2}\left(T^2-T_R^2\right)+\frac{\gamma}{3}\left(T^3-T_R^3\right)$$

where

$$\begin{aligned}
\Delta\alpha &= \alpha_{\mathrm{SO_3}}-0.5\alpha_{\mathrm{O_2}}-\alpha_{\mathrm{SO_2}}=35.634-0.5\cdot 23.995-30.178=-6.5415\\
\Delta\beta &= 0.02057\\
\Delta\gamma &= -1.0011\cdot 10^{-5}
\end{aligned}$$

n_{t0} is feed per cross-section area, that is

$$n_{t0}=\frac{0.2149}{0.00392}\frac{\mathrm{mol}}{\mathrm{m^2\cdot s}}=54.8214\frac{\mathrm{mol}}{\mathrm{m^2\cdot s}}$$

The inlet velocity can be found by using

$$u_0[\mathrm{m/s}]=\frac{n_{t0}RT_0}{P_0}$$