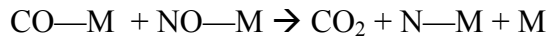


Figure 1.

- 1) The catalytic reaction ($A \rightarrow B$) takes place within a fixed bed containing spherical porous catalyst X22. Figure 1 shows the overall rates of reaction at a point in the reactor as a function of temperature for various entering total molar flow rates, F_{T0} .
 - a) Is the reaction limited by external diffusion?
 - b) If your answer to part (a) was “yes,” under what conditions [of those shown (i.e. T , F_{T0})] is the reaction limited by external diffusion?
 - c) Is the reaction “reaction-rate-limited”?
 - d) If your answer to part (c) was “yes,” under what conditions [of those shown (i.e. T , F_{T0})] is the reaction limited by the rate of the surf
 - e) Is the reaction limited by internal diffusion?
 - f) If your answer to part (e) was “yes,” under what conditions [of those shown (i.e. T , F_{T0})] is the reaction limited by the rate of internal diffusion?
 - g) For a flow rate of 10 mol/hr, determine (if possible) the overall effectiveness factor, Ω , at 360 K.
 - h) Estimate (if possible) the internal effectiveness factor, η , at 367 K.
 - i) If the concentration at the external catalyst surface is 1 mol/L, calculate (if possible) the concentration at $r = R/2$ inside the porous catalyst at 367 K.
 - j) If the reactor must achieve a conversion $X=0.05$, qualitatively sketch how the length of the reactor will have to vary with T and with F_{T0} . Assume the reactor is isothermal.

- 2) A large fraction of all the platinum-group metals that have ever been mined currently reside in catalytic converters on automobiles. As noble metals prices rise (prices remain near record high levels) and the number of vehicles in the world increases, it is imperative to minimize the amount of catalyst employed, while still meeting the emissions regulations. Your object in this problem is to first build a Matlab simulation of a catalytic converter, and then explore the geometrical tradeoffs involved that affect the total amount of catalyst employed.

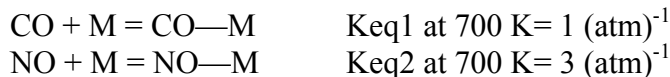
The input to the converter is the car exhaust stream; when it is running fuel-rich (e.g. during acceleration) it is 1200 moles/hr of N_2 , 200 moles/hr of CO_2 , 200 moles/hr of H_2O (steam), 20 moles/hr CO , and 4 moles/hr NO all at $T=700$ K and a total pressure of 1 atm. The most difficult requirement is that output needs to be < 0.4 moles/hr of NO . Assume that the rate-limiting (and essentially irreversible) elementary step is



Rate at 700 K = $(400 \text{ mole/hr-m}^2) \theta_{NO-M} \theta_{CO-M}$ (Area of noble metal/ volume porous material)

Rate has units of mol/hr-m^3 of porous material.

Where M is a noble metal site and the fraction of the surface covered by $CO-M$ and $NO-M$ is given by Langmuir-Hinshelwood equilibria:



The $N-M$ formed in the rate-controlling step rapidly combine to make and release N_2 .

For the purposes of this problem you can neglect the binding by the other gas-phase species at this temperature. (In the real system there are several other complications...). To make the numerical solution easier, we suggest that you assume that the partial pressure of CO is constant inside any pore, i.e.

$$[CO(\text{inside pore})] = [CO, s]$$

and that you also assume that $K_{eq2} * P_{NO}$ is negligible compared to $K_{eq1} * P_{CO}$. This is approximately correct even if the chemistry is fast because the CO is present in excess, and in any case $K_{eq2} * P_{NO}$ is always $\ll 1$. If you are a careful engineer, you can check the validity of these approximations after you have a solution in hand.

The converters are monolithic reactors, you can approximate the geometry as a lot of 8 mm i.d. pipes in parallel, with each pipe's walls lined with a thin layer of porous material (0.1 m^2 platinum/ ml porous material).

Assume the reactor is isobaric and isothermal.

Diffusivity of all species in bulk, $D = 1e-8 \text{ m}^2/\text{s}$

Diffusivity of all species in pores, $D_e = 1e-9 \text{ m}^2/\text{s}$

Assume gas density and viscosity constant along reactor at

$$\text{Density} = 0.5 \text{ kg/m}^3$$

$$\text{Viscosity} = 3 \times 10^{-5} \text{ Pa}\cdot\text{s}$$

Use the boundary layer approximation:

$$\Delta = 0.001 \text{ m} / (\text{Re}^{0.5})$$

$$\text{Re} = \text{density} \cdot (\text{superficial velocity}) \cdot \text{diameter} / \text{viscosity}$$

Use mass transfer approximation:

$$k_c = D / \Delta$$

- a) Rewrite the rate law so it is first order with respect to the NO concentration in the gas within the catalyst pores. It should have the form:

$$\text{Rate} = k' RT * [\text{NO}]$$

In which k' is derived from equilibrium balances and given k and area/volume term.

- b) Derive the Thiele modulus assuming the thin porous layer can be modeled as a slab. Derive the concentration profile of the NO inside the pore. What is the effectiveness factor?
- c) Use a flux balance to find the overall effectiveness factor, ω , for the reaction.
- d) Using your overall effectiveness factor, which allows you to write the reaction rate using the bulk NO and CO concentrations in the pipe, run a simulation for this base case: the porous layer is 1 μm thick, the pipes are 20 cm long, and there are 2000 identical pipes in parallel. Does this achieve the emission target for NO?
- e) Compute how the NO conversion varies if you double the thickness of the porous layer.
- f) Compute how the NO conversion varies if you double the number of parallel pipes.
- g) Compute how the NO conversion varies if you double the length of the pipes.
- h) Make a guess at a design that would achieve the same or better NO conversion as the base case but uses less noble metal. Run a simulation for this case to see if your estimate is right. Would the pressure drop be a lot different in your design than in the base case? (You do not need to simulate the pressure drop.)