Computer-Aided Reactor Design

Rechnерübung zur Vorlesung
Reaktordesign – Betrieb und Auslegung chemischer Reaktoren

version 1.5 – 21st May 2010

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Scope and Instructions

Scope

The scope of this course is to give the students an enhanced understanding of the theory of chemical reactors and enhanced skill in formulation and analysis of mathematical models in chemical engineering. The exercises and the computer laboratory exercises aim to enhance problem solving skills, both with and without computer usage. After you have worked through this course you should be able to:

- Use the principles, relationships and patterns of chemical reaction engineering for qualitative reasoning.
- Detect and analyse problems, which may be solved by the methods of chemical reaction engineering.
- Enhanced understanding of the theory of chemical reactors including formulation of mathematical models and their solution using computers.
- Transform calculation problems in chemical reaction engineering into mathematical models and, if necessary choose a numerical method for solving those models and, if necessary, choose suitable ready-made software and carry out the calculations on a computer.

Instructions

This course requires basic knowledge of chemical reaction engineering as well as basics in mathematics and numerical methods. All three „pillars“ will be established either in this practical course or in the corresponding lectures on „Reaktordesign – Betrieb und Auslegung chemischer Reaktoren“.

Please read and follow the rules listed below for this practical course carefully:

- The computer assignments are carried out in groups of 2 (preferably). The groups are formed at the first class problem meeting and they are kept throughout the course.
- Unless you register for the course, your credits cannot be reported. In order to register, simply fill in and sign registration card you’ll receive at the very first lecture.
- We recommend working with Scilab.
- You are required to submit all your work to get full credit, including any Scilab files that you have used. These may be emailed to the e-mail adresses listed on the title page. The sent Scilab files serve as supplementary material and are not acceptable in lieu of written/printed assignment.
Submit your own work only. No copying. Start each new question on a fresh page. It is implied, that in all types of group assignments, all group members participate in the work, understand the solutions and computer programs and consequently are able to outline the solutions, use the computer programs and answer questions. All group members must therefore sign individually the cover attached to each assignment to be handed in. Do not sign if you cannot fulfil this responsibility!

- The assignment is due by the end of the class on the due date.
- Failure to abide by the instructions will result in loss of credit.
Chapter 1

Homogeneous Reactor Models

1.1 Batch Reactor

The design equation for a batch reactor, in the limit of constant volume, is:

\[ \frac{dC_j}{dt} = R_j \]  
(1.1)

The rate of production of each component \( R_j \) is given by:

\[ R_j = \sum \nu_{ji} r_i \]  
(1.2)

If only one reaction is needed to describe the chemical transformations, the design equation can be integrated to give an analytical solution. If more than one linearly independent reaction is needed to describe the chemical transformations, a set of design equations will be needed to be solved numerically. This set of equations will not be greater than the number of components, and it could be less.

To illustrate the analytical solution consider a simple reversible first-order reaction:

\[ A \rightleftharpoons B \quad r = -\frac{dC_A}{dt} = k_1 \cdot C_A - k_2 \cdot C_B \]  
(1.3)

Introducing the stoichiometry into the rate equation we can eliminate \( C_B \):

\[ -\frac{dC_A}{dt} = (k_1 + k_2) \cdot C_A - k_2 \cdot (C_{A0} + C_{B0}) \]  
(1.4)

Therefore the rate depends only on the initial concentration of both species, the stoichiometry and the forward and reverse rate constants. Integrating this rate equation between the limits of \((C_{A0})\) and \((C_A,t_{\text{batch}})\) gives us the following analytical solution of \( C_A \):

\[ C_A = \frac{k_2}{k_1 + k_2} \cdot (C_{A0} + C_{B0}) + \frac{k_1 \cdot C_{A0} - k_2 \cdot C_{B0}}{k_1 + k_2} \cdot e^{-((k_1+k_2)t)} \]  
(1.5)

The concentration of \( C_B \) can be expressed in an identical way. More generally, we could write for any component in an isothermal batch reactor

\[ C_j(t) = f(\text{stoichiometry, initial conditions, kinetics}) \]  
(1.6)

If any of these change, the exact functional dependence in Equation [1.6] will change. The changes may necessitate reevaluating the integral. Alternately, a numerical solution can be
explored and the parameters can be easily changed to determine their effects. This simple reaction problem can be solved by the solution of an initial value ordinary differential equation (ODE) and a computer program to solve this problem has to be created. In this case we solve

\[-\frac{dC_A}{dt} = \frac{dC_B}{dt} = k_1 \cdot C_A - k_2 \cdot C_B\] (1.7)

subject to the initial conditions of \(C_{A0}\) and \(C_{B0}\).

THE PROBLEM STATEMENT

We want to explore how changing the initial conditions or the value of the (forward) rate constant changes the time for reaching equilibrium conversion. The reference case has \(C_{A0} = 5\) mole/liter, \(C_{B0} = 0\) mole/liter, \(k_1 = 0.5\) liter/(mole \cdot hr) and \(k_2 = 0.2\) liter/(mole \cdot hr).

1. Study the reference case. Can you explain why the curve for the concentration of B appears to be a mirror image of the curve for A?

2. Keeping the rate constant equal to 0.2 liter/(mole \cdot hr) and the concentration of A at 5 mole/liter, examine what happens as the concentration of B is increased.

3. Now explore what happens as the value of the rate constant is changed. Can you explain why increasing the value has the effect it does?

4. Now consider a possible pathway for species B to form species C:

\[A \rightleftharpoons B \rightarrow C\] (1.8)

How does the differential equation for \(C_B\) change? Consider a rate constant of \(k_3 = 0.05\) liter/(mole \cdot hr). How does the time dependent concentration profile of species B look like? How does the maximum in \(C_B\) change if we increase \(k_3\) to 0.2 liter/(mole \cdot hr)?
1.2 CSTR and PFR

In this section we will explore how to solve problems for a single steady state CSTR involving multiple reactions. We will also explore how closely one can approach the performance of a PFR with a finite number of identical CSTRs in series. Consider the following reaction sequence:

\[ \text{D} \leftarrow \text{A} \rightleftharpoons \text{B} \rightarrow \text{C} \quad (1.9) \]

where the values for the rate constants are those at 400 °C. The reaction rates are given in the following way:

\[ r_1 = k_\text{f} \cdot C_A - k_r \cdot C_B \quad (1.10) \]

\[ r_2 = k_2 \cdot C_B \quad (1.11) \]

\[ r_3 = k_3 \cdot C_A \quad (1.12) \]

For multiple reaction problems, the design equation for a steady state CSTR

\[ C_j \dot{V}_0 - C_j \dot{V}_{\text{out}} + R_j V_R = 0 \quad (1.13) \]

is written for each component, where

\[ R_j = \sum_{i} \nu_{ij} r_i \quad (1.14) \]

When \( \dot{V}_0 = \dot{V}_{\text{out}} \), the set of algebraic equations is solved for \( C_j \). If all of the reactions are first-order reactions, the set of equations will be linear and you should seek an analytical solution to the problem. This example involves first order reactions for each reaction so the material balances will all be linear equations. Therefore it will be possible to rearrange the materials balances and sort them such that a matrix representation of the balances of the following form results

\[ AC = C_0 \quad (1.15) \]

where \( C \) and \( C_0 \) are the component concentration and component feed concentration matrices. This problem can now easily be solved with the Scilab command \( C = A \backslash C_0 \).

THE QUESTIONS

1. Develop the set of algebraic equations that will permit you to determine the concentration of A, B, C, and D in the effluent of a 3 m³ CSTR operating at 400 °C (as you learned in class). The entering concentration of A is 0.35 mole/m³ and the volumetric feed rate is 1/30 m³/s.
2. A single 3 m$^3$ CSTR and a single 3 m$^3$ PFR have the effluent concentrations listed below. The reference case has $k_{f1} = 0.02$ s$^{-1}$, $k_{r1} = 0.001$ s$^{-1}$, $k_2 = 0.02$ s$^{-1}$ and $k_3 = 0.003$ s$^{-1}$.

<table>
<thead>
<tr>
<th>Component</th>
<th>Effluent Concentration from a CSTR (mole/m$^3$)</th>
<th>Effluent Concentration from a PFR (mole/m$^3$)</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>0.116</td>
<td>0.048</td>
</tr>
<tr>
<td>B</td>
<td>0.072</td>
<td>0.089</td>
</tr>
<tr>
<td>C</td>
<td>0.130</td>
<td>0.172</td>
</tr>
<tr>
<td>D</td>
<td>0.031</td>
<td>0.041</td>
</tr>
</tbody>
</table>

3. Now compute a simulation program to examine the effect of operating CSTRs-in-series on the final effluent concentration. The program should plot the effluent concentration from each CSTR so you can compare the cumulative effect of operation in series with the total volume fixed at 3 m$^3$ to the result in the 3 m$^3$ PFR. Notice how close you approach the PFR performance as the number in series increases. Can you explain why this happens?

(a) How many CSTRs come within 10% of the final effluent concentration of A for the PFR?

(b) How many CSTRs come within 5% of the final effluent concentration of A for the PFR?

(c) How many CSTRs come within 1% of the final effluent concentration of A for the PFR?

4. Plot the concentration versus volume diagram for the PFR.
Chapter 2

Transport Phenomena in Heterogeneous Catalysis (Spherical Catalyst Pellet)

2.1 Introduction – Use of Collocation for the Solution of Boundary Value Problems

Steady-state reaction with diffusion problems lead to second-order ordinary differential equations for one-dimensional situations, such as a spherical pellet. Since one does not know both boundary conditions at the same location, these problems fall into the general class known as boundary value problems. In reaction/diffusion problems we specify the concentration or match the fluxes at the pellet surface for one of the boundary conditions, and specify the gradient at the pellet center for the second boundary condition. In limited cases, such as single reactions, positive order kinetics and isothermal, the reaction/diffusion problem can be solved analytically.

Unfortunately the number of reaction/diffusion problems that can be solved analytically is very limited and numerical approaches are necessary. When the pellet has symmetry and can be reduced to a one dimensional problem, such as a spherical pellet, the collocation approach outlined here will work. If the pellet were a short cylinder, finite element methods or other techniques would be required. The collocation approach could be used for multiple reactions, for complex reaction rate expressions and for nonisothermal pellets. Indeed, collocation methods were used to generate the numerical solutions presented in the text.

Let’s use the analytical solution for a first-order reaction in an isothermal spherical pellet to illustrate the approach and to benchmark our solution. As illustrated in the text the differential equation and boundary conditions are

\[
\frac{d^2 \tau}{d\tau^2} + \frac{2}{\tau} \frac{d \tau}{d\tau} - \Phi^2 \tau = 0
\]

\[
\tau = 1 \text{ at } \tau = 3 \quad \frac{d \tau}{d\tau} = 0 \text{ at } \tau = 0
\]

\[
\tau(\tau) = \frac{3 \sinh \Phi \tau}{\tau \sinh 3\Phi}
\]
Equation 2.2 is plotted in Figure 2.1 for the case where $\Phi = 5$. We see how steep this curve is, meaning it has what appears to be a value of zero and then increases to a value of unity in the outer shell of the sphere. All functions, such as Eqn 2.2 can be expressed as a series of orthogonal functions, such as Fourier series, Legendre polynomials, Hermite polynomials, etc. The steeper the function, the higher the order of polynomial needed to describe it. Then to describe (or fit) the function, we need to select a high enough order and find the coefficients. This is essentially what collocation does.

We approximate the function by passing a polynomial through the function at selected points.

$$c(r) = \sum_{i}^{n_c} a_i c_i(r)$$  \hspace{1cm} (2.3)

where $c_i(r)$ is the $i^{th}$ orthogonal function. In the write up, five points are selected, and they are not sufficient when $\Phi = 5$. Ten points are sufficient as will be shown below. The placement of the points is done by the program \texttt{colloc} in Scilab. If you run \texttt{colloc}, you will find the five points, which are indicated in Figure 2.1, are located at the dimensionless radial positions $R$ (in the \texttt{colloc} program the variable is called $R$)

$$R = [0 \ 0.3381 \ 1.5000 \ 2.6619 \ 3.0000]$$

The derivatives of the polynomial interpolant can be computed as linear combinations of the values at the collocation points

$$\frac{dc}{dr} \bigg|_{r_i} = \sum_{j}^{n_c} A_{ij} c_j$$  \hspace{1cm} (2.4)

$$\frac{d^2c}{dr^2} \bigg|_{r_i} = \sum_{j}^{n_c} B_{ij} c_j$$  \hspace{1cm} (2.5)

For our problem, with five collocation points, there will be five values of $c$.

$$c = [c_1 \ c_2 \ c_3 \ c_4 \ c_5]$$  \hspace{1cm} (2.6)
We now use Equations 2.4 and 2.5 to satisfy the boundary conditions and the differential equation (Equation 2.1) at the appropriate points. We will be writing five algebraic equations and these will be solved simultaneously to find the five values of \( c \) in Equation 2.6. The program set the left-hand sides of these equations equal to a variable \( \text{retval}(n) \) so it will be used here. When running the program, we force the end points to the boundaries. Then the first collocation point \( n = 1 \) is at \( r = R(1) = 0.0 \) and here we must satisfy the boundary condition

\[
\frac{d\bar{c}}{dr} = 0
\]

This can be recast using Equation 2.4

\[
\text{retval}(1) = A_{11}c_1 + A_{12}c_2 + A_{13}c_3 + A_{14}c_4 + A_{15}c_5 \quad (2.7)
\]

or using Scilab syntax

\[
\text{retval}(1) = A(1,:) \ast c
\]

The values of the weighting coefficients \( A \) are generated by the program \text{colloc} based on our instructions to force the boundaries to the end points and that there were five collocation points. For this particular case the matrix \( A \) is given by

\[
A = \begin{bmatrix}
A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\
A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\
A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\
A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\
A_{51} & A_{52} & A_{53} & A_{54} & A_{55}
\end{bmatrix}
\]

\[
A = \begin{bmatrix}
-4.3333 & 4.9294 & -0.88889 & 0.62612 & -0.3333 \\
-1.7746 & 1.2910 & 0.68853 & -0.43033 & 0.22540 \\
0.50000 & -1.0758 & 0.0 & 1.0758 & -0.50000 \\
-0.22540 & 0.43033 & -0.68853 & -1.2910 & 1.7746 \\
0.33333 & -0.62612 & 0.88889 & -4.9294 & 4.3333
\end{bmatrix}
\]

Next we satisfy Equation 2.1 at any collocation point not at a boundary, i.e., \( \tau \neq 0 \) and \( \tau \neq 3 \). The algebraic equation becomes

\[
0 = \sum B_{ij}c_j + \frac{2}{r_i} \sum A_{ij}c_j - \Phi^2c_j
\]

and for collocation Point 2 \((R(2) = 0.3381)\)

\[
\text{retval}(2) = B_{21}c_1 + B_{22}c_2 + B_{23}c_3 + B_{24}c_4 + B_{25}c_5 \\
+ \frac{2}{R_2} A_{21}c_1 + \frac{2}{R_2} A_{22}c_2 + \frac{2}{R_2} A_{23}c_3 + \frac{2}{R_2} A_{24}c_4 + \frac{2}{R_2} A_{25}c_5 \\
- \Phi^2c_2
\]

or using Scilab syntax

\[
\text{retval}(2) = B(2,:) \ast c + \frac{2}{R(2)} \ast A(2,:) \ast c - \Phi^2 \ast c(2) \quad (2.8)
\]
As with the weights for $A$, there is a corresponding $(5 \times 5)$ $B$ matrix of weights for the second derivative that is generated by the program colloc. You can work out the specific forms of the two algebraic equations at the remaining interior collocations points, Point 3 and Point 4. These are represented here using Scilab syntax.

\[
\text{retval}(3) = B(3,:) \ast c + \frac{2}{R(3)} \ast A(3,:) \ast c - \Phi^2 \ast c(3) \tag{2.9}
\]

\[
\text{retval}(4) = B(4,:) \ast c + \frac{2}{R(4)} \ast A(4,:) \ast c - \Phi^2 \ast c(4) \tag{2.10}
\]

Finally at the last collocation point, $R(5) = 3.0$, we have to satisfy the boundary condition that $c = 1$.  $\text{retval}(5) = 1 - c(5)$ \tag{2.11}

As an aside, we might equally well apply the boundary condition at the surface $\frac{dc}{dr} = k_m a D_e (1 - c)$ and in Scilab syntax, $\text{retval}(5) = A(5,:) \ast c - \frac{k_m a}{D_e} \ast (1 - c(5))$

At this point the five concentrations in the $c$ vector are found using the Scilab function `fsolve` that minimizes the `retval` vector defined with the five equations, Equations 2.7 to 2.11.

You can explore how this works in the next section 2.2. Figures 2.1 and 2.2 illustrate the simulation for $\Phi = 5$, and five and ten collocation points, respectively. Notice that with ten points you cannot distinguish between the analytical and the numerical solutions. The analytical solution is scaled by the magnitude of $\Phi$ so you should explore the impact of how steep the curve for $c$ is on the necessary number of collocation points. One can always select a large number of collocation points and simply be patient while the computer churns away; having a sense of the steepness of the curves being approximated helps in selecting a number of collocation points.

Figure 2.2: Numerical solution for ten collocation points and the analytical solution when $\Phi = 5$.  

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2.2 First Order Reaction in a Spherical Pellet

The above section 2.1 Introduction – Use of Collocation for the Solutions of Boundary Value Problems describes in considerable detail how collocation is used to solve boundary value problems, such as reaction with diffusion in a spherical pellet. Here we will explore the effect of changing the value of the Thiele modulus on the concentration profile in a spherical pellet for a first-order reaction.

\[ A \rightarrow B \quad r = kc_A \]

As detailed in the text, increasing the value of the Thiele modulus leads to a steeper gradient of the concentration within the pellet. We will see that for even modest values of the Thiele modulus, the concentration within the pellet quickly becomes vanishingly small. Then by exploring this dependence you should get a sense of the importance of this parameter in deciding what is important or controlling in a given situation.

Since there is an analytical solution to this problem,

\[ \overline{c}(\overline{r}) = \frac{3 \sinh \Phi \overline{r}}{\overline{r} \sinh 3\Phi} \quad (2.12) \]

we can compare the numerical solution against the analytical solution. This will allow you to examine how the number of collocation points needs to increase as the concentration profile becomes steeper near the pellet surface.

Note that the curves should be plotted in a semilog format so you can better see the magnitude of the concentrations within the pellet. In the above Figures 2.1 and 2.2 the curves appear to approach zero, but they never do.

As you run the simulation you should be able to separately set the value of the Thiele modulus, \( \Phi \), and the number of collocation points.

**THE QUESTIONS**

1. Change the value of \( \Phi \) from the default. Select values that change by an order of magnitude to see how the concentration varies with \( \Phi \). This should give you a sense of when you could reasonable assume the reaction is kinetically controlled versus diffusion controlled.

2. Make a point of examining a value of \( \Phi = 10 \) and note how small the dimensionless concentration becomes within the pellet. What is the concentration of a gas at 1 atm and 200 °C? What is the absolute concentration within the pellet?

3. Holding \( \Phi \) at the same value, increase the number of collocation points to see how more points are needed to approximate the analytical solution. Notice that with enough points, the fit is very good. You should also notice that as you select more and more collocation points, the computations take longer and longer so there is a price to pay for selecting too many points.
2.3 Diffusion and Reaction in a Spherical Pellet

One does not necessarily know the concentration at the surface of a catalyst pellet. One does know the bulk fluid concentration. Therefore the most general boundary conditions to use in solving the equation of continuity for a first-order reaction

\[
\frac{d^2c}{dr^2} + \frac{2}{r} \frac{dc}{dr} - \Phi^2 \frac{c}{r} = 0
\]  

(2.13)

are

\[
\frac{dc}{d\tau} = B(1 - c) \text{ at } \tau = 3 \quad \text{where } B = \frac{k_m a}{D_e}
\]

(2.14)

and

\[
\frac{dc}{d\tau} = 0 \text{ at } \tau = 0
\]

(2.15)

As with the cases where the surface concentration is specified as the external boundary condition, there are limited situations for which an analytical solution can be found. Recognizing this we seek a numerical solution and will employ the collocation method.

In the above section 2.2 Numerical Approximation to Reaction with Diffusion - First Order Pellet the boundary condition (at Collocation Point 5) was given by

\[
\text{retval}(5) = 1 - c(5)
\]

(2.16)

As explained more fully in section 2.1 we now will simply replace this line of code with

\[
\text{retval}(5) = A(5,:) * c - B * (1 - c(5))
\]

(2.17)

For a catalyst pellet at steady-state the rate of diffusion into the pellet must equal the rate of reaction in the pellet. The collocation solution provides the gradient at the surface and this enables us to compute the value of \( R_{Ap} \). In dimensional form

\[
R_{Ap} = -\frac{D_e}{a} \left. \frac{dc}{dr} \right|_{r=R}
\]

(2.18)

Recasting this into Scilab syntax, and letting the variable npts be the number of collocation points

\[
R_{Ap} = -\left( \frac{D_e}{a} \right) * A(npts,:) * c
\]

We have selected a first-order reaction to examine here since there is an analytical solution and we can compare the numerical solution against the analytical solution. As you run the simulation the program should generate a curve that displays the concentrations at the collocation points and analytical solution, which can be used to compute the rate with

\[
R_{Ap} = -k c_{Aj} \left( \frac{1}{\Phi^2} \left[ \frac{1}{\text{tanh}(3\Phi)} - \frac{1}{3\Phi} \right] \right)
\]

(2.19)
THE PROBLEM STATEMENT

You should examine the impact of the size of the Biot number relative to the Thiele modulus. For this reason, if you make the Thiele modulus too large by selecting a rate constant greater than 100 s$^{-1}$, more collocation points are needed than the program has set. Hence, limit your values for the rate constant!

THE QUESTIONS

1. The program should written for the catalyst properties given in text Example 7.1. If you input a value of $k = 2.8$ s$^{-1}$, you will have a $\Phi = 2.0$. Then by selecting different values for the external mass transfer coefficient $k_m$ (cm/s) you can examine how the surface and bulk fluid concentrations begin to deviate. Set $k_m = 0.1, 1.0$ and100. Notice how the rate changes and the surface concentration differs from the bulk value. Thinking about what the Biot Number represents, does this make sense to you?

2. Work at the extreme of a large Thiele modulus by setting $k = 100$. Study the impact of the same values on $k_m$ and the Biot Number on the profiles and the differences in the bulk and surface concentration. What does this suggest to you about the interplay of internal and external gradients?

3. Make $\Phi$ take on values less than one and prove to yourself that even in this regime external gradients can be present. Remember this the next time you assume the bulk fluid and surface concentrations are equal.
Chapter 3

Heterogeneous Reactor Models
(Fixed Bed Reactor)

3.1 Fixed Bed Reactor

The design equation for a steady-state fixed bed reactor can be written as follows:

$$\frac{dQC_j}{dV} = \sum v_{ji}R_j \quad (3.1)$$

The energy balance can be neglected in terms of an isothermal operation of the reactor. Considering a second order heterogeneous reaction, the reaction rate is given by:

$$A \xrightarrow{k} B \quad r = k \cdot C_A^2 \quad (3.2)$$

This reaction rate is only valid for very small particles, without diffusion limitations. For industrial catalyst pellets it is often necessary to consider diffusion phenomena. The macrokinetic reaction rate is influenced by diffusion of reactants. Therefore the effectiveness factor is introduced into the global design equation:

$$R_A = -\frac{\rho_b}{\rho_p} \cdot \eta \cdot r \quad (3.3)$$

where for a spherical pellet we can write:

$$\eta = \frac{1}{\phi} \cdot \left( \frac{1}{\tanh (3\phi)} - \frac{1}{3\phi} \right) \quad (3.4)$$

with

$$\phi = a \cdot \left( \frac{3kC_A}{2D_e} \right)^{0.5} \quad (3.5)$$

Of course the above macrokinetic reaction rate is only valid if there is no gradient between fluid and external pellet surface concentration. In order to account for a possible gradient collocation can be used to calculate the difference between a reaction with and without such a gradient (see also the collocation primer and chapter 2). Please note, that a dimensioned form of equation 2.1 for a second order reaction, can be written as follows:

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dC_A}{dr} \right) - \frac{k}{D_e} C_A^2 = 0 \quad (3.6)$$

The flux boundary condition with external mass transfer becomes:

\[
\frac{dC_A}{dr} = \frac{k_m}{D_e} (C_A f - C_A)|_{r=R} \tag{3.7}
\]

Finally we have to couple the production rate \( R_A \) in the fluid phase to the production rate inside the particles, where the reaction takes place:

\[
R_A = -\frac{\rho_b}{\rho_p} \frac{D_e}{a} \frac{dC_A}{dr} \bigg|_{r=R} \tag{3.8}
\]

THE PROBLEM STATEMENT

We want to estimate the mass of catalyst required for 70% conversion of A. The gas feed consists of A and an inert, each with molar flowrate of 10 mole/s, the total pressure is 4.0 bar and the temperature is 500 K. The catalyst is a spherical pellet with a radius of 0.39 cm. The pellet density is \( \rho_p = 670 \text{ kg/m}^3 \) and the bed density is \( \rho_b = 590 \text{ kg/m}^3 \). The effective diffusivity of A is \( D_e = 0.0075 \text{ cm}^2/\text{s} \) and may be assumed to be constant. The external mass transfer coefficient is \( k_m = 1.1 \text{ cm/s} \). The rate constant is \( k = 2.55 \cdot 10^5 \text{ cm}^3/(\text{mole} \cdot \text{s}) \).

THE QUESTIONS

1. Estimate the mass of catalyst if you assume the fluid and pellet surface concentrations are equal. Also, use first the analytical approximation of \( \eta \) and utilize afterwards collocation to solve this problem. How many collocation points are needed to give the same result as for the analytical solution?

2. Estimate the mass of catalyst if you account for a possible gradient between the fluid concentration and the external surface concentration.