TKP4145 Reactor Technology, Project 3

In this project you are asked to simulate the steam methane reforming (SMR) process within a spherical porous pellet. The SMR reactions take place on the active sites within the pores of the particles, hence there will be heat- and mass transfer between the gas in the bulk and the pores of the catalyst pellets. Derive the governing equations comprising a set of differential-algebraic equations (DAE) on mass basis. The pellet equations are naturally formulated in spherical coordinates, and due to center symmetry only the r-coordinate is considered.

The pellet equations should be discretized by use of finite difference method. The diffusion terms can be discretized by a second order scheme. The resulting set of algebraic equations can be solved by several methods:

1. By the 2nd order Newton-Raphson method. You may code it yourself or possibly using the `fsolve` function in MATLAB.

2. By the 1st order Picard or 2nd order Newton methods. That is, linearizing the equations by the Picard or Newton methods and put the discretized equations into the vector form, $A\bar{x} = \bar{b}$. In the latter case the system can be iterated in MATLAB using a `while` loop and the $\bar{x} = A\backslash\bar{b}$ command updating the $A(\bar{x})$and $\bar{b}(\bar{x})$ after each iteration.

The set of equations should be implemented in MATLAB. The report handed in must contain the complete set of equations, printout of the MATLAB implementation and the results from the simulations in form of 2D-plots of the variable fields.

Boundary Conditions

$$\left.\frac{\partial \omega_i}{\partial \xi}\right|_{\xi=0} = 0$$

$$-D_i \left.\frac{\partial \omega_i}{\partial \xi}\right|_{\xi=r_p} = k_i \left(\omega_i - \omega_{i,bulk}\right)$$

$$\left.\frac{\partial T}{\partial \xi}\right|_{\xi=0} = 0$$

$$-\lambda_p \left.\frac{\partial T}{\partial \xi}\right|_{\xi=r_p} = h \left(T - T_{bulk}\right)$$

The catalyst data are given in table 1:

Table 1: Catalyst data

Catalyst density (ρ_b) :	2355.2	$[kg/m^3]$
Particle diameter (d_p) :	0.0173	$[m]$
Void in bulk (ϵ_b) :	0.528	
Heat transfer coefficient:	30000	$[W/m^2K]$
Particle conductivity (λ_p) :	50	$[W/mK]$

The operating conditions are given in the function *constant.m*. However, a more representative operating temperature for the reactor might be obtained by setting to 900 K.

Some useful relations are given in appendices 1-2.

Predefined functions in MATLAB

Some functions are implemented to simplify the work and these can be found on *itslearning*. You may still use the functions given for project 2, in addition a new function can be obtained.

- `masscoef.m` - A function which computes the binary diffusivities and the mass transfer coefficients for the different species.

Appendix I: Calculation of diffusivities and mass transfer coefficients

The molecular diffusivities may be computed from the relation:

$$D_i = \frac{1.0 \times 10^{-4} \left(0.00143 \cdot T^{1.75}\right)}{\left(P \cdot M_{ib}^{1/2} \left(\left(\sum \nu_i\right)^{1/3} + \left(\sum \nu_b\right)^{1/3}\right)\right)^2} \qquad (1)$$

in which M_{ib} is given as:

$$M_{ib} = 2\left(\frac{1}{M_a} + \frac{1}{M_b}\right)^{-1} \qquad (2)$$

The molecular constants $\sum \nu_b$ are listed in table 2.

Table 2: Molecular sums for diffusivity computations

i	$\sum \nu$
CH_4	25.14
CO	18.01
CO_2	26.90
H_2	6.12
H_2O	13.10
N_2	18.50

The mass transfer coefficients may for example be computed from the empirical relation:

$$k_i = u_z^s \times 1.17 \times \left(\frac{D_p u_z^s \rho_g}{\mu}\right)^{-0.42} \times \left(\frac{\mu}{\rho_g D_i}\right)^{-0.67} \qquad (3)$$

This parameter is computed by the `masscoef.m` function.

Symbols

k_i	$[m/s]$	Mass transfer coefficient, gas-solid
ν	$[-]$	Diffusion volumes