Example 6: Adiabatic Radial Flow Reactor (steady state)

Partial oxidation of methanol to formaldehyde

$CH_3OH + 1/2\ O_2 \longrightarrow CH_2O + H_2O$	R0
$CH_2O + 1/2\ O_2 \longrightarrow CO + H_2O$	R1

This example is based on Example 11 in Rase (1990). This model is for a radial flow reactor. The input data for this example are the same as given in Example 5 with the exception of the Feed Conditions and Reactor geometry. Therefore, the duplicate data are hidden to reduce printing.

▶ Hidden Area 1

Feed conditions

$T_0 := 525 \cdot K$ inlet temperature

$Ptot := 4 \cdot atm$ inlet pressure

$G_0 := .8 \cdot \frac{gm}{cm^2 \cdot s}$ mass flux

$M_f := molf \cdot Mw$ molecular weight of feed mixture

mole fractions in feed

$$molf := \begin{pmatrix} .0901 \\ .0991 \\ 0.0132 \\ 0.0051 \\ .0006 \\ .7918 \end{pmatrix}$$

$$\sum molf = 1$$

$$M_f = 0.029 \frac{kg}{mol}$$

Inlet conditions, dimensionless

$\omega_0 := \frac{\overrightarrow{(molf \cdot Mw)}}{M_f}$ convert mole fractions to weight fractions

$\theta_0 := 1$ feed temperature

$p_0 := 1$ *pressure*

Reactor geometry

$r_0 := 2 \cdot m$

$fluid := \text{"gas"}$ fluid is "gas" or "liquid"

$r_1 := 3 \cdot m$

Hidden Area 2

Adiabatic reactor model

$act := .2$

$$D(\eta, Y) := \begin{bmatrix} Rxn\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}, act\right)_0 \cdot Mw_0 \cdot \dfrac{\left[\eta \cdot \left(r_1 - r_0\right) + r_0\right] \cdot \left(r_1 - r_0\right)}{G_0 \cdot r_0} \\ Rxn\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}, act\right)_1 \cdot Mw_1 \cdot \dfrac{\left[\eta \cdot \left(r_1 - r_0\right) + r_0\right] \cdot \left(r_1 - r_0\right)}{G_0 \cdot r_0} \\ Rxn\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}, act\right)_2 \cdot Mw_2 \cdot \dfrac{\left[\eta \cdot \left(r_1 - r_0\right) + r_0\right] \cdot \left(r_1 - r_0\right)}{G_0 \cdot r_0} \\ Rxn\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}, act\right)_3 \cdot Mw_3 \cdot \dfrac{\left[\eta \cdot \left(r_1 - r_0\right) + r_0\right] \cdot \left(r_1 - r_0\right)}{G_0 \cdot r_0} \\ Rxn\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}, act\right)_4 \cdot Mw_4 \cdot \dfrac{\left[\eta \cdot \left(r_1 - r_0\right) + r_0\right] \cdot \left(r_1 - r_0\right)}{G_0 \cdot r_0} \\ Rxn\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}, act\right)_5 \cdot Mw_5 \cdot \dfrac{\left[\eta \cdot \left(r_1 - r_0\right) + r_0\right] \cdot \left(r_1 - r_0\right)}{G_0 \cdot r_0} \\ Qr\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}, act\right) \cdot \dfrac{\left[\eta \cdot \left(r_1 - r_0\right) + r_0\right] \cdot \left(r_1 - r_0\right)}{G_0 \cdot r_0 \cdot Cp\left(submatrix(Y,0,NC-1,0,0), Y_{NC}\right) \cdot T_0} \\ \dfrac{-f_k(\eta) \cdot \left(G_0 \cdot r_0\right)^2 \cdot \left(r_1 - r_0\right)}{d_p \cdot \rho_f\left(submatrix(Y,0,NC-1,0,0), Y_{NC}, Y_{NC+1}\right) \cdot Ptot \cdot \left[\eta \cdot \left(r_1 - r_0\right) + r_0\right]^2} \cdot \left(\dfrac{1-\varepsilon}{\varepsilon^3}\right) \end{bmatrix}$$

$NZ := 1000$ number of intervals in z to be saved

$Y_0 := stack\left(\omega_0, \theta_0, p_0\right)$ the initial value of Y

$S := Rkadapt\left(Y_0, 0, 1, NZ, D\right)$

ODE integration routine, the arguments are:

- initial value vector for Y
- initial value for z
- final value for z
- NZ
- function for right hand side of ODEs

results

$Z := S^{\langle 0 \rangle}$ independent variable values

$j := 0 .. NZ$ axial index variable

$n := 0 .. NC - 1$ component index

$\omega_{n,j} := \left(S^{\langle n+1 \rangle}\right)_j$ weight fractions

$\sum \omega^{\langle NZ \rangle} = 1$

check accuracy at reactor exit
sum weight fractions = 1?
even a small error may be an indication of model error

$\theta := S^{\langle NC+1 \rangle}$ temperature

$p := S^{\langle NC+2 \rangle}$ pressure

Fig E6.1: Temperature

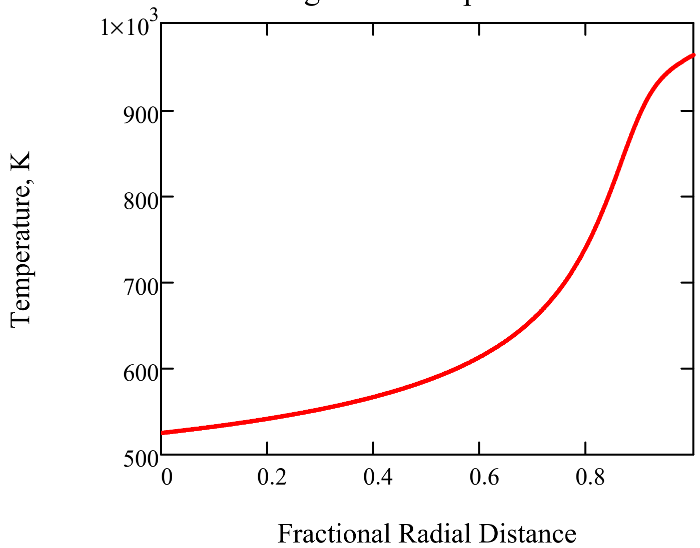


Fig E6.2: Mass Fractions

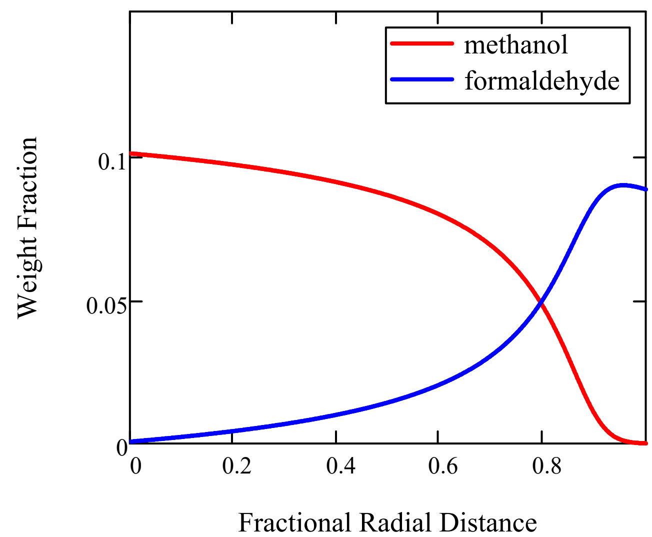
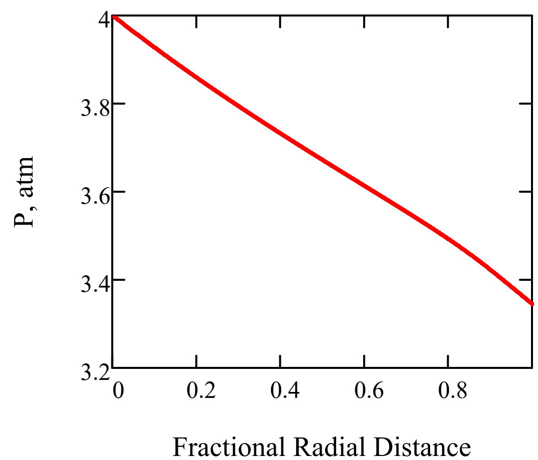


Fig E6.3: Pressure



check interphase temperature difference using results with Dp/Dt

$$\Delta T_c := Rg \cdot \frac{\left(max(\theta) \cdot T_0\right)^2}{Ea_0} \cdot ln(1.1) = 14.515\,K$$

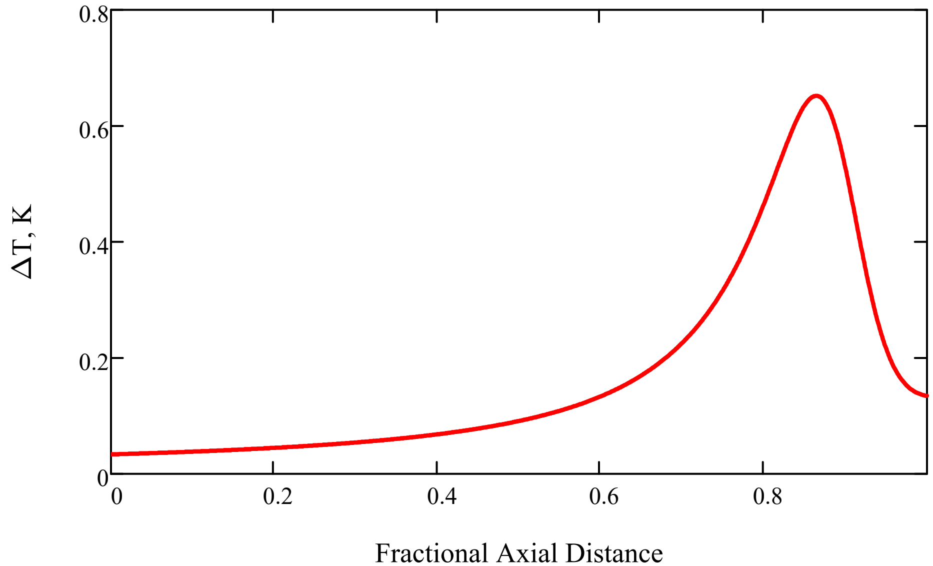
maximum temperature difference for <10% error in the reaction rate, Rase (1990) p 109

The peak in the curve below needs to be less than 1 . If not, then decrease L/G or include the particle energy balance in the model.

$$\Delta T_j := \frac{Qr\left(\omega^{\langle j \rangle}, \theta_j, p_j, act\right)}{a_p \cdot h_s \cdot \Delta T_c}$$

temperature difference ratio from the particle energy balance

Fig E6.4: Temperature Difference between Particle and Fluid



Conclusion: For the conditions modeled, the assumption of a pseudo homogeneous temperature is acceptable.

References:

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Bird, R.B., W.E. Stewart, and E.N. Lightfoot, "Transport Phenomena", Ed 2, Wiley (2002)

MacDonald, I.F., M.S. El_Sayed, K. Mow, and F.A.L. Dullien, *Ind. Eng. Chem. Fundam.,* **18**, 199 (1979)

Rase, H.F., "Fixed-bed Reactor Design and Diagnostics: Gas Phase Reactions", Butterworths (1990)

Reid, R.C., The Properties of Gases and Liquids", Ed 3, McGraw-Hill (1977)

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Exercise:

The example assumed that flow was in the radial outward direction. How would you change the flow direction to inward?

Answer To see answers in Mathcad, open the collapsed area below. To see them in pdf file, open in Adobe and click on the redacted area. Then click on the trash bin to remove the black highlight. The answers will then be visible.

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