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APPENDICES

APPENDIX A

THE KINETIC PARAMETERS OF RATE CONSTANTS

The kinetic data of dehydrogenation of ethylbenzene to styrene by Abdalla *et al.*, (1993, 1994 and 1994a) are used in the models. They observed this reaction in conventional packed-bed reactor experiments with a commercial catalyst composed by Fe_2O_3 doped with K_2O. The properties of commercial catalyst are shown in Table A-1.

Table A-1 Properties of commercial catalyst.

Properties	Value	Dimension
Pellet size	0.2	Mm
Packed-bed void fraction	0.5	-
Pellet density	1500	kg_{cat}/m^3

The six reactions taken into consideration are listed as follow:

$$C_6H_5CH_2CH_3 \xleftrightarrow{r_1} C_6H_5CHCH_2 + H_2 \qquad \text{(A-1)}$$

$$C_6H_5CH_2CH_3 \xrightarrow{r_2} C_6H_6 + C_2H_4 \qquad \text{(A-2)}$$

$$C_6H_5CH_2CH_3 + H_2 \xrightarrow{r_3} C_6H_5CH_3 + CH_4 \qquad \text{(A-3)}$$

$$2H_2O + C_2H_4 \xrightarrow{r_4} 2CO + 4H_2 \qquad \text{(A-4)}$$

$$H_2O + CH_4 \xrightarrow{r_5} CO + 3H_2 \qquad \text{(A-5)}$$

$$H_2O + CO \xrightarrow{r_6} CO_2 + H_2 \qquad \text{(A-6)}$$

The rate equations are given by:

$$R_1 = k_1\left(p_{EB} - p_S p_H / K_{EB}\right) \quad \text{(A-7)}$$

$$R_2 = k_2 p_{EB} \quad \text{(A-8)}$$

$$R_3 = k_3 p_{EB} p_H \quad \text{(A-9)}$$

$$R_4 = k_4 p_{HO} p_H^{0.5} \quad \text{(A-10)}$$

$$R_5 = k_5 p_{HO} p_{MET} \quad \text{(A-11)}$$

$$R_6 = k_6\left(P_T / T^3\right) p_{HO} p_{CO} \quad \text{(A-12)}$$

The rate constants of these reactions are given by:

$$k_i = exp\left(A_i - (E_i / RT\right) \quad \text{(A-13)}$$

and

$$K_{EB} = exp\left(? E_0 / RT\right) \quad \text{(A-14)}$$

where;

$$\Delta F_0 = a + bT + cT^2$$

$$a = 122725.157 \text{ kJ/kmol}$$

$$b = -126.27 \text{ kJ/kmol K}$$

$$c = -2.194 \ 10^{-3} \text{ kJ/molK}^2$$

The kinetic parameters of rate constants for the six reactions obtained are given in Table A-2

Table A-2 Kinetic parameters

Reaction No.	Commercial catalyst	
	A_I	E_I
1	0.851	90891
2	14.00	207989
3	0.56	91515
4	0.12	103996
5	-3.21	65723
6	21.24	73628

The kinetic with surface oxidation of hydrogen

The rate expression for the surface oxidation of hydrogen through the membrane as follow; (Itoh *et al.*, 1997)

$$r_{oxidation} = 0.00418 \cdot \exp(-9580/T) \cdot p_{O_2} p_{H_2,sep} \text{ [mol/m}^2\text{s]} \qquad \text{(A-15)}$$

APPENDIX B

CHARACTERISTICS OF THE COMPOSITE PALLADIUM MEMBRANE

The characteristics of the membrane employed in this thesis work is taken from form Abdalla *et al.*, (1994). The membrane is a ceramic-based membrane with separative layer of palladium coated at the outer part of the membrane. The characteristics of membrane have been shown in Table B-1.

Table B -1 Characteristics of composite palladium membrane

Inner diameter of ceramic support	0.025	[m]
outer diameter of ceramic support	0.029	[m]
Palladium layer thickness	0.00001	[m]
Total length of membrane	0.15	[m]

Permeation rate

The permeation rate of hydrogen through the composite palladium membrane was found to obey the half pressure law by Sieverts. Consequently, the permeation rate of hydrogen read:

$$Q_H = \frac{\alpha_H}{L}\left[p_{H_2,R}^{0.5} - p_{H_2,S}^{0.5} \right] \qquad \text{(B-1)}$$

with the permeability coefficient of hydrogen through the composite palladium membrane,α_H, related to the diffusivity of hydrogen, D_H, and the concentration of dissolved hydrogen, C_0, in the palladium. It holds:

$$\alpha_H = \frac{D_H C_0}{ln\left(r_o / r_i\right)\sqrt{P_0}} \qquad \text{(B-2)}$$

where D_H and C_0 for the pure palladium are determined as a function of temperature according to:

$$D_H = 2.30 \times 10^{-7} \bullet exp\left(\frac{-21700}{RT}\right) \quad \text{(B-3)}$$

$$C_0 = 3.03 \times 10^{2} \bullet T^{-1.0358} \quad \text{(B-4)}$$

APPENDIX C

CONVENTIONAL PACKED-BED REACTOR MODEL

A schematic representation of the conventional packed-bed reactor used in the development of the mathematical models is given in Figures C-1 and C-2. Two conventional packed-bed reactor models were considered namely models with and without radial effect. Details are discussed as follows.

A. Plug flow model

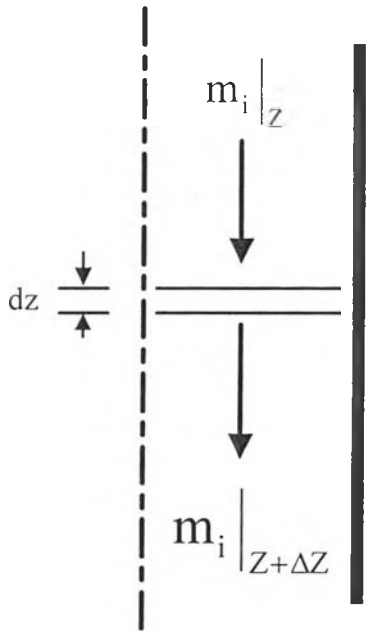

Figure C-1 Schematic diagram of mass balance of plug flow model for conventional packed-bed reactor

Model equations of the conventional packed-bed reactor are given by the mole and heat balance equations of the component i between z and $z + \Delta z$ are expressed as follow:

Mass balance

$$M_i\Big|_z - M_i\Big|_{z+\Delta z} + A_c \Delta z \rho_c r_i = 0 \qquad \text{(C-1)}$$

Energy balance

$$\sum(M_i c_{p,i})[T|_z - T|_{z+\Delta z}] + 2\pi r_1 \Delta z U_{ss}(T_{ss} - T_z) + A_c \Delta z \rho_c \sum(r_i \times \Delta H_{R,i}) = 0 \quad \text{(C-2)}$$

then;

$$\frac{dM_i}{dz} = \rho_c A_c r_i \quad \text{(C-3)}$$

$$\Sigma\left(M_i C_{pi}\right)\frac{dT}{dz} = U_{SS} 2\pi r_1 (T_{ss} - T) + \rho_c A_c \Sigma\left(r_i \times \Delta H_{R,i}\right) \quad \text{(C-4)}$$

Dimensionless form:

Eq. C-3 to C-4 can be converted to a dimensionless form by basing molar flow rate of species i and bed length with initial molar flow rate of ethylbenzene, total bed length and initial feed temperature, respectively.

$$\frac{d\overline{M}_i}{dL} = c_1 r_i \quad \text{(C-5)}$$

$$\sum(M_i c_{p,i})\frac{d\overline{T}}{dL} = c_2(\overline{T}_{ss} - \overline{T}) + c_3 \Sigma\left(r_i \times \Delta H_{R,i}\right) \quad \text{(C-6)}$$

The dimensionless and constant terms are below.

$$c_1 = \frac{\rho_c A_c l_0}{M_{T,0}}$$

$$c_2 = U_{SS} 2\pi r_1 l_0$$

$$c_3 = \pi r_1^2 l_0 \rho_c$$

$$\overline{M_i} = \frac{M_i}{M_{T,0}}, \qquad \overline{T} = \frac{T}{T_0}, \qquad \overline{T_s} = \frac{T}{T_0}$$

B. Radial flow model

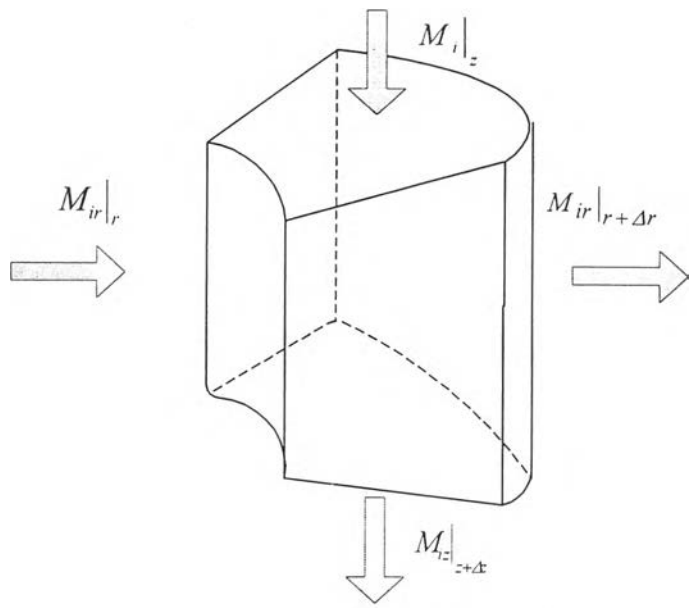

Figure C-2 Schematic diagram of mass balance of radial diffusion model

Mole balance

Mole balance on component i in the conventional packed-bed reactor segment between z and z + Δz and r and r + Δr with rate of formation, r_i,
then partial differential equation will be obtained;

$$\frac{\partial C_i}{\partial t} = \frac{D_{er}}{r}\frac{\partial}{\partial r}(r\frac{\partial C_i}{\partial r}) + D_e(\frac{\partial^2 C_i}{\partial z^2}) - \frac{1}{A_c}\frac{\partial M_i}{\partial z} + \rho_c r_i \qquad \text{(C-7)}$$

In this case, the diffusion in z-direction and convection in r-direction ignored, then a general partial differential equation at steady state condition is;

$$\frac{1}{A_c}\frac{\partial M_i}{\partial z} = D_{er}(\frac{1}{r}\frac{\partial C_i}{\partial r} + \frac{\partial^2 C_i}{\partial r^2}) + \rho_c r_i \qquad \text{(C-8)}$$

For fixed-bed reactor $A_c = \pi r_1^2$ and $C_i = \frac{P_i}{RT} = \frac{M_i}{M_T}\frac{P_t}{RT}$

A general partial different equation (PDE), Eq. C-8, and substitute C_i is used to apply on conventional packed-bed reactor system, PDE and its boundary condition are;

$$\frac{\partial M_i}{\partial z} = D_{er} A_c \frac{P_T}{R}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{M_i}{M_T T}\right) + \frac{\partial^2}{\partial r^2}\left(\frac{M_i}{M_T T}\right)\right] + \rho_c A_c r_i$$

Boundary conditions:

$$\begin{aligned} &\text{at}: \quad z = 0 \;; && C_i = C_{i,0} && \text{for all } r \\ &\qquad r = 0 \;; && \left.\frac{\partial C_i}{\partial r}\right|_{r=0} = 0 && \text{for all } z \\ &\qquad r = r_1 \;; && \left.\frac{\partial C_i}{\partial r}\right|_{r=r_1} = 0 && \text{for all } z \end{aligned} \qquad \text{(C-9)}$$

Heat balance

According to mole balance, partial differential equation and boundary condition for heat balance in the conventional packed-bed reactor is;

$$\sum\left(\frac{C_{p,i} M_i}{A_c}\right)\frac{\partial T}{\partial z} = \lambda_{er}\left(\frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2}\right) + \rho_c \sum\left(r_i \times \Delta H_{R,i}\right)$$

Boundary conditions:

$$\begin{aligned} &\text{at}: \quad z = 0 \;; && T = T_0 && \text{for all } r \\ &\qquad r = 0 \;; && \left.\frac{\partial T_i}{\partial r}\right|_{r=0} = 0 && \text{for all } z \\ &\qquad r = r_1 \;; && \lambda_{er}\left.\frac{\partial T_i}{\partial r}\right|_{r=r_1} = U_{ss}(T_{ss} - T) && \text{for all } z \end{aligned} \qquad \text{(C-10)}$$

Dimensionless form

The set of partial differential equations in Eq. C-10 and Eq. C-11 were converted to dimensionless form.

Mole balance:

$$\frac{\partial \overline{M_i}}{\partial L} = c_4\left[\frac{1}{R}\frac{\partial}{\partial R}\left(\frac{\overline{M}_i}{\overline{M}_T \overline{T}}\right) + \frac{\partial^2}{\partial R^2}\left(\frac{\overline{M}_i}{\overline{M}_T \overline{T}}\right)\right] + c_5 r_i$$

Boundary conditions:

$$\begin{aligned}
&\text{at}: \quad L = 0 \;; && \overline{M}_i = \overline{M}_{i,0} && (0 < R < 1) \\
&\qquad R = 0 \;; && \frac{\partial}{\partial r}\left(\frac{\overline{M}_i}{\overline{M}_T \overline{T}}\right)\Big|_{r=0} = 0 && (0 < L < 1) \\
&\qquad R = 1 \;; && \frac{\partial}{\partial r}\left(\frac{\overline{M}_i}{\overline{M}_T \overline{T}}\right)\Big|_{r=r_1} = 0 && (0 < L < 1)
\end{aligned} \qquad \text{(C-11)}$$

Energy balance:

$$\frac{\partial \overline{T}}{\partial L} = c_6\left[\frac{1}{R}\frac{\partial \overline{T}}{\partial R} + \frac{\partial^2 \overline{T}}{\partial R^2}\right] + c_7 \Sigma\left(r_i \times \Delta H_{R,i}\right)$$

Boundary conditions:

$$\begin{aligned}
&\text{At}: \quad L = 0 \;; && \overline{T} = 1 \; (0 < R < 1) \\
&\qquad R = 0 \;; && \frac{\partial \overline{T}}{\partial R} = 0 \\
&\qquad R = 1 \;; && -2\pi L \lambda_{er} \frac{\partial \overline{T}}{\partial R} = 2\pi r_1 L U_{SS}\left(\overline{T}_{R=1} - \overline{T}_{ss}\right)
\end{aligned} \qquad \text{(C-12)}$$

The dimensionless and constant term in Eq. C-12 and Eq. C-13 are ;

$$\overline{M}_i = \frac{\overline{M}_i}{\overline{M}_{T,0}}; \qquad \overline{T} = \frac{T}{T_0}; \qquad \overline{T_{ss}} = \frac{T_{ss}}{T_0}; \qquad L = \frac{z}{l_0}; \qquad R = \frac{r}{r_1}$$

$$c_4 = \frac{D_{er} A_c l_0 P_T}{F_{T,0} T_0 R r_1^2}; \qquad c_5 = \rho_c\left(\frac{A_c l_0}{F_{T,0}}\right)$$

$$c_6 = \frac{\lambda_{er} l_0}{r_1^2}\frac{A_c}{\Sigma(C_{p,i} M_i)}; \qquad c_7 = \rho_c \frac{l_0}{T_0}\frac{A_c}{\Sigma(C_{p,i} M_i)}$$

APPENDIX D

MEMBRANE REACTOR MODEL

A schematic representation of the membrane reactor used in the development of the mathematical models is given in Figures D-1 and D-2. Two membrane reactor models were considered namely models with and without radial effect. Details are discussed as follows.

A. Plug flow model

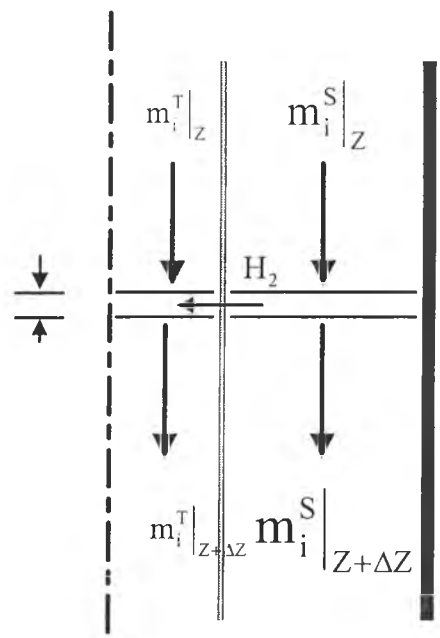

Figure D-1 schematic diagram of mass balance of plug flow model

Model equations of the membrane reactor are given by the mole and heat balance equations of the component i between z and $z + \Delta z$ are expressed as follow:
Shell side:

$$M_i^S\Big|_Z - M_i^S\Big|_{Z+\Delta Z} + A_C^S \Delta z \rho_C R_i - (\Delta z) Q_H = 0 \qquad \text{(D-1)}$$

$$\sum(M_i^S c_{p,i}^S)[T|_Z^S - T|_{Z+\Delta Z}^S] + 2\pi r_3 \Delta z U_{ss}(T_{ss} - T_Z^S) + 2\pi r_1 \Delta z U_m(T^t - T^S)$$
$$+ (\Delta z) H_m^S Q_H + A_c^S \Delta z \rho_c \sum(R_i \times \Delta H_{R,i}) \qquad \text{(D-2)}$$

then;

$$\frac{dM_i^S}{dz} = \rho_c A_C^S R_i - Q_H \qquad \text{(D-3)}$$

$$\Sigma\left(M_i^S C_{p,i}^S\right)\frac{dT^S}{dz} = U_{SS} 2\pi r_3 (T_{ss} - T^S) + U_m 2\pi r_1 (T^T - T^S)$$
$$+ H_m^S Q_H + \rho_c A_C^S \Sigma\left(R_i \times \Delta H_{R,i}\right) \qquad \text{(D-4)}$$

Tube side :

Similarly, the following equation for the tube side could be obtained:

$$\frac{dM_i^T}{dz} = Q_H \qquad \text{(D-5)}$$

$$\Sigma\left(M_i^T C_{p,i}^T\right)\frac{dT^T}{dz} = -U_m 2\pi r_1 (T^T - T^S) + H_m^S Q_H \qquad \text{(D-6)}$$

when $A_C^S = \pi(r_3^2 - r_2^2)$

B. **Radial flow model**

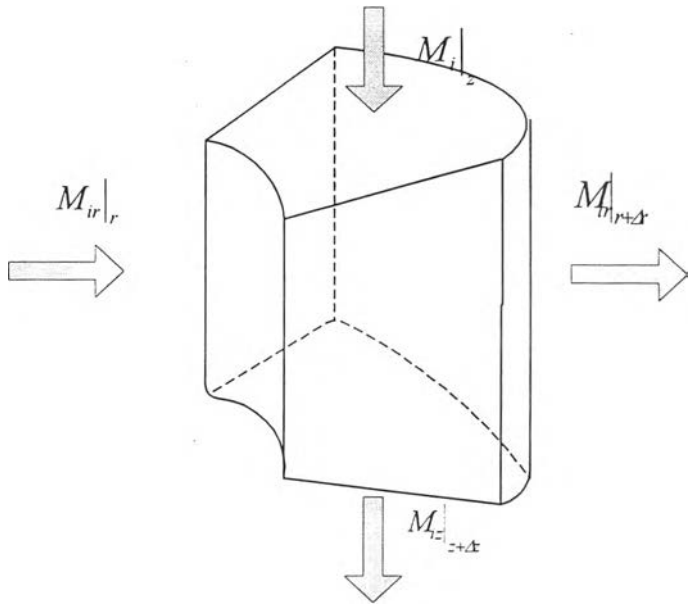

Figure D-2 Schematic diagram of mass balance of radial diffusion model

The same balance is similar in fixed-bed reactor and included permeation term.

Shell side:

Mass balance

$$\frac{\partial M_i^S}{\partial z} = D_{er}^S A_C^S \frac{P_S}{R}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{M_i^S}{M_t^S T^S}\right) + \frac{\partial^2}{\partial r^2}\left(\frac{M_i^S}{M_t^S T^S}\right)\right] + \rho_c A_C^S R_i$$

Boundary conditions:

at : $z = 0$; $M_i^S = M_{i,0}^S$ for all r

$r = r_2$; $\frac{P_S}{R}\frac{\partial}{\partial r}\left(\frac{M_i^S}{M_t^S T^S}\right) = -\frac{1}{D_{er}^S 2\pi r_3} Q_H$ for all z (D-7)

$r = r_3$; $\frac{\partial}{\partial r}\left(\frac{M_i^S}{M_t^S T^S}\right) = 0$ for all z

Heat balance

$$\sum\left(\frac{C_{p,i}M_i^S}{A_C^S}\right)\frac{\partial T^S}{\partial z} = \lambda_{er}^S\left(\frac{1}{r}\frac{\partial T^S}{\partial r} + \frac{\partial^2 T^S}{\partial r^2}\right) + \sum\left(R_i(\Delta H_{R,i})\right)$$

Boundary conditions:

at : $z = 0$; $T^S = T_0^S$ for all r

$r = r_2$; $-\lambda_{er}^S\frac{\partial T^S}{\partial r} = U_m(T^T - T^S) - \frac{1}{2\pi r_2}H_m^S Q_H$ for all z (D-8)

$r = r_3$; $-\lambda_{er}^S\frac{\partial T^S}{\partial r} = U_{ss}(T_{ss} - T^S)$ for all z

Tube side:

Mole balance

$$\frac{\partial M_i^T}{\partial z} = D_{er}^T A_C^T\frac{P_T}{R}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{M_i^T}{M_t^T T^T}\right) + \frac{\partial^2}{\partial r^2}\left(\frac{M_i^T}{M_t^T T^T}\right)\right]$$

at : $z = 0$; $M_i^S = M_{i,0}^S$ for all r

$r = r_1$; $\frac{P_T}{R}\frac{\partial}{\partial r}\left(\frac{M_i^T}{M_t^T T^T}\right) = \frac{1}{D_{er}^T 2\pi r_1}Q_H$ for all z (D-9)

$r = 0$; $\frac{\partial}{\partial r}\left(\frac{M_i^T}{M_t^T T^T}\right) = 0$ for all z

Heat balance:

$$\Sigma\left(\frac{C_{p,i}M_i^T}{A_C^T}\right)\frac{\partial T^T}{\partial z} = \lambda_{er}^T\left(\frac{1}{r}\frac{\partial T^T}{\partial r} + \frac{\partial^2 T^T}{\partial r^2}\right)$$

Boundary conditions:

$$\text{at}: \quad z = 0\ ; \qquad T^Y = T_0^T \qquad \text{for all } r$$

$$r = r_1\ ; \quad -\lambda_{er}^T\frac{\partial T^T}{\partial r} = -U_m(T^T - T^S) + \frac{1}{2\pi r_1}H_m^T Q_H \qquad \text{for all } z \qquad \text{(D-10)}$$

$$r = 0\ ; \qquad \frac{\partial T^T}{\partial r} = 0 \qquad \text{for all } z$$

Dimensionless form:

The set of mass and heat equation for fixed-bed and membrane reactor can be converted to a dimensionless .

Plug flow model

Shell side **;**

$$\frac{d\overline{M}_i^S}{dL} = a_1 R_i + a_2 Q_H \qquad \text{(D-11)}$$

$$\Sigma\left(M_i^S C_{p,i}^S\right)\frac{d\overline{T}^S}{dL} = a_3(\overline{T}_{ss} - \overline{T}^S) + a_4(\overline{T}^T - \overline{T}^S) + a_5\Sigma\left(R_i \times \Delta H_{R,i}\right) + a_6 H_m^S Q_H \qquad \text{(D-12)}$$

Tube side;

$$\frac{d\overline{M}_i^T}{dL} = a_7 Q_H \qquad \text{(D-13)}$$

$$\Sigma\left(\overline{M}_i^T C_{p,i}\right)\ \frac{d\overline{T}^T}{dL} = -a_8(\overline{T}^T - \overline{T}^S) + a_9 H_m^T Q_H \qquad \text{(D-14)}$$

Radial flow model

Shell side:

$$\frac{\partial \overline{M}_i^S}{\partial L} = a_{S,1}\left[\frac{1}{R^S + R_2}\frac{\partial}{\partial R^S}\left(\frac{\overline{M}_i^S}{\overline{M}_T^S \overline{T}^S}\right) + \frac{\partial^2}{\partial R^{S2}}\left(\frac{\overline{M}_i^S}{\overline{M}_T^S \overline{T}^S}\right)\right] + a_{S,2}R_i$$

Boundary conditions:

$$\text{at}: \quad L = 0 \; ; \qquad \overline{M}_i^S = \overline{M}_{i,0}^S \qquad (0 < R^S < 1)$$

$$R^S = 0 \; ; \quad -D_{er}^S \frac{P_S}{RT_0^S}\frac{\partial}{\partial R^S}\left(\frac{\overline{M}_i^S}{\overline{M}_T^S \overline{T}^S}\right) = \frac{l_0}{2\pi r_2 l_0} Q_H \qquad (0 < l_0 < 1) \qquad \text{(D-15)}$$

$$R^S = 1 \; ; \qquad \frac{\partial}{\partial R^S}\left(\frac{\overline{M}_i^S}{\overline{M}_T^S \overline{T}^S}\right) = 0 \qquad (0 < l_0 < 1)$$

Energy balance:

$$\frac{\partial \overline{T}^S}{\partial L} = a_{S,3}\left[\frac{1}{R^S + R_2}\frac{\partial \overline{T}^S}{\partial R^S} + \frac{\partial^2 \overline{T}^S}{\partial R^{S2}}\right] + a_{S,4}\Sigma\left(R_i \times \Delta H_{R,i}\right)$$

Boundary conditions:

$$\text{At}: \quad L = 0 \; ; \qquad \overline{T}^S = 1 \qquad (0 < R^S < 1)$$

$$R^S = 0 \; ; \quad -\frac{\partial \overline{T}^S}{\partial R^S} = a_{S,5}U_m\left(\overline{T}^T - \overline{T}^S\right) + a_{S,5}\frac{l_0}{2\pi r_2 l_0 T_0^S} Q_H \qquad (0 < l_0 < 1) \qquad \text{(D-16)}$$

$$R^S = 1 \; ; \quad -\frac{\partial \overline{T}^S}{\partial R^S} = a_{S,5}U_{SS}\left(\overline{T}_{ss} - \overline{T}_{R=1}^S\right) \qquad (0 < l_0 < 1)$$

Tube side:

$$\frac{\partial \overline{M}_i^T}{\partial L} = a_{T,1}\left[\frac{1}{R^T}\frac{\partial}{\partial R^T}\left(\frac{\overline{M}_i^T}{\overline{M}_T^T \overline{T}^T}\right) + \frac{\partial^2}{\partial R^{T2}}\left(\frac{\overline{M}_i^T}{\overline{M}_T^T \overline{T}^T}\right)\right]$$

Boundary conditions:

at : $L = 0$; $\overline{M}_i^T = \overline{M}_{i,0}^T$ $(0 < R^T < 1)$

$R^T = 1$; $-D_{er}^T \frac{P_T}{RT_0^T}\frac{\partial}{\partial R^T}\left(\frac{\overline{M}_i^T}{\overline{M}_T^T \overline{T}^T}\right) = \frac{l_0}{2\pi r_1 l_0} Q_H$ $(0 < l_0 < 1)$ (D-16)

$R^T = 0$; $\frac{\partial}{\partial R^T}\left(\frac{\overline{M}_i^T}{\overline{M}_T^T \overline{T}^T}\right) = 0$ $(0 < l_0 < 1)$

Energy balance:

$$\frac{\partial \overline{T}^T}{\partial L} = a_{T,2}\left[\frac{1}{R^T}\frac{\partial \overline{T}^T}{\partial R^T} + \frac{\partial^2 \overline{T}^T}{\partial R^{T2}}\right]$$

Boundary conditions:

At : $L = 0$; $\overline{T}^T = 1$ $(0 < R^T < 1)$

$R^T = 1$; $-\frac{\partial \overline{T}^T}{\partial R^T} = -a_{T,3} U_m (\overline{T}^T - \overline{T}^S) + a_{T,3}\frac{l_0}{2\pi r_1 l_0 T_0^T} Q_H$ $(0 < l_0 < 1)$ (D-17)

$R^T = 0$; $\frac{\partial \overline{T}^T}{\partial R^T} = 0$ $(0 < l_0 < 1)$

The dimensionless and constant terms are below.

$$\overline{M}_i^S = \frac{M_i^S}{M_{T,0}^S} \; ; \qquad \overline{M}_i^T = \frac{\overline{M}_i^T}{\overline{M}_{T,0}^T} ; \qquad \overline{T}^S = \frac{T^S}{T_0^S} ; \qquad \overline{T}_{ss} = \frac{T_{ss}}{T_0^S} ;$$

$$\overline{T}^T = \frac{T^T}{T_0^S}$$

$$a_1 = \frac{\rho_c A_C^S l_0}{M_{T,0}^S} \; ; \; a_2 = \frac{l_0}{M_{T,0}^S} ; \qquad a_3 = U_{SS} 2\pi r_3 l_0 ; \qquad a_4 = U_m 2\pi r_1 l_0$$

$$a_5 = \frac{A_C l_0 \rho_C}{T_0^S} \; ; \; a_6 = \frac{l_0}{T_0^S} ; \qquad a_7 = \frac{l_0}{\overline{M}_{T,0}^T} \qquad a_8 = U_m 2\pi r_1 l_0 ;$$

$$a_9 = \frac{l_0}{T_0^T}$$

The dimensionless and constant term in radial flow model are ;

$$A_C^S = \pi(r_3^2 - r_2^2) ; \qquad A_C^T = \pi r_1^2 ; \qquad \overline{M}_i^S = \frac{M_i^S}{M_{T,0}^S} ; \qquad \overline{M}_i^T = \frac{M_i^T}{M_{T,0}^T} \; ;$$

$$\overline{T}^S = \frac{T^S}{T_0^S} \; ; \qquad \overline{T}^T = \frac{T^T}{T_0^T} ; \qquad \overline{T}_{ss} = \frac{T_{ss}}{T_0^S} ; \qquad L = \frac{z}{l_0} \; ;$$

$$R^S = \frac{r^2}{(r_3^2 - r_2^2)} \; ; \qquad R^T = \frac{r^2}{r_1^2} ; \qquad R_2 = \frac{r_2^2}{(r_3^2 - r_2^2)} \; ;$$

$$a_{S,1} = \frac{D_{er}^S \times \pi l_0 P_S}{T_0^S F_{T,0}^S R} \; ; \qquad a_{S,2} = \rho_c (\frac{A_C^S l_0}{F_{T,0}^S}) ; \qquad a_{S,3} = \frac{l_0 \pi \lambda_{er}^S}{\sum (F_{T,0}^S C_{P,i})} ;$$

$$a_{S,4} = \rho_c \frac{A_C^S l_0}{T_0^S} \frac{1}{\sum (F_{T,0}^S C_{p,i})} ; \qquad a_{S,5} = \frac{A_C^S}{\lambda_{er}^S \pi}$$

$$a_{T,1} = \frac{D_{er}^{T} \times \pi l_0 P_T}{T_0^T F_{T,0}^T R}; \qquad a_{T,2} = \frac{l_0 \pi \lambda_{er}^T}{\sum (F_{T,0}^T C_{P,i})}; \qquad a_{T,3} = \frac{A_C^T}{\lambda_{er}^T \pi}$$

APPENDIX E

PHYSICAL PROPERTIES DATA

Physical and thermodynamic property data for organic and inorganic chemicals are of special value to engineers in the processing and petroleum refining industries. The engineering design of process equipment often requires knowledge of such properties as viscosity, heat capacity, enthalpy, thermal conductivity, diffusion coefficient, and others.

Viscosity of gas

The correlation for gas viscosity as a function of temperature is given by the equation shown below

$$\mu_i = (A_i + B_i T + C_i T^2) \times 10^{-7} \qquad \text{(E-1)}$$

Table E-1 Viscosity of gas

Species	*A*	*B*	*C*
Ethylbenzene	-4.267	2.4735E-1	-5.4264E-5
Styrene	-10.035	2.5191E-1	-3.7932E-5
Benzene	-0.151	2.5706E-1	-8.9797E-6
Toluene	1.787	2.3566E-1	-9.3508E-6
Methane	3.844	4.0112E-1	-1.4303E-4
Ethylene	-3.985	3.8726E-1	-1.1227E-4
Carbon dioxide	11.336	4.9918E-1	-1.0876E-4
Carbon monoxide	35.086	5.0651E-1	-1.3314E-4
Water	-36.826	4.29E-1	-1.62E-4
Hydrogen	27.758	2.12E-1	-3.28E-5
Oxygen	44.224	5.62E-1	-1.13E-4
Nitrogen	42.606	4.75E-1	-9.88E-5

Viscosity for multicomponent gas mixture are provided by Bird *et al.*, (1960)

$$\mu_{mix} = \sum \frac{x_i \mu_i}{\sum x_i \Phi_{ij}} \tag{E-2}$$

in which

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1+\frac{M_i}{M_j}\right)^{-1/2} \left[1+\left(\frac{\mu_i}{\mu_j}\right)^{1/2} \left(\frac{M_j}{M_i}\right)^{1/4}\right]^2 \tag{E-3}$$

Diffusion coefficients

Fuller-scherttler-griddings present correlation of binary diffusion coefficients:

$$D_{ij} = \frac{1.43 \times 10^{-7} T^{1.75} \sqrt{\frac{1}{M_i} + \frac{1}{M_j}}}{P\left[\left(\sum V_i\right)^{1/3} + \left(\sum V_j\right)^{1/3}\right]^2} \tag{E-4}$$

Table E-2 Diffusion coefficient

Species	$\sum V_i$	Species	$\sum V_i$
Ethylbenzene	132	Carbon dioxide	26.9
Styrene	127.38	Carbon monoxide	18
Benzene	90.96	water	13.1
Toluene	111.14	Hydrogen	6.12
Methane	24.42	Oxygen	16.6
Ethylene	40.92	Nitrogen	18.5

A binary diffusion coefficient is the usual starting point for the calculation of ordinary diffusion in multicomponent gas mixture.

$$\frac{1 - x_i}{D_{i,m}} = \sum_{j=2}^{n} \frac{x_i}{D_{ij}} \tag{E-5}$$

The effective radial diffusion coefficient can be described in the following correlation (Itoh *et al.*, 1994).

$$1/Pe_r = 0.4/(Re_pSc)0.8+0.009/\{1+10/(Re_pSc)\} \quad \text{(E-6)}$$

for $0.4 < Re_p < 500$, $0.77 < Sc < 1.2$

where

$D_{i,m}$ = diffusion coefficient of gas mixture, m^2/s

D_{er} = effective radial diffusion coefficient, m^2/s

y_i, y_j = mole fraction of components i and j

Pe_r = Peclet number, ud_p/D_{er}

Sc = Schmidt number, $\mu/(\rho D_{i,m})$

$$Re_p = \frac{\rho u d_p}{\mu_m}$$

u = velocity of gas, m/s

d_p = particle diameter, m

Thermal conductivity

Pure component

The correlation for thermal conductivity of pure gas component and solid catalyst are given by Carl L. Yaws (1999).

$$\lambda_i = A_i + B_i T + C_i T^2 \qquad \text{(E-7)}$$

Table E-3 Thermal conductivity

Species	*A*	*B*	*C*
Ethylbenzene	-0.00979	4.0572E-5	6.7289E-8
Styrene	-0.00712	4.5538E-5	3.9529E-8
Benzene	-0.00565	3.44E-5	6.9298E-8
Toluene	-0.00776	4.4905E-5	6.4514E-8
Methane	-0.00935	1.4028E-4	3.318E-8
Ethylene	-0.00123	3.6219E-5	1.2459E-7
Carbon dioxide	-0.012	1.0208E-4	-2.2403E-8
Carbon monoxide	0.00158	8.2511E-5	-1.9081E-8
Water	0.00053	4.7093E-5	4.9551E-8
Hydrogen	0.03951	4.5918E-4	-6.4933E-8
Oxygen	0.00121	8.6157E-5	-1.3346E-8
Nitrogen	0.00309	4.75E-1	-1.1014E-8

Gas mixture and effective radial thermal conductivity

$$\lambda_m = \sum_{i=1}^{n} \frac{y_i \lambda_i}{\sum_{j=1}^{n} y_j A_{ij}} \qquad \text{(E-8)}$$

λ_m = thermal conductivity of the gas mixture, W/(m K)

λ_{sc} = thermal conductivity of solid catalyst, assume equal to MgO, W/(m K)

λ_{er} = effective radial thermal conductivity, W/(m K)

y_i, y_j = mole fraction of components i and j

$$A_{ij} = \frac{\left[1 + \left(\varphi_{tri}/\varphi_{trj}\right)^{1/2}\left(M_i/M_j\right)^{1/4}\right]^2}{\left[8\left(1 + M_i/M_j\right)\right]^{1/2}} \tag{E-9}$$

$$A_{ii} = 1$$

where φ_{tr} is monatomic value of the thermal conductivity.

$$\frac{\varphi_{tri}}{\varphi_{trj}} = \frac{\Lambda_j\left[\exp(0.0464T_{ri}) - \exp(-0.2412T_{ri})\right]}{\Lambda_i\left[\exp(0.0464T_{rj}) - \exp(-0.2412T_{rj})\right]} \tag{E-10}$$

and Λ is defined by the following equation.

$$\Lambda = 210\left(\frac{T_c M^3}{P_c^4}\right)^{1/6} \tag{E-11}$$

The effective radial thermal conductivity is considered to consist of two contributions, the first static and the second dynamic (i.e., dependent on the flow conditions), so that (Froment, G. F. and Bischoff, K. B. (1990))

$$\lambda_{er} = \lambda_{er}^0 + \lambda_{er}^t \tag{E-12}$$

$$\frac{\lambda_{er}^0}{\lambda_m} = \left(1 - \sqrt{1-\varepsilon}\right)\left(1 + \varepsilon\frac{\alpha_{rs}d_p}{\lambda_m}\right) + \frac{2\sqrt{1-\varepsilon}}{1 + \left(\frac{\alpha_{rs}d_p}{\lambda_m} - B\right)\frac{\lambda_m}{\lambda_{sc}}}\theta \tag{E-13}$$

$$\alpha_{rs} = 0.227\frac{\varepsilon_r}{2-\varepsilon_r}\left(\frac{T}{100}\right)^3 \tag{E-14}$$

where ε_r is the emissivity of the solid and α_{rs} is radiation coefficient for the solid.

(E-15)

$$\theta = \frac{\left[1 + \left(\frac{\alpha_{rs}d_p}{\lambda_m} - 1\right)\frac{\lambda_m}{\lambda_{sc}}\right]B}{\left[1 + \left(\frac{\alpha_{rs}d_p}{\lambda_m} - B\right)\frac{\lambda_m}{\lambda_{sc}}\right]^2}\ln\left(\frac{1 + \frac{\alpha_{rs}d_p}{\lambda_{sc}}}{B\frac{\lambda_m}{\lambda_{sc}}}\right) - \frac{B-1}{1 + \left(\frac{\alpha_{rs}d_p}{\lambda_m} - B\right)\frac{\lambda_m}{\lambda_{sc}}} + \frac{B+1}{2B}\left(\frac{\alpha_{rs}d_p}{\lambda_m} - B\right)$$

$$B = b\left[\frac{1-\varepsilon}{\varepsilon}\right]^{10/9} \tag{E-16}$$

b = 1.25 for spheres

$$\lambda_{er}^t = \varepsilon\rho C_p D_{er} \tag{E-17}$$

Table E-4 The property data of gases by Robert C. Reid, John M. Prausnitz and Bruce E. Poling (1988).

No.	Species	M g/mole	T_b (K)	T_c (K)	$P_c \times 10^{-2}$ KPa	$V_c \times 10^6$ m^3/mol	Acentric factor	Dipm$\times 10^3$ Debye
1	Ethylbenzene	106.17	409.4	617.2	36.1	374	0.304	0.59
2	Styrene	104.15	418.3	648.2	40.0	352	0.261	0.13
3	Benzene	78.11	353.2	562.2	48.9	259	0.211	0.00
4	Toluene	92.14	383.8	591.8	41.1	316	0.264	0.36
5	Methane	16.043	111.7	190.6	46.0	99	0.011	0.00
6	Ethylene	28.054	169.5	282.4	50.3	129	0.085	0.00
7	Carbon dioxide	44.010	194.7	304.2	73.8	94	0.228	0.00
8	Carbon monoxide	28.010	81.7	132.9	34.9	93	0.066	0.11
9	Water	18.051	373.2	647.1	220.6	56	0.345	1.85
10	Hydrogen	2.016	20.39	33.2	13.1	64.2	-0.220	0.00
11	Oxygen	31.999	90.2	154.6	50.4	73.4	0.022	0.00
12	Nitrogen	28.013	77.35	126.1	33.9	90.1	0.040	0.00

Enthalpy of formation

The correlation for enthalpy of formation of the ideal gas is a series expansion in temperature:

$$\Delta H_{f,i} = (A_i + B_i T + C_i T^2) \times 10^3 \qquad \text{(E-18)}$$

Table E-5 Enthalpy of formation

Species	*A*	*B*	*C*
Ethylbenzene	58.099	-1.1129E-1	5.3183E-5
Styrene	167.879	-8.0354E-2	3.7418E-5
Benzene	101.403	-7.2136E-2	3.2877E-5
Toluene	74.320	-9.5998E-2	4.7011E-5
Methane	-63.425	-4.3355E-2	1.722E-5
Ethylene	63.053	-4.1076E-2	1.6598E-5
Carbon dioxide	-393.422	1.5913E-2	-1.3945E-6
Carbon monoxide	-112.19	8.1182E-2	-8.0425E-6
Water	-	-	-
Hydrogen	-	-	-
Oxygen	-	-	-
Nitrogen	-	-	-

Heat capacity

The correlation for heat capacity

$$C_{pl} = A_l + B_l T + C_l T^2 \qquad \text{(E-19)}$$

Table E-6 Thermal conductivity

Species	*A*	*B*	*C*
Ethylbenzene	-20.527	5.9578E-1	-3.0849E-4
Styrene	71.201	5.4767E-2	6.4793E-4
Benzene	-31.368	4.746E-1	-3.1137E-4
Toluene	-24.097	5.2187E-1	-2.9827E-4
Methane	34.942	-3.9957E-2	1.9184E-4
Ethylene	32.083	-1.4831E-2	2.4774E-4
Carbon dioxide	27.427	4.2315E-2	-1.9555E-5
Carbon monoxide	29.556	-6.5807E-3	2.013E-5
Water	33.933	-8.4186E-3	2.9906E-5
Hydrogen	25.399	2.0178E-2	-3.8549E-5
Oxygen	29.526	-8.899E-3	3.8083E-5
Nitrogen	29.342	-3.5395E-3	1.0076E-5

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