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$$F = \frac{D}{D_H} \quad , \quad K = \frac{C_s b}{k_D}$$
$$P = k_D D_H \left[1 + \frac{F K}{(1 + b p_o)(1 + b p_L)} \right] \quad ()$$
$$D_L \left[\frac{m^2}{s} \right] \quad D_H \left[\frac{m^2}{s} \right]$$

$$C_s \left[\frac{cc(gas)}{cc(polymer)} \right]$$

$$b [pa^{-1}]$$

$$k_D \left[\frac{cc(gas)}{cc(polymer).pa} \right]$$

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p_L, p_o

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$$\frac{r}{\lambda} < 0.05$$

$$\frac{r}{\lambda} = 0.05 - 50$$

$$\frac{r}{\lambda} > 50$$

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$$\lambda = \frac{RT}{\sqrt{2}\pi d^2 N \bar{p}} \quad ()$$

$$R \quad \bar{p} \text{ [pa]}$$

$$d \text{ [m]} \quad T \text{ [°K]}$$

N

$$N(r) = \frac{N_t}{\sqrt{2\pi}\sigma} \exp\left[-0.5\left(\frac{r-\bar{r}}{\sigma}\right)^2\right] \quad ()$$

$$N_t \quad \bar{r} \text{ [m]}$$

$$() r_{max}$$

σ [m]

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$$q_K = \frac{2\pi r^3}{3} \left[\frac{8RT}{\pi M} \right]^{\frac{1}{2}} \left[\frac{\Delta p}{LRT} \right] = \left[\frac{32\pi}{9MRT} \right]^{\frac{1}{2}} \frac{r^3 \Delta p}{L} \quad ()$$

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$$q_V = \frac{\pi r^4 \bar{p} \Delta p}{8\eta RTL} \quad ()$$

$$q_{sl} = \frac{\pi r^3 \Delta p}{M \bar{C} L} \quad ()$$

$$\eta \text{ [pa.s]} \quad L \text{ [m]}$$

$$\bar{C} \text{ [m/s]} \quad M$$

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$$\bar{C} = (8RT / \pi M)^{\frac{1}{2}} \quad ()$$

$$(Q_g \text{ [kmol/s]})$$

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$$Q_g = Q_K + Q_{sl} + Q_V \quad ()$$

$$Q_g = \sum_{r=0}^{0.05\lambda} N(r)q_k + \sum_{r=0.05\lambda}^{50\lambda} N(r)q_{sl} + \sum_{r=50\lambda}^{r_{max}} N(r)q_V \quad ()$$

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$$Q_g = \frac{N_t}{L} [G_1 I_1 + G_2 I_2 + G_3 I_3] \Delta p \quad ()$$

$$(r \text{ [m]})$$

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I G

$$(\lambda \text{ [m]})$$

$$\begin{aligned} & \left(\right) \left(\right) \\ & : \end{aligned}$$

$$Q_S = \frac{RT\rho_{app}}{2000\tau C_R L^2} \frac{I_4}{I_5} \int_{p_L}^{p_0} \frac{X^2}{p} dp \quad ()$$

$$X = k_D p \quad ()$$

$$C_R = \frac{Q_S}{\bar{r}, L, \sigma, \tau, \rho_{app}} \quad ()$$

$$\left(\right) :$$

$$X = k_D p \quad ()$$

$$Q_S = \frac{RT\rho_{app}}{2000\tau C_R L^2} \frac{I_4}{I_5} \int_{p_L}^{p_0} k_D^2 p dp = A_2' \frac{I_4}{I_5} \bar{p} \Delta p \quad ()$$

$$A_2' = \frac{RT\rho_{app}}{2000\tau C_R L^2} k_D^2 \quad ()$$

$$Q_{ota} = Q_S + Q_g$$

$$Q_{total} = Q_g + Q_S = \frac{N_t}{L} [G_1 I_1 + G_2 I_2 + G_3 I_3] \Delta p + \dots$$

$$A_2' \frac{I_4}{I_5} f(p, \dots)$$

$$(J \text{ [kmol/(m}^2 \cdot s \cdot Pa)])$$

$$J_{total} = \frac{Q_{total}}{S_{total} \Delta p} = A_1 [G_1 I_1 + G_2 I_2 + G_3 I_3] + \dots$$

$$A_2 \frac{I_4}{I_5} \frac{f(p, \dots)}{\Delta p}$$

$$A_1 [m^{-3}] \quad S_{total} [m^2]$$

$$A_2 \left[\frac{Kmol}{m^3 \cdot s \cdot Pa^2} \right]$$

$$A_1 = \frac{N_t}{S_{total} L}, \quad A_2 = \frac{RT\rho_{app}}{2000\tau C_R L^2 S_{total}} S^2 \quad ()$$

$$\left(\right) :$$

$$A_p = \pi I_4, \quad S_S = 2\pi LI$$

$$J_{total} = A_1 [G_1 I_1 + G_2 I_2 + G_3 I_3] + A_2 \frac{I_4}{I_5} \bar{p} \quad ()$$

$$L = \tau L_p$$

$$G_1 = \left[\frac{32\pi}{9MRT} \right]^{\frac{1}{2}}, \quad G_2 = \frac{\pi}{MC}, \quad G_3 = \frac{\pi \bar{p}}{8\eta RT} \quad ()$$

$$I_1 = \frac{1}{\sqrt{2\pi\sigma}} \int_{r=0}^{0.05\lambda} r^3 \exp \left[-\frac{1}{2} \left(\frac{r-\bar{r}}{\sigma} \right)^2 \right] dr \quad ()$$

$$I_2 = \frac{1}{\sqrt{2\pi\sigma}} \int_{r=0.05\lambda}^{50\lambda} r^3 \exp \left[-\frac{1}{2} \left(\frac{r-\bar{r}}{\sigma} \right)^2 \right] dr \quad ()$$

$$I_3 = \frac{1}{\sqrt{2\pi\sigma}} \int_{r=50\lambda}^{r_{max}} r^4 \exp \left[-\frac{1}{2} \left(\frac{r-\bar{r}}{\sigma} \right)^2 \right] dr \quad ()$$

$$r_{max} > 50\lambda$$

$$:$$

$$:$$

$$\frac{Q_S}{A_p} = \frac{RT\rho_{app}}{1000\tau C_R S_S L_p} \int \frac{X^2}{p} dp \quad ()$$

$$Q_S \text{ [kmol/s]}$$

$$\rho_{app} \text{ [kg/m}^3]$$

$$C_R \text{ [kg/(s.m}^2)]$$

$$X \text{ [kmol/kg]}$$

$$S_S \text{ [m}^2/\text{kg]}$$

$$A_p \text{ [m}^2]$$

$$:$$

$$A_p = \pi I_4, \quad S_S = 2\pi LI$$

$$I_4 = \int_{r=0}^{r_{max}} N(r) r^2 dr, \quad I_5 = \int_{r=0}^{r_{max}} N(r) r dr \quad ()$$

$$:$$

$$L = \tau L_p$$

$$:$$

$$L = \tau L_p$$

$$\left(\begin{array}{c} \\ \end{array} \right) \quad \left(\begin{array}{c} \\ \end{array} \right)$$

$(R_3 \cong 0)$ [] Rangarajan

[] Tremblay
Simplex Rangarajan

$$I_{total} = I_1 + I_2, \quad Q_{total} = Q_1 + Q_2 \quad () \quad [] \quad \text{Wang}$$

$$Q_1 \quad Q_{total} \left[\frac{kmol}{s} \right]$$

$$Q_2$$

$$Q_2 = \frac{N_t}{L} (G_1 I_1 + G_2 I_2 + G_3 I_3) \Delta p + A_2' \frac{I_4}{I_5} p \Delta p \quad ()$$

$$\left(\begin{array}{c} \\ \end{array} \right)$$

$$Q_1 = P S_1 \frac{\Delta p}{L_{eff}} \quad ()$$

$$L_{eff} [m] \quad S_1 [m^2] \quad \Delta p [pa] \quad P \left[\frac{kmol \cdot m}{m^2 \cdot pa \cdot s} \right]$$

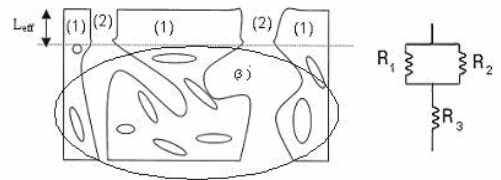
$$()$$

$$\left(\begin{array}{c} \\ \end{array} \right) \left(\begin{array}{c} \\ \end{array} \right)$$

$$Q_{total} = \frac{N_t}{L} (G_1 I_1 + G_2 I_2 + G_3 I_3) \Delta p + A_2' \frac{I_4}{I_5} p \Delta p + \dots$$

$$P S_1 \frac{\Delta p}{L_{eff}} \quad ()$$

$$J_{total} = \frac{Q_{total}}{\Delta p S_{total}} \quad ()$$



$$\left(\begin{array}{c} \\ \end{array} \right) L_{eff} \quad \left(\begin{array}{c} \\ \end{array} \right)$$

$$\begin{aligned}
 & \sigma, \bar{r}, A_2, A_1 \\
 & (J_{total}) \\
 & \left(\frac{S_1}{S_{total}} \right)^p \\
 & J_{total} = \frac{N_t}{L S_{total}} (G_1 I_1 + G_2 I_2 + G_3 I_3) + \frac{A_2'}{S_{total}} \frac{I_4}{p} + \dots \\
 & \frac{S_1}{S_{total}} \frac{P}{L_{eff}} \\
 & J_{total} \quad S_{total} \quad [m^2] \\
 & (J_{calc}) \\
 & (J_{exp}) \\
 & \varepsilon = \frac{S_2}{S_{total}} \Rightarrow \frac{S_1}{S_{total}} = 1 - \varepsilon \\
 & SS_R = \sum_{i=0}^n (J_{exp i} - J_{calci})^2 \\
 & SS_R \quad n \\
 & \varepsilon \quad S_2 \quad [m^2] \\
 & \varepsilon < 10^{-5} \\
 & \frac{S_1}{S_{total}} = 1 - \varepsilon \cong 1 \Rightarrow S_1 \cong S_{total} \\
 & (\sigma, \bar{r}, A_2, A_1) \\
 & J_{total} = A_1 (G_1 I_1 + G_2 I_2 + G_3 I_3) + A_2 \frac{I_4}{I_5} \frac{P}{L_{eff}} \\
 & A_1 = \left[\frac{1}{m^3} \right], A_2 = \frac{A_2'}{S_{total}}, A_1 = \frac{N_t}{L S_{total}} \\
 & A_2 = \left[\frac{kmol}{m^3 \cdot s \cdot pa^2} \right] \\
 & P, G_3, G_2, G_1 \\
 & L_{eff} \\
 & SEM \\
 & \sigma, \bar{r}, A_2, A_1 \quad \sigma \quad \bar{r} \quad I_5 \quad I_4 \quad I_3 \\
 & (J_{total}) \\
 & \int_0^{\infty} f(r) dr = 1 \\
 & r_{max} \\
 & \int_0^{r_{max}} f(r) dr = 1 \\
 & \bar{r}(\sigma) \\
 & (A_1, A_2) \\
 & J_{total} \quad X_1 \quad X_2 \quad A_1 \quad A_2
 \end{aligned}$$

Quasi

Newton

Y

:

$$Y_i = a_i X_1 + b_i X_2 + c_i \quad ()$$

:

$$a_i = G_1 I_{1,i} + G_2 I_{2,i} + G_3 I_{3,i}$$

$$b_i = \frac{I_{4,i}}{I_{5,i}} p_i \quad c_i = \frac{P_i}{L_{\text{eff}}}$$

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$c_i \quad b_i \quad a_i$

:

$$SS_R = \sum_{i=1}^n [Y_{\text{exp}i} - (a_i X_1 + b_i X_2 + c_i)]^2 \quad ()$$

$X_2 \quad X_1$

:

$$\frac{\partial SS_R}{\partial X_1} = 0, \quad \frac{\partial SS_R}{\partial X_2} = 0 \quad ()$$

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Rangarajan

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Wang

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min $SS_R(A_1, A_2, \bar{r}, \sigma)$ subject to:

$$LB_{A_1} < A_1 < UB_{A_1}$$

$$LB_{A_2} < A_2 < UB_{A_2}$$

$$0 < \bar{r} < r_{\text{max}}$$

$$\int_0^{r_{\text{max}}} \frac{N(r)}{N_t} dr = 1$$

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$A_2 \quad A_1$

$$(LB_{A_1} \quad UB_{A_1} \quad LB_{A_2} \quad UB_{A_2})$$

	Ar	N_2
$k_D \left(\frac{cm^3}{cm^3 \cdot atm} \right)$	0.15	0.0753
$C_s \left(\frac{cm^3}{cm^3} \right)$	6.72	9.98
$b \left(\frac{1}{atm} \right)$	0.0317	0.0156
$D_H \times 10^8 \left(\frac{cm^2}{s} \right)$	1.7	1.03
$D_L \times 10^8 \left(\frac{cm^2}{s} \right)$	0.639	0.468

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:

	$d \text{ [}^\circ\text{A]}$	$\eta \times 10^7 \text{ [pa.s]}$
Ar	3.542	222
N_2	3.798	178

(constrained method)

Matlab7

Fmincon

Quasi Newton

Quasi Newton

(Local Minimums)

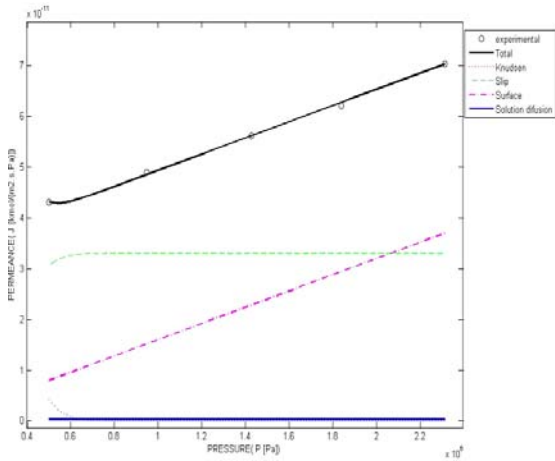
Quasi Newton

$\cdot L_{eff} = 20000^\circ A$

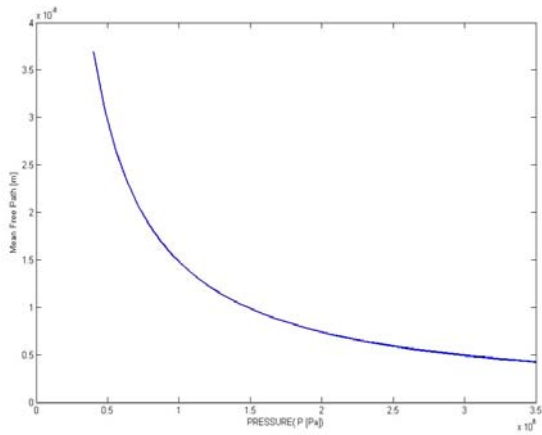
$A_1 \times 10^{-16} [l/m^3]$	6.13
$A_2 \times 10^{10} [Kmol/m^3.s.pa^2]$	8.40
$\bar{r} (^\circ A)$	47.34
$\sigma (^\circ A)$	5.05

$\cdot L_{eff} = 5000^\circ A$

$A_1 \times 10^{-19} [l/m^3]$	2.74
$A_2 \times 10^8 [Kmol/m^3.s.pa^2]$	1.74
$\bar{r} (^\circ A)$	17.61
$\sigma (^\circ A)$	3.46



$\cdot (L_{eff}=5000^\circ A)$



$(C_s \ S \ b)$

$(D_L \ D_H)$

$G_3 (\lambda)$

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$P_o \times 10^{-5} [pa]$	$J_{exp} \times 10^{11} [Kmol/m^2.s.pa^2]$
1.15	0.216
1.28	0.216
1.73	0.205
1.93	0.220
2.40	0.233
3.00	0.227
3.43	0.259
3.96	0.255
4.47	0.281
5.00	0.277
5.53	0.286
6.04	0.307
6.57	0.324

$p_L = 1 \times 10^5 \text{ pa} \quad (\quad) *$

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$P_o \times 10^{-6} [pa]$	$J_{exp} \times 10^{10} [Kmol/m^2.s.pa^2]$
0.50	0.431
0.95	0.485
1.43	0.526
1.84	0.628
2.31	0.703

$p_L = 0 \text{ pa} \quad (\quad) *$

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$$r_{\max} > 50\lambda$$

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- 1 - Solution-diffusion Model
2 - Pore Flow Model
3 - Microvoids
4 - Slip Flow
5 - Scanning Electron Microscopy (SEM)
6 - Probability Density Function
7 - Hybrid Algorithm
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