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APPENDICES

APPENDIX A

MASS TRANSFER COEFFICIENT DETERMINATION

A.1 The mass transfer coefficient in the aqueous phase for the tube side, k_i

In this process, the physical properties of water are calculated as the physical properties of aqueous solution because the copper ions in aqueous solution are diluted.

A.1.1 Calculation of the Reynolds number.

The Reynolds (Re) was calculated from

$$\mathrm{Re} = \frac{\rho v d}{\mu} \qquad \text{(A.1)}$$

where d is the inner diameter of tube = 2.4×10^{-4} m

Q is the volumetric flow rate in tube side = 3.33×10^{-6} m^3/s

ρ is the density of water at 25 °C = 1000 kg/ m^3

μ is the dynamic viscosity of water at 25 °C = 9.5×10^{-4} kg m/s

v is the mean flow velocity in tube side = $\frac{Q}{NA}$

N is the number of fibers in module = 10,000 tubes

A is the cross section area of tube

$$v = \frac{3.33 \times 10^{-6}}{10{,}000\pi \times (\frac{2.4 \times 10^{-4}}{2})^2}$$

$= 7.3 \times 10^{-3}$ m/s

$$\mathrm{Re} = \frac{1000 \times 7.3 \times 10^{-3} \times 2.4 \times 10^{-4}}{9.5 \times 10^{-4}}$$

$= 1.84$

A.1.2 Calculation of mass transfer coefficient, k_i

Due to the Reynolds number in the tube side is less than 10, hence the flow through the tube side is laminar flow. Within this region, the mass transfer coefficient in the aqueous phase(k_i) is calculated by

$$k_i = \frac{1.62D}{2r_i} \times \left(\frac{4r_i^2 v}{DL} \right)^{1/3} \qquad \text{(A.2)}$$

in this correlation, r_i is the inner radius of tube, L is effective length of the module and the diffusivity of copper ion in the bulk solution D is estimated by the Hayduk-Minhas equation.

$$D_{AB} = 1.25 \times 10^{-8} (V_A^{0.19} - 0.292) T^{1.52} \eta_w^{\varepsilon^*} \qquad \text{(A.3)}$$

$$\eta_w^{\varepsilon^*} = (9.58/V_A) - 1.12 \qquad \text{(A.4)}$$

In this correlation, subscripts A and B denote copper ion and water, respectively. V_A is the molar volume of solute A at its normal boiling point(cm^3/mol), T is temperature in degree Kelvin and η_w is the dynamic viscosity of water(cP).

$V_A = 7.11$ cm^3/mol, T = 298 K, $\eta_w = 0.95$ cP

$\varepsilon^* = (9.58 / 7.11) - 1.12 = 0.2274$

$D_{AB} = 1.25 \times 10^{-8} (7.11^{0.19} - 0.292) 298^{1.52} 0.95^{0.2274}$

$= 2.83 \times 10^{-5}$ $cm^2/s = 2.83 \times 10^{-9}$ m^2/s

Equation(A.3) will be used. The quantities for substitution are

$D = 2.83 \times 10^{-9}$ m^2/s, $r_i = 1.2 \times 10^{-4}$ m, v = 7.3×10^{-3} m/s, L = 0.193 m

$$k_i = \frac{1.62 \times 2.83 \times 10^{-9}}{2 \times 1.2 \times 10^{-4}} \times \left(\frac{4 \times (1.2 \times 10^{-4})^2 \times 7.3 \times 10^{-3}}{2.83 \times 10^{-9} \times 0.193} \right)^{1/3}$$

$$k_i = 1.746 \times 10^{-5} \text{ m/s}$$

A.2 The mass transfer coefficient in the membrane, k_m

The mass transfer coefficient in the membrane can be approximated by

$$k_m = \frac{\varepsilon D}{\tau^2 r_i \ln(r_o / r_i)} \qquad \text{(A.5)}$$

where ε and τ are the porosity and tortuosity of the membrane, respectively. D is the diffusivity of copper complex in liquid membrane.

In liquid membrane phase, D2EHPA is diluted by kerosene. In this solution, the solute is very dilute hence the physical properties of membrane phase are substituted with kerosene.

The diffusivity of copper complex in liquid membrane is estimated by

$$D_{AB} = \frac{1.55 \times 10^{-8} T^{1.29} (P_B^{0.5} / P_A^{0.42})}{\eta_B^{0.92} V_B^{0.23}} \qquad \text{(A.6)}$$

In this correlation, subscripts A and B denote copper complex and membrane phase, respectively. where P_A and P_B are parachors for the solute and solvent.

Equation (A.6) will be used. The quantities for substitution are

$P_A = 791.5$, $P_B = 511$, $\eta_B = 7.46 \times 10^{-7}$, $V_B = 278.5$ cm^3/mol, T = 298 K

$$D_{AB} = \frac{1.55 \times 10^{-8} \times 298^{1.29}(511^{0.5} / 791.5^{0.42})}{(7.46 \times 10^{-7})^{0.92} \times 278.5^{0.23}}$$

$$= 2.93 \times 10^{-6} \text{ cm}^2/\text{s} = 2.93 \times 10^{-10} \text{ m}^2/\text{s}$$

The mass transfer coefficient in the membrane is calculated by eq. (A.5) The quantities for substitution are

$$\varepsilon = 0.4,\ \tau = 2.25,\ \text{D} = 2.93 \times 10^{-10} \text{ m}^2/\text{s},\ r_i = 1.2 \times 10^{-4} \text{ m}$$

$$k_m = \frac{0.4 \times 2.93 \times 10^{-10}}{2.25 \times 1.2 \times 10^{-4} \ln(\frac{1.5 \times 10^{-4}}{1.2 \times 10^{-4}})}$$

$$= 1.945 \times 10^{-6} \text{ m/s}$$

A.3 The mass transfer coefficient in the aqueous phase for the shell side, k_o

For the shell side, the mass transfer correlation is

$$(d_H k_o / D) = 5.8(1 - \phi)(d_H / L)(d_H u_{shell} / \nu)^{0.6}(\nu / D)^{0.33} \qquad \text{(A.7)}$$

where ν is the kinematic viscosity of the medium and ϕ is the fiber packing density within the module. The u_{shell} is given as the volumetric flow rate divided by the cross sectional flow area. d_H is the hydraulic diameter of the shell, defined as the cross sectional flow area divided by the wetted parameter.

A.3.1 Calculation of u_{shell}

$$u_{tube} = \frac{Q}{A} \qquad \text{(A.8)}$$

$$A = \pi(R_i^2 - Nr_o^2) \tag{A.9}$$

in which R_i is the inner radius of shell and N is the number of fiber.

$$u_{tube} = \frac{3.33 \times 10^{-6}}{\pi[(3.15 \times 10^{-2})^2 - 10000\,(1.5 \times 10^{-4})]} = 1.4 \times 10^{-3}\ \text{m/s}$$

A.3.2 Calculation of d_H

$$d_H = 2(R_i^2 - Nr_o^2)/(R_i + Nr_o) \tag{A.10}$$

$$= 2[(3.15\times 10^{-2})^2 - 10000(1.5\times 10^{-4})^2]/[\,3.15\times 10^{-2}+10000(1.5\times 10^{-4})]$$
$$= 0.001\ \text{m}$$

A.3.3 Calculation of the mass transfer coefficient in the shell side, k_o

$$k_o = 5.8(1-\phi)(d_H/L)(d_H u_{shell}/\nu)^{0.6}(\nu/D)^{0.33}(D/d_H) \tag{A.11}$$

$$= 5.8(1-0.15)\left(\frac{0.001}{0.193}\right)\left(\frac{0.001 \times 1.4 \times 10^{-3}}{9.2 \times 10^{-7}}\right)^{0.6}\left(\frac{9.2 \times 10^{-7}}{2.83 \times 10^{-9}}\right)^{0.33}\left(\frac{2.83 \times 10^{-9}}{0.001}\right)$$

$$= 6.114 \times 10^{-7}$$

APPENDIX B

THE PROPERTIES OF COPPER

B.1 Atomic Structure

Atomic radius: 1.57 °A

Atomic volume: 7.1 cm^3/mol

Covalent radius: 1.17 °A

Crystal structure: cubic face centered

Electron configuration: $1s^2\ 2s^2p^6\ 3\ s^2p^6\ 4s^1$

Electrons per energy level: 2, 8, 18, 1

Ionic radius: 0.73 °A

Number of electrons: 29

Number of neutrons: 35

Number of protons: 29

Oxidation states: 2, 1

B.2 Chemical properties

Electrochemical Equivalent: 1.1855 g/amp-hr

Electron work function: 4.65 eV

Electronegative: 1.9

Heat of fusion: 13.05 kJ/mol

Incompatibilities: oxidizers, alkalis, sodium azide and acetylene

Ionization potential

First: 7.726

Second: 20.292

Third: 36.83

Valance electron potential(-eV): 34

B.3 Physical properties

Atomic mass average: 63.546

Boiling point: 2567 °C

Coefficient of linear thermal expansion: 1.66×10^{-5} cm/cm·°C

Conductivity

Electrical: 5.69×10^{7} /cm Ω

Thermal: 4.01 W/cm K

Density: 8.96 g/cm^3 at 300 K

Elastic modulus

Bulk: 140/GPa

Rigidity: 48/Gpa

Youngs: 130/GPa

Enthalpy of atomization: 338.9 kJ/mole at 25 °C

Enthalpy of fusion: 13.01 kJ/mole

Enthalpy of vaporization: 304.6 kJ/mole

Flammability class: non-combustible solid (except as dust)

Hardness scale

Brinell: 874 MN/m^2

Mohs: 3 MN/m^2

Vickers: 369 MN/m^2

Heat of vaporization: 300.3 kJ/mole

Melting point: 1084.6 °C

Optical reflectivity: 90 %

Physical state(at 20 °C, 1 atm): Solid

Specific heat: 0.38 J/g K

Vapor pressure: 0.0505 Pa at melting point

APPENDIX C

LEAST SQUARES METHOD

The method of least squares is used to solve a set of linear equations having more equations than unknown variables. Since there are more equations than variables, the solution will not be exactly correct for each equation; rather, the process minimizes the sum of the squares of the residual errors. The method is very powerful and can be applied to numerous applications.

In the general case, the least-squares method is often used to solve a set of non-linear equations that have been linearized using a first-order Taylor-series expansion. Solving non-linear equations is an iterative process using Newton's method. The speed of convergence is dependent on the quality of an initial guess for the solution. The non-linear least-squares method is often referred to as a bundle adjustment since all of the values of an initial guess of the solution are modified together (adjusted in a bundle). This technique is also occasionally referred to as the Gauss-Newton method.

C.1 General Technique

The general least squares process can be used to solve a set of equations for a set of unknowns. The only requirement is that there are at least as many equations as there are unknowns.

If the equations are linear, the least-squares process will produce a direct solution for the unknowns. If the equations are not linear, an initial guess of the unknowns is required, and the result is an adjustment to the initial parameters. This is repeated until the results converge (the adjustments become very close to zero). The linear case is an adjustment using zero as the initial guess of all parameters.

The process requires a set of equations with the unknowns on one side and some known quantity on the other. Let x_i be the set of unknowns, and let the equations be of the form

$$F_i(x_1,x_2,x_3,...) = k_i \tag{C.1}$$

where k_i is the observation (value) whose least-squares error will be minimized. Since there are more equations than unknowns, the solution of the unknowns will not be exact. Using the solution to compute the equation, $F_i(x_1,x_2,x_3,...)$, will not generate the exact observation value, k_i. The square of the difference between the evaluated equation and the observation is minimized.

There is typically one equation for each observation. In photogrammetry, this might be one equation for each x pixel coordinate and one equation for each y pixel coordinate. Each equation is not required to have all of the unknowns in it.

The Jacobian matrix, **J**, is the matrix of the partial differentials of each equation with respect to each unknown. That is,

$$\mathbf{J} = \begin{bmatrix} \frac{\partial F_1}{\partial x_1} & \frac{\partial F_1}{\partial x_2} & \frac{\partial F_1}{\partial x_3} & \cdots \\ \frac{\partial F_2}{\partial x_1} & \frac{\partial F_2}{\partial x_2} & \frac{\partial F_2}{\partial x_3} & \cdots \\ \frac{\partial F_3}{\partial x_1} & \frac{\partial F_3}{\partial x_2} & \frac{\partial F_3}{\partial x_3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{C.2}$$

In general, the height of the Jacobian matrix will be larger than the width, since there are more equations than unknowns.

Furthermore, let the vector **K** be the vector of the residuals. A residual is the difference between the observation and the equation calculated using the initial values. That is

$$\mathbf{K} = \begin{bmatrix} k_1 - F_1(x_{10}, x_{20}, x_{30}, \ldots) \\ k_2 - F_2(x_{10}, x_{20}, x_{30}, \ldots) \\ k_3 - F_3(x_{10}, x_{20}, x_{30}, \ldots) \\ \vdots \end{bmatrix} \tag{C.3}$$

One further parameter is a weighting matrix, **W**. This is a matrix which includes the expected confidence of each equation and also includes any dependence of the equations. A larger value in the weighting matrix increases the importance of the corresponding equation (larger values indicate greater confidence). It is a square symmetric matrix with one row per equation. The main diagonal contains the weights of the individual equations, while the off-diagonal entries are the dependencies of equations upon one another. If all of the observations are independent, this will be a diagonal matrix. The cofactor matrix, **Q**, is the inverse of the weighting matrix (i.e., $\mathbf{Q}=\mathbf{W}^{-1}$).

Let x_{i0} be an initial guess for the unknowns. The initial guesses can have any finite real value, but the system will converge faster if the guesses are close to the solution. Also, let **X** be the vector of these initial guesses. That is

$$\mathbf{X} = \begin{bmatrix} x_{10} \\ x_{20} \\ x_{30} \\ \vdots \end{bmatrix} \tag{C.4}$$

It is desirable to solve for the adjustment values, D**X**. This is the vector of adjustments for the unknowns

$$\Delta \mathbf{X} = \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \\ \vdots \end{bmatrix} \tag{C.5}$$

where, based on the initial guess, **X**, and an adjustment, D**X**, a set of new values are computed

$$\mathbf{X}' = \mathbf{X} + \mathrm{D}\mathbf{X} \tag{C.6}$$

To solve for D**X**,

$$\mathrm{D}\mathbf{X} = (\mathbf{J}^t\mathbf{W}\mathbf{J})^{-1}\mathbf{J}^t\mathbf{W}\mathbf{K} \tag{C.7}$$

The normal matrix, **N**, is defined as

$$\mathbf{N} = \mathbf{J}^t\mathbf{W}\mathbf{J}, \tag{C.8}$$

and the covariance matrix (sometimes referred to as the variance-covariance matrix), $\mathbf{Q}_{xx}$, is defined as

$$\mathbf{Q}_{xx} = (\mathbf{J}^t\mathbf{W}\mathbf{J})^{-1} = \mathbf{N}^{-1} \tag{C.9}$$

If the weighting matrix is diagonal, then D**X** can be solved by row reduction of the matrix

$$\left[\begin{array}{cccc|c}
\sum_i\left(\frac{\partial F_i^2}{\partial x_1}w_i\right) & \sum_i\left(\frac{\partial F_i}{\partial x_1}\frac{\partial F_i}{\partial x_2}w_i\right) & \sum_i\left(\frac{\partial F_i}{\partial x_1}\frac{\partial F}{\partial x_3}w_i\right) & \cdots & \sum_i\left(\frac{\partial F_i}{\partial x_1}(k_i - F_i(x_{10}, x_{20}, x_{30}, \ldots))w_i\right) \\
\sum_i\left(\frac{\partial F_i}{\partial x_1}\frac{\partial F_i}{\partial x_2}w_i\right) & \sum_i\left(\frac{\partial F_i^2}{\partial x_2}w_i\right) & \sum_i\left(\frac{\partial F_i}{\partial x_2}\frac{\partial F_i}{\partial x_3}w_i\right) & \cdots & \sum_i\left(\frac{\partial F_i}{\partial x_2}(k_i - F_i(x_{10}, x_{20}, x_{30}, \ldots))w_i\right) \\
\sum_i\left(\frac{\partial F_i}{\partial x_1}\frac{\partial F_i}{\partial x_3}w_i\right) & \sum_i\left(\frac{\partial F_i}{\partial x_2}\frac{\partial F_i}{\partial x_3}w_i\right) & \sum_i\left(\frac{\partial F_i^2}{\partial x_3}w_i\right) & \cdots & \sum_i\left(\frac{\partial F_i}{\partial x_3}(k_i - F_i(x_{10}, x_{20}, x_{30}, \ldots))w_i\right) \\
\vdots & \vdots & \vdots & \ddots & \vdots
\end{array}\right]$$

(C.10)

where w_1, w_2, w_3, ... are the diagonal elements of the weighting matrix. Note that the left side of the matrix is the normal matrix, **N**.

The initial guesses, x_{i0}, are updated using the solution of the adjustment matrix, D**X**, as follows

$$\mathbf{X}' = \mathbf{X} + \mathrm{D}\mathbf{X} \tag{C.11}$$

or

$$x'_i = x_{i0} + \mathrm{D}x_i$$

The process is repeated using the new values, x'_i, as the initial guesses until the adjustments are close to zero.

Practically, an adjustment is close to zero when it is small compared to the absolute magnitude of the value it is adjusting, i.e., $\mathrm{D}x_i < x_{i0}\, e$, where e is a small value. The actual value for e can be selected based on the number of decimal digits of precision used in the calculations. Typically, the order of magnitude of e will be a few less than the number of digits of precision. For example, if the calculations are done on a computer using standard double precision (8-byte) values, the computer can hold around 15 digits of precision; therefore e is about 10^{-12}.

C.2 Potential Problems

There are conditions where the solution will not converge or will converge to undesirable values. This process finds a local minimum. As such, there may be a better solution than the one found. A solution is dependent on the equations, $F_i(x_1,x_2,x_3,...)$, being continuous in $x_1,x_2,x_3,....$ The first and second derivatives do not need to be continuous, but if the equations are not continuous, there is no guaranty that the process will converge. Also, in certain circumstances, even if the equations are continuous, the solution may not converge. This can happen when the first and second derivatives of the equations have significantly different values at the initial values than at the solution.
In any case where the solution does not converge, a solution may still be able to be obtained if different starting values, x_{i0}, are used.

C.3 Linear Technique

For sets of linear equations, the least-squares process will produce a direct solution for the unknowns. The linear case is mathematically the same as the general case where an adjustment is performed using zero as the initial guess of all parameters. Only a single iteration is required for convergence.

The equations must be of the form

$$F_i(x_1,x_2,x_3,...) = a_1x_1 + a_2x_2 + a_3x_3 + ... = k_i \qquad \text{(C.12)}$$

The Jacobian matrix, **J**, is therefore

$$\mathbf{J} = \begin{bmatrix} a_{11} & a_{21} & a_{31} & \cdots \\ a_{12} & a_{22} & a_{32} & \cdots \\ a_{13} & a_{23} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \qquad \text{(C.13)}$$

where a_{ij} is the ith coefficient of the jth equation.

Since the initial guesses are all zero, the vector of residuals, **K**, is

$$\mathbf{K} = \begin{bmatrix} k_1 \\ k_2 \\ k_3 \\ \vdots \end{bmatrix} \tag{C.14}$$

If the weighting matrix is diagonal, then D**X** can be solved by row reduction of the matrix

$$\left[\begin{array}{cccc|c} \sum_i (a_{1i}^2 w_i) & \sum_i (a_{1i}a_{2i}w_i) & \sum_i (a_{1i}a_{3i}w_i) & \cdots & \sum_i (a_{1i}k_i w_i) \\ \sum_i (a_{1i}a_{2i}w_i) & \sum_i (a_{2i}^2 w_i) & \sum_i (a_{2i}a_{3i}w_i) & \cdots & \sum_i (a_{2i}k_i w_i) \\ \sum_i (a_{1i}a_{3i}w_i) & \sum_i (a_{2i}a_{3_i w_i}) & \sum_i (a_{3i}^2 w_i) & \cdots & \sum_i a_{3i}k_i w_i \\ \vdots & \vdots & \vdots & \ddots & \vdots \end{array}\right] \tag{C.15}$$

The final solution will be the adjustment values. That is

$$\mathbf{X} = \mathrm{D}\mathbf{X} \quad \text{or} \quad \mathrm{x_i} = \mathrm{Dx_i} \tag{C.16}$$

C.4 Error Residuals, Ellipsoids, and Confidence

The covariance matrix, $\mathbf{Q}_{xx}$, contains the variance of each unknown and the covariance of each pair of unknowns. The quantities in $\mathbf{Q}_{xx}$ need to be scaled by a reference variance. This reference variance, S_0^2, is related to the weighting matrix and the residuals by the equation

$$S_O^2 = \frac{K^t WK}{r} \tag{C.17}$$

where r is the number of degrees of freedom (i.e., the number of equations minus the number of unknowns).

For any set of quantities, an error ellipse can be calculated. The dimensions and orientations of the ellipse are calculated from the coefficients of the covariance matrix. Only the coefficients of the covariance matrix in the relevant rows and columns are used. This is the appropriate n x n sub-matrix, where n is the number of dimensions for the error ellipse. The sub-matrix is symmetric.

The ellipse matrix is composed of entries from the covariance matrix. For example, a three-dimensional error ellipsoid is computed from

$$Q'_{xx} = \begin{bmatrix} q_{xx_{aa}} & q_{xx_{ab}} & q_{xx_{ac}} \\ q_{xx_{ba}} & q_{xx_{bb}} & q_{xx_{bc}} \\ q_{xx_{ca}} & q_{xx_{cb}} & q_{xx_{cc}} \end{bmatrix} \qquad \text{(C.18)}$$

where $q_{xx_{jj}}$ are values from the covariance matrix $\mathbf{Q}_{xx}$, and a, b, and c are the indices for the unknowns for which the ellipse is computed.

The error ellipse semi-axes are given by

$$S_{axis} = \pm\sqrt{S_0^2 eigenvalue_{axis}(Q'_{xx})} \qquad \text{(C.19)}$$

The orientation of the error ellipse is the column eigenvectors of $\mathbf{Q}'_{xx}$.

To determine the error to a specific confidence level, the length of the semi-axis is multiplied by a confidence factor based on the Fisher distribution using the formula

$$S_{axis\%} = S_{axis}\sqrt{2Fisher(1-confidence, \#of\ unknown, r)} \qquad \text{(C.20)}$$

where the confidence is a number from 0 to 1, with 1 being complete confidence, and r is the number of degrees of freedom. The Fisher distribution is determined from the equation

$$\alpha = \int_{Fisherr(\alpha,\nu_1,\nu_2)}^{\infty} \frac{\Gamma((\nu_1+\nu_2)/2)}{\Gamma(\nu_1/2)\Gamma(\nu_2/2)}\left(\frac{\nu_1}{\nu_2}\right)\frac{x^{[\nu_1-2]/2}}{1+(\nu_1/\nu_2)x^{(\nu_1+\nu_2)/2}}dx \quad \text{(C.21)}$$

where the Gamma function, G(ν), is given by

$$\Gamma(\nu) = \int_0^{\infty} u^{\nu-1}e^{-u}du \quad \text{(C.22)}$$

APPENDIX D

FSOLVE TOOLBOX

FSOLVE solves nonlinear equations by a least square method. It solve equations of the form :

$$F(X) = 0 \tag{D.1}$$

where F and X may be vector or matrices.

Syntax

X = FSOLVE(FUN, X0) starts at the matrix X0 and tries to solve the equation in FUN. FUN accepts input X and returns a vector (or matrix) of equation values F evaluated at X.

X=FSOLVE(FUN,X0,OPTIONS) minimizes with the default optimization parameters replaced by values in the structure OPTIONS, an argument created with the OPTIMSET function. Used options are Display, TolX, TolFun, DerivativeCheck, Diagnostics, Jacobian, JacobMult, JacobPattern, LineSearchType, LevenbergMarquardt, MaxFunEvals, MaxIter, DiffMinChange and DiffMaxChange, LargeScale, MaxPCGIter, PrecondBandWidth, TolPCG, TypicalX. Use the Jacobian option to specify that FUN also returns a second output argument J that is the Jacobian matrix at the point X. If FUN returns a vector F of m components when X has length n, then J is an m-by-n matrix where J(i,j) is the partial derivative of F(i) with respect to x(j). (Note that the Jacobian J is the transpose of the gradient of F.)

X=FSOLVE(FUN,X0,OPTIONS,P1,P2,...) passes the problem-dependent parameters P1,P2,... directly to the function FUN: FUN(X,P1,P2,...). Pass an empty matrix for OPTIONS to use the default values.

[X,FVAL]=FSOLVE(FUN,X0,...) returns the value of the objective function at X.

[X,FVAL,EXITFLAG]=FSOLVE(FUN,X0,...) returns a string EXITFLAG that describes the exit condition of FSOLVE.

If EXITFLAG is:

> 0 then FSOLVE converged to a solution X.

0 then the maximum number of function evaluations was reached.

< 0 then FSOLVE did not converge to a solution.

[X,FVAL,EXITFLAG,OUTPUT]=FSOLVE(FUN,X0,...) returns a structure OUTPUT with the number of iterations taken in OUTPUT.iterations, the number of function evaluations in OUTPUT.funcCount, the algorithm used in OUTPUT.algorithm, the number of CG iterations (if used) in OUTPUT.cgiterations, and the first-order optimality (if used) in OUTPUT.firstorderopt.

[X,FVAL,EXITFLAG,OUTPUT,JACOB]=FSOLVE(FUN,X0,...) returns the Jacobian of FUN at X.

APPENDIX E

SIMULATION DATA

Part 1. Initial concentration of D2EHPA variables

Experimental condition

Once-through mode

Feed phase

pH: 7

Volumetric flow rate: 200 ml/min

Initial concentration of copper: 10, 50, 100, 300, 500 and 1,000 ppm

Membrane phase

Solvent: kerosene

Initial concentration of D2EHPA: 2, 3, 4, 5, 10, 15, 20, 25, 35, 50 and 70 % v/v

Stripping phase

Initial concentration of H^+: 0.1 mol/l

Volumetric flow rate: 200 ml/min

Δx: 1, 2 and 5 cm

Table E.1 Calculation of removal efficiency percentage of copper-ion extraction at various initial concentrations of D2EHPA and Δx

%D2EHPA	Δx = 1 cm		Δx = 2 cm		Δx = 5 cm	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
2	73.78	26.22	68.92	31.08	30.46	69.54
3	70.39	29.61	30.27	39.73	16.53	83.47
4	60.94	39.06	45.57	54.43	0	100
5	52.94	47.06	31.68	68.32	0	100
10	20.68	79.32	0	100	0	100
15	0	100	0	100	0	100
20	0	100	0	100	0	100
25	0	100	0	100	0	100

Table E.2 Calculation of removal efficiency percentage of copper-ion extraction at various initial concentrations of D2EHPA (Δx = 1 cm, C^f = 10, 50 and 100 ppm)

%D2EHPA	C^f = 10 ppm		C^f = 50 ppm		C^f = 100 ppm	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
2	1.16	88.39	34.27	31.47	73.78	26.22
5	0	100	12.42	75.16	52.94	47.06
10	0	100	0	100	20.68	79.32
15	0	100	0	100	0	100
20	0	100	0	100	0	100
55	0	100	0	100	0	100
35	0	100	0	100	0	100
50	0	100	0	100	0	100
75	0	100	0	100	0	100

Table E.3 Calculation of removal efficiency percentage of copper-ion extraction at various initial concentrations of D2EHPA (Δx = 1 cm, C^f = 300, 500 and 1000 ppm)

%D2EHPA	C^f = 300 ppm		C^f = 500 ppm		C^f = 1000 ppm	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
2	272.04	9.32	463.50	7.30	949.40	5.08
5	252.06	15.98	443.85	11.23	919.90	8.81
10	215.55	28.15	396.30	20.74	862.50	13.75
15	157.47	47.51	386.30	26.34	822.40	17.67
20	111.21	62.93	324.30	35.14	787.90	21.21
25	81.42	72.86	301.00	39.80	757.50	24.25
35	73.47	75.51	178.45	64.31	690.90	30.91
50	46.68	84.44	143.85	75.23	610.90	38.91
75	0	100	0	100	490.80	50.92

Part 2. Initial concentration of copper ion in feed solution variables

Experimental condition

Once-through mode

Feed phase

pH: 7

Volumetric flow rate: 200 ml/min

Initial concentration of copper: 10, 50, 100, 300, 500 and 1,000 ppm

Membrane phase

Solvent: kerosene

Initial concentration of D2EHPA: 2, 5, 10, 15, 20, 25, 35, 50 and 70 % v/v

Stripping phase

Initial concentration of H^+: 0.1 mol/l

Volumetric flow rate: 200 ml/min

Δx: 1

Table E.4 Calculation of removal efficiency percentage of copper-ion extraction at various initial concentrations of copper-ion in feed solution (Δx = 1 cm, B_O = 2, 5 and 10 % v/v)

C^f (ppm)	B_O = 2 % v/v		B_O = 5 % v/v		B_O = 10 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
10	1.16	88.39	0	100	0	100
50	34.27	31.47	12.42	75.16	0	100
100	73.78	26.22	52.94	47.06	20.68	79.32
300	272.04	9.32	252.06	15.98	215.55	28.15
500	463.50	7.30	443.85	11.23	396.30	20.74
1000	949.20	5.08	911.90	8.81	862.50	13.75

Table E.5 Calculation of removal efficiency percentage of copper-ion extraction at various initial concentrations of copper-ion in feed solution (Δx = 1 cm, B_O = 15, 20 and 25 % v/v)

C^f (ppm)	B_O = 15 % v/v		B_O = 20 % v/v		B_O = 25 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
10	0	100	0	100	0	100
50	0	100	0	100	0	100
100	0	100	0	100	0	100
300	157.47	47.51	111.21	62.93	81.42	72.86
500	386.30	26.34	324.30	35.14	301.00	39.80
1000	822.40	17.76	787.90	21.21	757.50	24.25

Table E.6 Calculation of removal efficiency percentage of copper-ion extraction at various initial concentrations of copper-ion in feed solution (Δx = 1 cm, B_O = 35, 50 and 75 % v/v)

C^f (ppm)	B_O = 35 % v/v		B_O = 50 % v/v		B_O = 75 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
10	0	100	0	100	0	100
50	0	100	0	100	0	100
100	0	100	0	100	0	100
300	73.47	75.51	46.68	84.44	0	100
500	178.45	64.31	143.85	71.23	0	100
1000	690.90	30.91	610.90	38.91	490.80	50.92

Part 3. pH in feed solution variables

Experimental condition

Once-through mode

Feed phase

pH: 1, 2, 3, 4, 5, 6, 7, 8

Volumetric flow rate: 200 ml/min

Initial concentration of copper: 100 ppm

Membrane phase

Solvent: kerosene

Initial concentration of D2EHPA: 2, 5, 10, 15, 20 and 25 % v/v

Stripping phase

Initial concentration of H^+ : 0.1 mol/l

Volumetric flow rate: 200 ml/min

Δx: 1

Table E.7 Calculation of removal efficiency percentage of copper-ion extraction at various pH in feed solution (Δx = 1 cm, B_O = 2, 5 and 10 % v/v)

pH in feed solution	B_O = 2 % v/v		B_O = 5 % v/v		B_O = 10 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
1	100	0	100	0	99.99	0.01
2	100	0	100	0	97.08	2.92
3	93.72	6.28	82.23	17.77	73.59	26.41
4	85.97	14.03	74.28	25.72	60.63	39.37
5	84.70	15.30	62.95	37.05	36.16	63.84
6	82.16	17.84	52.73	47.27	21.00	79.00
7	73.78	26.22	52.61	47.39	20.68	79.32
8	74.05	25.95	52.67	47.33	22.45	77.55

Table E.8 Calculation of removal efficiency percentage of copper-ion extraction at various pH in feed solution (Δx = 1 cm, B_O = 15, 20 and 25 % v/v)

pH in feed solution	B_O = 15 % v/v		B_O = 20 % v/v		B_O = 25 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
1	99.97	0.03	99.62	0.38	99.48	0.52
2	93.59	6.41	60.91	9.09	86.54	13.46
3	57.78	42.22	56.05	43.95	44.57	55.43
4	49.27	50.73	44.25	55.75	40.70	59.30
5	36.63	72.37	21.83	78.17	18.58	81.42
6	0	100	0	100	0	100
7	0	100	0	100	0	100
8	0	100	0	100	0	100

Part 4. Hydrogen ion in stripping solution variables

Experimental condition

Once-through mode

Feed phase

pH: 7

Volumetric flow rate: 200 ml/min

Initial concentration of copper: 100 ppm

Membrane phase

Solvent: kerosene

Initial concentration of D2EHPA: 2, 5, 10, 15, 20 and 25 % v/v

Stripping phase

Initial concentration of H^+: 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 0.1, 1 and 10 mol/l

Volumetric flow rate: 200 ml/min

Δx: 1

Table E.9 Calculation of removal efficiency percentage of copper-ion extraction at various hydrogen ion concentration in stripping solution (Δx = 1 cm, B_O = 2, 5 and 10 % v/v)

H^+ in stripping solution (mol/l)	B_O = 2 % v/v		B_O = 5 % v/v		B_O = 10 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
10^{-5}	100	0	100	0	100	0
10^{-4}	99.17	0.83	98.92	1.08	97.71	2.29
10^{-3}	84.76	15.24	67.24	32.76	42.03	57.97
10^{-2}	76.38	23.62	66.41	33.59	25.78	74.22
0.1	73.78	26.22	53.94	46.06	20.68	79.32
1	73.57	26.43	52.92	47.08	20.63	79.37
10	73.57	26.43	52.22	47.78	20.63	79.37

Table E.10 Calculation of removal efficiency percentage of copper-ion extraction at various hydrogen ion concentration in stripping solution (Δx = 1 cm, B_O = 15, 20 and 25 % v/v)

H^+ in stripping solution (mol/l)	B_O = 15 % v/v		B_O = 20 % v/v		B_O = 25 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
10^{-5}	100	0	100	0	100	0
10^{-4}	98.03	1.97	95.43	4.57	94.92	5.08
10^{-3}	43.03	56.97	21.67	78.33	5.39	94.61
10^{-2}	0	100	0	100	0	100
0.1	0	100	0	100	0	100
1	0	100	0	100	0	100
10	0	100	0	100	0	100

Part 5. Volumetric flow rate in feed solution variables

Experimental condition

Once-through mode

Feed phase

pH: 7

Volumetric flow rate: 5, 10, 50, 100, 200, 500 and 1,000 ml/min

Initial concentration of copper: 100 ppm

Membrane phase

Solvent: kerosene

Initial concentration of D2EHPA: 2, 5, 10, 15, 20 and 25 % v/v

Stripping phase

Initial concentration of H^+: 0.1 mol/l

Volumetric flow rate: 200 ml/min

Δx: 1

Table E.11 Calculation of removal efficiency percentage of copper-ion extraction at various volumetric flow rate in feed solution (Δx = 1 cm, B_O = 2, 5 and 10 % v/v)

Volumetric flow rate (ml/min)	B_O = 2 % v/v		B_O = 5 % v/v		B_O = 10 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
5	0	100	0	100	0	100
10	0	100	0	100	0	100
50	47.76	52.24	0	100	0	100
100	62.64	37.36	26.86	73.14	0	100
200	73.78	26.22	52.94	47.06	19.68	80.32
500	89.71	10.29	77.66	22.34	59.27	40.73
1000	93.97	6.03	87.29	12.71	80.02	19.98

Table E.12 Calculation of removal efficiency percentage of copper-ion extraction at various volumetric flow rate in feed solution (Δx = 1 cm, B_O = 15, 20 and 25 % v/v)

Volumetric flow rate (ml/min)	B_O = 15 % v/v		B_O = 20 % v/v		B_O = 25 % v/v	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
5	0	100	0	100	0	100
10	0	100	0	100	0	100
50	0	100	0	100	0	100
100	0	100	0	100	0	100
200	0	100	0	100	0	100
500	43.61	56.39	29.37	70.63	15.71	84.29
1000	67.46	32.54	58.57	41.43	51.02	48.98

Part 6. Circulating rate in feed solution variables

Experimental condition

Recycling mode

Feed phase

pH: 7

Volumetric flow rate: 50, 100, 200, 400 and 600 ml/min

Initial concentration of copper: 300 ppm

Membrane phase

Solvent: kerosene

Initial concentration of D2EHPA: 25 % v/v

Stripping phase

Initial concentration of H^+: 1 mol/l

Volumetric flow rate: 200 ml/min

Δx: 1

Table E.13 Calculation of removal efficiency percentage of copper-ion extraction at various circulating rate in feed solution (Δx = 1 cm, t = 2, 4 and 6 min)

Circulating rate (ml/min)	t = 2 min		t = 4 min		t = 6 min	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
50	298.42	0.53	283.61	5.46	269.38	10.21
100	283.23	5.59	255.97	14.68	230.92	23.03
200	270.46	9.85	236.74	21.09	206.12	31.29
400	259.76	13.41	226.36	24.55	184.99	38.34
600	251.21	16.42	251.29	28.74	173.85	42.05

Table E.14 Calculation of removal efficiency percentage of copper-ion extraction at various circulating rate in feed solution (Δx = 1 cm, t = 8, 10 and 12 min)

Circulating rate (ml/min)	t = 8 min		t = 10 min		t = 12 min	
	C_o (ppm)	% Remove	C_o (ppm)	% Remove	C_o (ppm)	% Remove
50	255.71	14.74	243.06	18.98	231.17	22.94
100	208.77	30.41	188.55	37.28	170.24	43.25
200	173.47	42.18	146.96	51.01	121.34	59.55
400	149.43	50.19	117.74	60.75	85.60	71.47
600	134.37	55.21	99.51	66.83	71.55	76.45

VITA

Mr. Sarawut Jitpinit was born on June 15, 1974 in Nakhossrithammarat Province, Thailand. He graduated high school from Kanlayanee Srithammarat School. He graduated in Bachelor Degree in Chemical Engineering from Prince of Songkhla University in 1997. He has worked as a lecturer in Department of Chemical Engineering, Faculty of Engineering, Rajamangala Institute of Technology since 1997.