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APPENDICES

APPENDIX A

PROPERTIES OF ETBE

A.1 Liquid Heat Capacity

In the energy balance equation, it requires the liquid heat capacity of all substances in the system. ETBE is the newly invented substance and there is not much data about its properties. The properties of all other substances in this research are basically available in Perry's Chemical Engineer's Handbook. In this research, the liquid heat capacity of ETBE was calculated by the empirical correlation (John Garvin, 2002) as following described.

$$C_{pl} = \sum n[a(1/T_r - 1)^k + bT_r^m] \tag{A.1}$$

Where *a*, *b* = coefficients for each group

C_{pl} = liquid specific heat at saturation, kJ/mol.K

k, *m* = exponents for each group

n = number of instances of each group

n_c = number of carbon atoms in molecule

T = absolute temperature, K

T_c = critical temperature, K

T_r = reduced temperature = T/T_c

The parameters *a*, *b*, *k* and *m* are tabulated in Table1 (John Garvin, 2002). These parameters are constants for each group except in the case of -OH (alcohols), where *a* and *b* are also functions of n_c (the number of carbon atoms in the molecule).

The coefficients, *a* and *b*, were found by least-squares minimization. The exponents, *k* and *m*, were found by iteration. The accuracy of the correlation was relatively uniform over the entire reduced temperature range. The average absolute error for Equation (A.1) over the entire database was 3.52%.

From the equation (A.1), note that there is an additional parameter required, the critical temperature, T_c, which is calculated by the method described below in the section **A.2**.

A.2 Critical Temperature

In this research, the critical temperature, T_C [K], of ETBE was calculated by Joback's method (Dragon Technology, Inc., 1995) as follows:

$$T_C = T_B / [0.584 + 0.965 \Sigma\Delta T_J - (\Sigma\Delta T_J)^2] \qquad (A.2)$$

The additional parameter required is the normal boiling point, T_B, which is calculated by the method described below in the section **A.3**.

A.3 Normal Boiling Point

In this research, the normal boiling point, T_B [K], of ETBE was calculated by Joback's method (Dragon Technology, Inc., 1995) as follows:

$$T_B = 198 + \Sigma\Delta B_J \qquad (A.3)$$

A.4 Heat of Formation

In this research, the standard heat of formation, ΔH_F^{298} [J/ mol], of ETBE was calculated by Joback's method (Dragon Technology, Inc., 1995) as follows:

$$\Delta H_F^{298} = \Sigma\Delta H_J + 68.29 \qquad (A.4)$$

Where, ΔT_J, ΔB_J and ΔH_J are the group contributions from appendix table7 (Dragon Technology, Inc., 1995).

APPENDIX B

FILTERS

B.1 Analog Filters

The filters are utilized to smooth the noisy experimental data by damping out the high-frequency fluctuations due to the electrical noise. They are also called low-pass filters, described by a first-order transfer function, or equivalently, a first-order differential equation as follows:

$$\tau_F \frac{dy(t)}{dt} + y(t) = x(t) \tag{B.1}$$

Where, t denotes the continuous time domain

x is the measured value

y is the filtered value (filter output)

τ_F is time constant of the filter

τ_F should be much smaller than the dominant time constant of the process, τ_{MAX}, to avoid introducing a significant dynamic lag in the feedback control loop. For example, choosing $\tau_F < 0.1\ \tau_{MAX}$, but if the noise amplitude is high, the larger τ_F may be required.

B.2 Digital Filters

The analog filters are not available for implementation. The digital filters are required for that. There are many types of the digital filters, but for the IMC loop, an exponential filter is required which can be expressed as follow:

$$\tau_F \frac{y_{(k)} - y_{(k-1)}}{\Delta t} + y_{(k)} = x_{(k)} \tag{B.2}$$

Where, k denotes the discrete time steps

The equation (B.2) can be transformed as follows:

$$y_{(k)} = \frac{\Delta t}{\tau_F + \Delta t} x_{(k)} + \left[1 - \frac{\Delta t}{\tau_F + \Delta t}\right] y_{(k-1)} \tag{B.3}$$

Let $\alpha = \dfrac{1}{\dfrac{\tau_F}{\Delta t} + 1}$

Then $$y_{(k)} = \alpha x_{(k)} + (1-\alpha) y_{(k-1)} \tag{B.4}$$

If τ_F=0, then α=1 and $y_{(k)}=x_{(k)}$. This is mean, no filtering.

If $\tau_F=\infty$, then α=0 and $y_{(k)}=y_{(k-1)}$. This is mean, the measurement signal is ignored.

APPENDIX C

BLACK BOX MODELING PERFORMANCE INDEX

The backpropagation algorithm requires the error goal to be criteria for stop the training. Typically, the square errors are used for this. The reason is this criterion will penalize the responses which have large errors, which are not desired for the prediction result. The backpropagation algorithm is a gradient descent optimization procedure in which minimizes the Mean Square Error (MSE) performance index. The algorithm is provided with a set of examples proper network behaviour as follows:

$$\{p_1, t_1\}, \{p_2, t_2\}, \{p_3, t_3\}, \ldots, \{p_i, t_i\}, \ldots, \{p_n, t_n\} \qquad (C.1)$$

Where, p_i is an input to the network, and t_i is the corresponding target output. As each input is applied to the network, the network output is compared to the target and the algorithm adjusts the network parameter in order to minimize the Sum Square Error (SSE):

$$SSE = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (t_i - a_i)^2 \qquad (C.2)$$

And, MSE is the mean value of SSE as follows:

$$MSE = \frac{1}{n}\sum_{i=1}^{n} e_i^2 = \frac{1}{n}\sum_{i=1}^{n} (t_i - a_i)^2 \qquad (C.3)$$

Where, a_i is the neural network prediction output.

MSE is used as a criterion for choosing the appropriate network architecture.

APPENDIX D

CONTROL PERFORMANCE INDICES

A measured integral error indicates the cumulative deviation of the controlled variable from its set point during the transient response. The following formulations of the integral can be proposed.

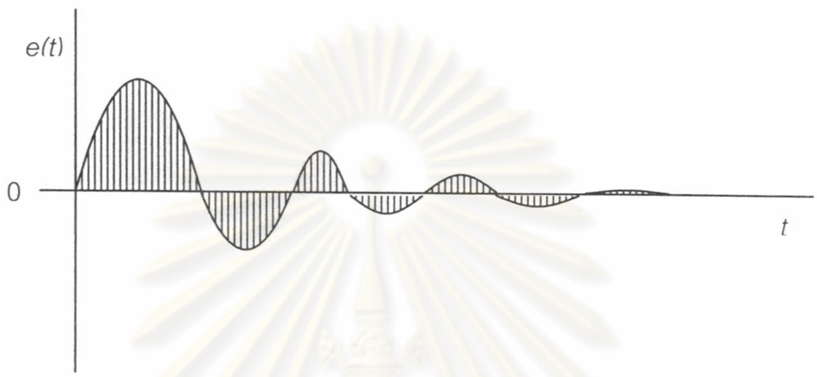

Figure D.1 Definition of error integrals

Integral of Absolute Error (IAE)

$$IAE = \int_0^\infty |e(t)|\, dt \tag{D.1}$$

Integral of Square Error (ISE)

$$ISE = \int_0^\infty |e^2(t)|\, dt \tag{D.2}$$

Integral of Time-weighted Absolute Error (ITAE)

$$ITAE = \int_0^\infty |e(t)|\, t dt \tag{D.3}$$

Where, e is the usual error between set point and control variable.

Each formulations of the error have different purposes. The ISE will penalize the response that has large errors, which usually occur at the beginning of a response, because the error is squared. The ITAE will penalize a response which has errors that persist for a long time. The IAE will be less severe in penalizing a response for large errors and treat all errors (large or small, persist for a long or short time) in a uniform manner.

APPENDIX E

UNIFAC METHOD

Activity coefficients play a key role in the calculation of vapor-liquid equilibria. They are used to estimate the vapor-liquid equilibria for nonideal mixtures when experimental data are not available and when the assumption of regular solutions is not valid because polar compounds are present. In this study, UNIFAC method is used to estimate activity coefficients.

The UNIFAC (UNIQUAC Functional-group Activity Coefficients) groupcontribution method, first presented by Fredenslund, Jones, and Prausnitz and further developed for use in practice by Fredenslund, Gmehling, and Rasmussen, has several advantages over other group-contribution methods: (1) It is theoretically based on the UNIQUAC method; (2) the parameters are essentially independent of temperature; (3) size and binary interaction parameters are available for a wide range of types of functional groups; (4) predictions can be made over a temperature range of 275 to 425 K and for pressures up to a few atmospheres; and (5) extensive comparisons with experimental data are available. All components in the mixture must be condensable.

The UNIFAC method for estimation of activity coefficients depends on the concept that a liquid mixture may be considered a solution of the structural units from which the molecules are formed rather than a solution of the molecules themselves. These structural units are called subgroups, and all of which concerned in this study are listed in the second column of Table E.1. A number, designated k, identifies each subgroup. The relative volume R_k and relative surface area Q_k are properties of the subgroups, and values are listed in columns 4 and 5 of Table E.1. When it is possible to construct a molecule from more than one set of subgroups, the set containing the least number of different subgroups is the correct set. The great advantage of the UNIFAC method is that a relatively small number of subgroups combine to form a very large number of molecules.

Main group	Subgroup	k	R_k	Q_k
1. "CH_2"	CH_3	1	0.9011	0.848
	CH_2	2	0.6744	0.540
5. "OH"	OH	15	1.0000	1.200
7. "H_2O"	H_2O	17	0.9200	1.400
11. "CCOO"	CH_3COO	22	1.9031	1.728
20. "COOH"	COOH	43	1.3013	1.224

Table E.1: UNIFAC-VLE Subgroup Parameter for all studied components

Activity coefficients depend not only on the subgroup properties R_k and Q_k, but also on interactions between subgroups. Here, similar subgroups are assigned to a main group, as shown in the first two columns of Table E.1. All subgroups belonging to the same main group are considered identical with respect to group interactions. Therefore parameters characterizing group interactions are identified with pairs of main groups. Parameter values a_{mk} for a few such pairs are given in Table E.2.

Main group	1. "CH_2"	5. "OH"	7. "H_2O"	11. "CCOO"	20. "COOH"
1. "CH_2"	0.00	986.500	1318.000	232.100	663.500
5. "OH"	156.400	0	353.500	101.100	199.000
7. "H_2O"	300.00	-229.100	0	14.420	-14.090
11. "CCOO"	114.800	245.400	100000.000	0	660.200
20. "COOH"	315.300	-151.000	-66.170	-256.300	0

Table E.2: UNIFAC-VLE Interaction Parameters, a_{mk} for all studied components, in kelvins

The UNIFAC method for predicting liquid-phase activity coefficients is based on the UNIQUAC equation, for which the activity coefficients are given by the following equations:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \tag{E.1}$$

$$\ln \gamma_i^C = 1 - J_i + \ln J_i - 5q_i\left(1 - \frac{J_i}{L_i} + \ln \frac{J_i}{L_i}\right) \tag{E.2}$$

$$\ln \gamma_i^R = q_i\left[1 - \sum_k\left(\theta_k \frac{\beta_{ik}}{s_k} - e_{ki} \ln \frac{\beta_{ik}}{s_k}\right)\right] \tag{E.3}$$

$$J_i = \frac{r_i}{\sum_j r_j x_j} \tag{E.4}$$

$$L_i = \frac{q_i}{\sum_j q_j x_j} \tag{E.5}$$

$$r_i = \sum_k \nu_k^{(i)} R_k \tag{E.6}$$

$$q_i = \sum_k \nu_k^{(i)} Q_k \tag{E.7}$$

$$e_{ki} = \frac{\nu_k^{(i)} Q_k}{q_i} \tag{E.8}$$

$$\beta_{ik} = \sum_m e_{mi} \tau_{mk} \tag{E.9}$$

$$s_k = \sum_m \theta_m \tau_{mk} \tag{E.10}$$

$$\tau_{mk} = \exp \frac{-a_{mk}}{T} \tag{E.11}$$

Subscript i identifies species, and j is a dummy index running overall species. Subscript k identifies subgroups, and m is a dummy index running over all subgroups. The quantity $\nu_k^{(i)}$ is the number of subgroups of type k in a molecule of species i. Values of the subgroups parameters R_k and Q_k and of the group interaction parameters a_{mk} come from tabulations in the literature.

VITA

Mister Chawat Siwaranon was born in Bangkok on March 10, 1980. He received the Bachelor Degree of Engineering in Chemical Engineering from Chulalongkorn University in 2001. He continued the Graduate School of Chulalongkorn University to pursue the Master of Engineering in Chemical Engineering in 2002.