**Appendix C**

**Models** Scripts for Multicomponent Systems in **MATLAB**

function Gamma=UNIQUAC(DATA,Optimized)

% DATA containd experimental x-data and temperature

% each x(i) corresponds to each component

% Optimized in the values of variables (Aij) from Optimization method,

% for first iteration of Optimization method, Optimzed is set randomly

NT=length(DATA.x); % determining number of experimental data

T=DATA.T; % determining temperature

R=1.98721; % Gas constant cal/mol K

R(1:NT)=[000 0000 ]; % Volume parameters of pure components (cm^3/mol)

Q(1:NT)=[000 0000 ]; % Area parameters of pure components(cm^3/mol)

z=10; % Coordination number

L=z/2\*(R-Q)-(R-1); % UNIQUAC Parameter

id=1:NT; % index

A=Optimized; % Binary interaction parameters Aij (cal/mol)

% from Optimization script, NT\*NT matrix with

% independent Aij estimations

A(id,id)=0; % for Aii=0;

Tau=exp(-A./(R\*T)); % Binary interaction parameters

for i=id

theta(i)=Q(i)\*x(i)./sum(Q(id)\*x(id));

% Area fraction of pure components

phi(i)=R(i)\*x(i)./sum(R(id)\*x(id));

% Volume fraction of pure components

% Activity coefficients (combinatorial part)

lnGc(i)=log(phi(i)./x(i)) + z/2\*Q(i)\*log(theta(i)./phi(i)) + L(i)...

- (phi(i)./x(i)).\*sum(x(id).\*L(id));

% Activity coefficients (residual part)

lnGr(i)=Q(i).\*(1-log(sum(theta(i).\*Tau(i,id)))...

-sum(theta(i).\*T(i,id)./sum(theta(i).\*T(i,id))));

% Activity coefficients

G(i)=exp(Gc(i)+Gr(i));

end

Gamma=G;

end

function Gamma=Wilson(DATA,Optimized)

% DATA containd experimental x-data and temperature

% each x(i) corresponds to each component

% Optimized in the values of variables (Aij) from Optimization method,

% for first iteration of Optimization method, Optimzed is set randomly

NT=length(DATA.x); % determining number of experimental data

T=DATA.T; % determining temperature

R=1.98721; % Gas constant cal/mol K

id=1:NT; % index

A=Optimized; % Binary interaction parameters Aij (cal/mol)

% from Optimization script, NT\*NT matrix with

% independent Aij estimations

A(id,id)=0; % for Aii=0;

for i=id

L(i,:)=V(id)./V(i).\*exp(-A(i,id)./(R\*T));

% Binary interaction parameters

G(i)=exp(1-log(sum(x(i).\*L(i,id)))-sum(x(i).\*L(i,id)/sum(x(i).\*L(i,id))));

% Activity coefficients

end

Gamma=G;

end

function Gamma=NRTL(DATA,Optimized)

% DATA containd experimental x-data and temperature

% each x(i) corresponds to each component

% Optimized in the values of variables (Aij) from Optimization method,

% for first iteration of Optimization method, Optimzed is set randomly

NT=length(DATA.x); % determining number of experimental data

T=DATA.T; % determining temperature

R=1.98721; % Gas constant cal/mol K

id=1:NT; % index

A=Optimized; % Binary interaction parameters Aij (cal/mol)

% from Optimization script

A(id,id)=0; % Aii=0;

Tau=exp(-A./(R\*T)); % Binary interaction parameters

alpha=rand(NT,NT); % Alpha interaction parameter

alpha(id,id)=0; % for Alpha ii=0

G=exp(-alpha.\*Tau); % Binary interaction parameters, Gji

for i=id

% Activity coefficients

lnG(i)=sum(Tau(i,id).\*G(id,i).\*x(i))./sum(G(i,id).\*x(i))+...

sum((G(i,id).\*x(i)).\*(Tau(i,id)-sum(Tau(i,id).\*G(i,id)...

.\*x(i))./sum(G(i,id).\*x(i)))./sum(G(i,id).\*x(i)));

% Activity coefficients

Gam(i)=exp(lnG(i));

end

Gamma=Gam;

end