%input: Temperature (K) and mass fraction

%output: Saturation thermodynamic properties for the given P and x

function [hb,hd,Tb,Td,sb,sd,vb,vd] = Px(P,x)

M=18.01528\*17.0306/((1-x)\*17.0306+x\*18.01528);

y=x\*18.01528/(x\*18.01528+(1-x)\*17.0306);

Tb=Bubble\_T(P,x);

Td=Dew\_T(P,x);

% sat liq h

hb=enthalpy\_mixture\_l(Tb,P,y)/M;

% sat vap h

hd=enthalpy\_mixture\_g(Td,P,y)/M;

% sat liq s

sb=entropy\_mixture\_l(Tb,P,y)/M;

% sat vap s

sd=entropy\_mixture\_l(Td,P,y)/M;

% sat liq v

vb=volume\_mixture\_l(Tb,P,y)/M;

% sat vap v

vd=volume\_mixture\_g(Td,P,y)/M;

end

%input: Temperature (K) and mass fraction

%output: Bubble point pressure of the mixture (bar)

function [T,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov,iter,maxiter] = hPx(h,P,x)

T=400;

incr2=10;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=1;

maxiter=1000;

while ((abs(h-hm)>0.1)&&(iter<maxiter))

while ((hm>h)&&(iter<maxiter))

T=T-incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

while ((hm<h)&&(iter<maxiter))

T=T+incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

end

if (iter==maxiter)

T=400;

incr2=10;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=1;

% maxiter=1000;

while ((abs(h-hm)>0.5)&&(iter<maxiter))

while ((hm>h)&&(iter<maxiter))

T=T-incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

while ((hm<h)&&(iter<maxiter))

T=T+incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

end

end

if (iter==maxiter)

T=400;

incr2=10;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=1;

% maxiter=1000;

while ((abs(h-hm)>1)&&(iter<maxiter))

while ((hm>h)&&(iter<maxiter))

T=T-incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

while ((hm<h)&&(iter<maxiter))

T=T+incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

end

end

end

%input: Temperature (K) and mass fraction

%output: Bubble point pressure of the mixture (bar)

function [hm,T,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov,iter,maxiter] = Psx(P,s,x)

T=400;

incr2=10;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=1;

maxiter=1000;

while ((abs(s-sm)>.001)&&(iter<maxiter))

while ((sm>s)&&(iter<maxiter))

T=T-incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

while ((sm<s)&&(iter<maxiter))

T=T+incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

end

if (iter==maxiter)

T=400;

incr2=10;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=1;

% maxiter=1000;

while ((abs(s-sm)>.01)&&(iter<maxiter))

while ((sm>s)&&(iter<maxiter))

T=T-incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

while ((sm<s)&&(iter<maxiter))

T=T+incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

end

end

if (iter==maxiter)

T=400;

incr2=10;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=1;

% maxiter=1000;

while ((abs(s-sm)>.1)&&(iter<maxiter))

while ((sm>s)&&(iter<maxiter))

T=T-incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

while ((sm<s)&&(iter<maxiter))

T=T+incr2;

[hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov]=PTx(P,T,x);

iter=iter+1;

end

incr2=incr2/10;

end

end

end

%input: Temperature (K) and mass fraction

%output: Bubble point pressure of the mixture (bar)

function [hm,sm,vm,qm,istate,NH3l,H2Ol,NH3v,H2Ov] = PTx(P,T,x)

M=18.01528\*17.0306/((1-x)\*17.0306+x\*18.01528);

y=x\*18.01528/(x\*18.01528+(1-x)\*17.0306);

Tb=Bubble\_T(P,x);

Td=Dew\_T(P,x);

if(T<Tb)

istate=1;

hm=enthalpy\_mixture\_l(T,P,y)/M;

sm=entropy\_mixture\_l(T,P,y)/M;

vm=volume\_mixture\_l(T,P,y)/M;

NH3v=0;H2Ov=0;NH3l=x;H2Ol=1-x;

qm=0.0;

elseif (T>Td)

istate=3;

hm=enthalpy\_mixture\_g(T,P,y)/M;

sm=entropy\_mixture\_g(T,P,y)/M;

vm=volume\_mixture\_g(T,P,y)/M;

NH3l=0;H2Ol=0;NH3v=x;H2Ov=1-x;

qm=100;

else

istate=2;

xb=Bubble\_x(P,T);

xd=Dew\_x(P,T);

qm=(x-xb)/(xd-xb); % quality of mixture

yb=xb\*18.01528/(xb\*18.01528+(1-xb)\*17.0306);

yd=xd\*18.01528/(xd\*18.01528+(1-xd)\*17.0306);

Mb=18.01528\*17.0306/((1-xb)\*17.0306+xb\*18.01528);

Md=18.01528\*17.0306/((1-xd)\*17.0306+xd\*18.01528);

hm=(1-qm)/Mb\*enthalpy\_mixture\_l(T,P,yb)+qm/Md\*enthalpy\_mixture\_g(T,P,yd); %kJ/kg(mix at current state)

sm=(1-qm)/Mb\*entropy\_mixture\_l(T,P,yb)+qm/Md\*entropy\_mixture\_g(T,P,yd); %kJ/kg K(mix at current state)

vm=(1-qm)/Mb\*volume\_mixture\_l(T,P,yb)+qm/Md\*volume\_mixture\_g(T,P,yd); % m3/kg(mix at current state)

NH3v=(x-xb)/(xd-xb)\*xd; % mass NH3 vap per mass total

H2Ov=(x-xb)/(xd-xb)\*(1-xd);

NH3l=(1-(x-xb)/(xd-xb))\*xb;

H2Ol=(1-(x-xb)/(xd-xb))\*(1-xb);

qm=qm\*100;

end

end

%input: Temperature (K) and mass fraction

%output: Bubble point pressure of the mixture (bar)

function [hb,hd,Pb,Pd,sb,sd,vb,vd] = Tx(T,x)

M=18.01528\*17.0306/((1-x)\*17.0306+x\*18.01528);

y=x\*18.01528/(x\*18.01528+(1-x)\*17.0306);

Pb=Bubble\_P(T,x);

Pd=Dew\_P(T,x);

% sat liq h

hb=enthalpy\_mixture\_l(T,Pb,y)/M;

% sat vap h

hd=enthalpy\_mixture\_g(T,Pd,y)/M;

% sat liq s

sb=entropy\_mixture\_l(T,Pb,y)/M;

% sat vap s

sd=entropy\_mixture\_g(T,Pd,y)/M;

% sat liq v

vb=volume\_mixture\_l(T,Pb,y)/M;

% sat vap v

vd=volume\_mixture\_g(T,Pd,y)/M;

end

%input: Temperature (K) and Temperature (K)

%output: Saturation thermodynamic properties for the given P and T

function [hb,hd,sb,sd,vb,vd,xb,xd] = PT(P,T)

xb=Bubble\_x(P,T); %xb is the sat liq mass fraction

xd=Dew\_x(P,T); %xd is the sat vap mass fraction

if(xb<0)

% sat liq h \* sat vap h \* sat liq s \* sat vap s \* sat liq v \* sat vap v

hb=0;hd=0;sb=0;sd=0;vb=0;vd=0;

elseif (xd>1)

% sat liq h \* sat vap h \* sat liq s \* sat vap s \* sat liq v \* sat vap v

hb=0;hd=0;sb=0;sd=0;vb=0;vd=0;

xd=1;

else

x=xb;

y=x\*18.01528/(x\*18.01528+(1-x)\*17.0306);

M=18.01528\*17.0306/((1-x)\*17.0306+x\*18.01528);

yd=xd\*18.01528/(xd\*18.01528+(1-xd)\*17.0306);

Md=18.01528\*17.0306/((1-xd)\*17.0306+xd\*18.01528);

% sat liq h

hb=enthalpy\_mixture\_l(T,P,y)/M;

% sat vap h

hd=enthalpy\_mixture\_g(T,P,yd)/Md;

% sat liq s

sb=entropy\_mixture\_l(T,P,y)/M;

% sat vap s

sd=entropy\_mixture\_g(T,P,yd)/Md;

% sat liq v

vb=volume\_mixture\_l(T,P,y)/M;

% sat vap v

vd=volume\_mixture\_g(T,P,yd)/Md;

end

end

%input: Temperature (K) and pressure (bar)

%output: Bubble point mass fraction of the mixture

function [x] = Bubble\_x(P,T)

x=0;

Tb=10000;

incr=0.1;

xx=0;xxx=0;

while ((abs(T-Tb)>.0001)&&(xxx~=-1)&&(xx~=2))

while (T-Tb<0)

x=x+incr;

if(x>1)

x=2;

xx=x;

break;

end

Tb=Bubble\_T(P,x);

end

x=x-incr;

if(x<0)

x=-1;

xxx=x;

break;

end

Tb=Bubble\_T(P,x);

incr=incr/10;

end

if (xxx==-1)

x=xxx;

elseif (xx==2)

x=xx;

end

end

%input: pressure (bar) and mass fraction

%output: Bubble point temperature (K)

function [Tb] = Bubble\_T(P,x)

%Cij sub values

cijsub1=[-462.460321366 23739.9986309 -194504.35292 639383.528867 -523748.057636 -2328271.47551 7562418.53499 -9668295.89504 5922081.87086 -1432405.52125];

cijsub2=[421.443122208 -14560.354925 53051.4495633 382763.793582 -3583589.86875 12243265.3815 -22307970.0156 22896656.8499 -12483324.8091 2813311.71633];

cijsub3=[-248.783804168 4807.07241098 13565.1003309 -466407.780832 2827083.44764 -8469715.15799 14459588.8962 -14281087.5331 7596403.59678 -1684002.64482];

cijsub4=[126.965580728 -2090.45270574 1993.17101166 100706.510396 -687388.808612 2132412.46959 -3699199.65914 3688365.22546 -1975122.39296 440201.446068];

cijsub5=[-33.5343446156 601.878586689 -3064.82070658 71.7954752052 51780.666659 -209714.899856 405011.985355 -428310.461566 238153.698326 -54497.0973336];

cijsub6=[3.97454953787 -77.026846469 541.19105807 -1696.60270972 1713.45942707 4019.01019872 -14844.7928004 19481.0094551 -12107.0794501 2966.92804386];

cijsub7=[-.170806170177 3.48182859299 -27.7957587743 113.762064546 -258.750496922 311.002585218 -123.917993454 -123.480627492 154.375042114 -48.508382870];

%Cij values

Cij=[cijsub1;cijsub2;cijsub3;cijsub4;cijsub5;cijsub6;cijsub7];

%Ci values

Ci=[153.634521459 -13.0305543892 -1.14845282991 .550358094447 -.0753450148427 .0048111666267 -.000120433757177];

%bubble T calculation

[Pc] = Criticalmix\_P(x);

[Tc] = Criticalmix\_T(x);

sum2 = 0;

for i = 1:7

sum1 = 0;

for j = 1:10

sum1 = sum1 + Cij(i,j)\*x^j;

end

sum2 = sum2 + (Ci(i) + sum1)\*(log(Pc/P))^i;

end

Tb=Tc-sum2/1.8; %unit conversion -- bubble point temperature (K)

end

%input: mass fraction of ammonia in mixture

%output: critical pressure (bar)

function [Pc] = Criticalmix\_P(x)

Pcw = 3206.79; %critical properties of water (R and psia)

b=[0.368105523897 -3.6679548875 46.6000470809 -262.921061996 732.99536936 -1076.0613489 797.948078048 -235.903904222];

sum1 = 0; i = 1;

while (i <= 8)

sum1 = sum1 + b(i)\*x^i;

i = i + 1;

end

Pc = Pcw\*exp(sum1)/(14.696/1.01325); %convert from psia to bar

end

%input: mass fraction of ammonia in mixture

%output: critical temperature (K)

function [Tc] = Criticalmix\_T(x)

Tcw = 1165.14 ; %critical properties of water (R and psia)

a=[205.8889 280.930556 -317.0138889 263.194444];

sum1 = 0; i = 1;

while (i <= 4)

sum1 = sum1 + (a(i)\*x^i);

i = i + 1;

end

Tc = (Tcw - sum1)/1.8; %convert from R to K

end

%input: Temperature (K) and pressure (bar)

%output: Bubble point mass fraction of the mixture

function [x] = Dew\_x(P,T)

x=0;

Td=10000;

incr=0.1;

xx=0;xxx=0;

while ((abs(T-Td)>.0001)&&(xxx~=-1)&&(xx~=2))

while (T-Td<0)

x=x+incr;

if(x>1)

x=2;

xx=x;

break;

end

Td=Dew\_T(P,x);

end

x=x-incr;

if(x<0)

x=-1;

xxx=x;

break;

end

Td=Dew\_T(P,x);

incr=incr/10;

end

if (xxx==-1)

x=xxx;

elseif (xx==2)

x=xx;

else

x=x;

end

end

%input: pressure (bar) and mass fraction

%output: Dew point temperatures (K)

function [Td] = Dew\_T(P,x)

%aij sub values

aijsub1=[194.793913463 74.236124188 9.84103819552 .436843852745];

aijsub2=[-74.3508283362 -33.2941879809 -4.78866918581 -.225416733476];

aijsub3=[13.0175447367 6.1586564117 .789740337141 .0321510834958];

aijsub4=[-0.90857587517 -.356752691147 .0238067275502 .00495593933952];

aijsub5=[-0.00071863574153 -.0251026383533 -.0191664613304 -.0017014253867];

aijsub6=[0.00195441702983 .00280533348937 .0013899436563 .000116422611616];

%Aij values

Aij=[aijsub1;aijsub2;aijsub3;aijsub4;aijsub5;aijsub6];

%Ai values

Ai=[153.17055346 -11.7705687461 -1.78126355957 0.647385455059 -0.0719950751898 0.00285423950786];

%dew T calculation

%calculate critical temperature and pressure of the mixture

[Pc] = Criticalmix\_P(x);

[Tc] = Criticalmix\_T(x);

sum2 = 0;

for i = 1:6

sum1 = 0;

for j = 1:4

sum1 = sum1 + Aij(i,j)\*(log(1.0001-x))^j;

end

sum2 = sum2 + (Ai(i) + sum1)\*(log(Pc/P))^i;

end

Td = Tc - sum2/1.8; %unit conversion -- dew point temperature (K)

end

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: enthalpy of the mixture (in liquid phase) kJ/kmol(mix)

function [enthalpymix\_l] = enthalpy\_mixture\_l(T,P,y)

%constants

la=enthalpy\_la(T,P);

lw=enthalpy\_lw(T,P);

mix=enthalpyex\_liquidm(T,P,y);

enthalpymix\_l=y\*la+(1-y)\*lw+mix; %kJ/kmol(mix)

end

%input: pressure (bar) and temperature (K)

%output: pure liquid ammonia enthalpy kJ/kmol (ammonia)

function [enthalpyla] = enthalpy\_la(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

hlroa=4.878573;

Troa=3.2252;

Proa=2.0;

Aa=[3.971423\*10^(-2) -1.790557\*10^(-5) -1.308905\*10^(-2) 3.752836\*10^(-3)];

Ba=[1.634519\*10 -6.508119 1.448937];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

enthalpyla=-R\*T\_B\*(-hlroa+Ba(1)\*(Troa-Tr)+Ba(2)/2\*(Troa\*Troa-Tr\*Tr)+Ba(3)/3\*(power(Troa,3)-power(Tr,3))-(Aa(1)+Aa(4)\*Tr\*Tr)\*(Pr-Proa)-Aa(2)/2\*(Pr\*Pr-Proa\*Proa)); %kJ/kmol (ammonia)

end

%input: pressure (bar) and temperature (K)

%output: pure liquid water enthalpy kJ/kmol (water)

function [enthalpylw] = enthalpy\_lw(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

hlrow=21.821141;

Trow=5.0705;

Prow=3.0;

Aw=[2.748796\*10^(-2) -1.016665\*10^(-5) -4.452025\*10^(-3) 8.389246\*10^(-4)];

Bw=[1.214557\*10 -1.898065 2.911966\*10^(-1)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

enthalpylw=-R\*T\_B\*(-hlrow+Bw(1)\*(Trow-Tr)+Bw(2)/2\*(Trow\*Trow-Tr\*Tr)+Bw(3)/3\*(power(Trow,3)-power(Tr,3))-(Aw(1)+Aw(4)\*Tr\*Tr)\*(Pr-Prow)-Aw(2)/2\*(Pr\*Pr-Prow\*Prow)); %kJ/kmol (water)

end %enthalpylw=enthalpylwmolar/18.01528;

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: excess enthalpy of the mixture (in liquid phase) kJ/kmol (mix)

function [enthalpyex\_liquidmix] = enthalpyex\_liquidm(T,P,y)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

E=[-41.733398 0.02414 6.702285 -0.011475 63.608967 -62.490768 1.761064 0.008626 0.387983 -0.004772 -4.648107 0.836376 -3.553627 0.000904 24.361723 -20.736547];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

enthalpyex\_liquidmix=-R\*T\_B\*(1-y)\*y\*(-E(1)-E(2)\*Pr-2\*E(5)/Tr-3\*E(6)\*power(Tr,-2)+(2\*y-1)\*(-E(7)-E(8)\*Pr-2\*E(11)/Tr-3\*E(12)\*power(Tr,-2))+power((2\*y-1),2)\*(-E(13)-E(14)\*Pr-2\*E(15)/Tr-3\*E(16)\*power(Tr,-2))); %kJ/kmol (mix)

end %enthalpyex\_liquidmix=enthalpyex\_liquidmixmolar/(18.01528\*(1-y)+17.0306\*y);%kJ/kg

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: enthalpy of the mixture (in gaseous phase) kJ/kmol (mix)

function [enthalpymix\_g] = enthalpy\_mixture\_g(T,P,y)

%constants

ga=enthalpy\_ga(T,P);

gw=enthalpy\_gw(T,P);

enthalpymix\_g=y\*ga+(1-y)\*gw;

end %kJ/kmol (mix)

%input: pressure (bar), temperature (K)

%output: pure ammonia vapor enthalpy kJ/kmol (ammonia)

function [enthalpyga] = enthalpy\_ga(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

hgroa=26.468879;

Troa=3.2252;

Proa=2.0;

Ca=[-1.049377\*10^(-2) -8.288224 -6.647257\*10^(2) -3.045352\*10^(3)];

Da=[3.673647 9.989629\*10^(-2) 3.617622\*10^(-2)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

enthalpyga=-R\*T\_B\*(-hgroa+Da(1)\*(Troa-Tr)+Da(2)/2\*(Troa\*Troa-Tr\*Tr)+Da(3)/3\*(power(Troa,3)-power(Tr,3))-Ca(1)\*(Pr-Proa)-4\*Ca(2)\*(Pr\*power(Tr,-3)-Proa\*power(Troa,-3))-12\*Ca(3)\*(Pr\*power(Tr,-11)-Proa\*power(Troa,-11))-4\*Ca(4)\*(power(Pr,3)\*power(Tr,-11)-power(Proa,3)\*power(Troa,-11))); %kJ/kmol (ammonia)

end %enthalpyga=enthalpygamolar/17.0306;%kJ/kg (ammonia)

%input: pressure (bar) and temperature (K)

%output: pure water vapor enthalpy kJ/kmol (water)

function [enthalpygw] = enthalpy\_gw(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

hgrow=60.965058;

Trow=5.0705;

Prow=3.0;

Cw=[2.136131\*10^(-2) -3.169291\*10^(1) -4.634611\*10^(4) 0.0];

Dw=[4.019170 -5.175550\*10^(-2) 1.951939\*10^(-2)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

enthalpygw=-R\*T\_B\*(-hgrow+Dw(1)\*(Trow-Tr)+Dw(2)/2\*(Trow\*Trow-Tr\*Tr)+Dw(3)/3\*(power(Trow,3)-power(Tr,3))-Cw(1)\*(Pr-Prow)-4\*Cw(2)\*(Pr\*power(Tr,-3)-Prow\*power(Trow,-3))-12\*Cw(3)\*(Pr\*power(Tr,-11)-Prow\*power(Trow,-11))-4\*Cw(4)\*(power(Pr,3)\*power(Tr,-11)-power(Prow,3)\*power(Trow,-11))); %kJ/kmol (water)

end %enthalpygw=enthalpygwmolar/18.01528; %kJ/kg (water)

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: entropyof the mixture (in liquid phase) kJ/kmol K (mix)

function [entropymix\_l] = entropy\_mixture\_l(T,P,y)

%constants

la=entropy\_la(T,P);

lw=entropy\_lw(T,P);

lex=entropyex\_liquidm(T,P,y);

mix=entropy\_mix(y);

entropymix\_l=y\*la+(1-y)\*lw+lex+mix;

end %kJ/kmol K (mix)

%input: pressure (bar) and temperature (K)

%output: pure ammonia liquid entropy kJ/kmol K (ammonia)

function [entropyla] = entropy\_la(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

slroa=1.644773;

Troa=3.2252;

Proa=2.0;

Aa=[3.971423\*10^(-2) -1.790557\*10^(-5) -1.308905\*10^(-2) 3.752836\*10^(-3)];

Ba=[1.634519\*10 -6.508119 1.448937];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

entropyla=-R\*(-slroa-Ba(1)\*log(Tr/Troa)+Ba(2)\*(Troa-Tr)+Ba(3)/2\*(Troa\*Troa-Tr\*Tr)+(Pr-Proa)\*(Aa(3)+2\*Aa(4)\*Tr)); %kJ/kmol K (ammonia)

end %entropyla=entropylamolar/17.0306; %kJ/kgK

%input: pressure (bar) and temperature (K)

%output: pure water liquid entropy kJ/kmol K (water)

function [entropylw] = entropy\_lw(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

slrow=5.733498;

Trow=5.0705;

Prow=3.0;

Aw=[2.748796\*10^(-2) -1.016665\*10^(-5) -4.452025\*10^(-3) 8.389246\*10^(-4)];

Bw=[1.214557\*10 -1.898065 2.911966\*10^(-1)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

entropylw=-R\*(-slrow-Bw(1)\*log(Tr/Trow)+Bw(2)\*(Trow-Tr)+Bw(3)/2\*(Trow\*Trow-Tr\*Tr)+(Pr-Prow)\*(Aw(3)+2\*Aw(4)\*Tr)); % kJ/kmol K (water)

end %entropylw=entropylwmolar/18.01528; %kJ/kg K (water)

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: excess entropy of the mixture (in liquid phase) %kJ/kmol K(mix)

function [entropyex\_liquidmix] = entropyex\_liquidm(T,P,y)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

E=[-41.733398 0.02414 6.702285 -0.011475 63.608967 -62.490768 1.761064 0.008626 0.387983 -0.004772 4.648107 0.836376 -3.553627 0.000904 24.361723 -20.736547];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

entropyex\_liquidmix=-R\*(1-y)\*y\*(E(3)+E(4)\*Pr-E(5)\*power(Tr,-2)-2\*E(6)\*power(Tr,-3)+(2\*y-1)\*(E(9)+E(10)\*Pr-E(11)\*power(Tr,-2)-2\*E(12)\*power(Tr,-3))+power((2\*y-1),2)\*(-E(15)\*power(Tr,-2)-2\*E(16)\*power(Tr,-3))); %kJ/kmol K(mix)

end %entropyex\_liquidmix=entropyex\_liquidmixmolar/(18.01528\*(1-y)+17.0306\*y); %kJ/kmol K(mix)

%input: molar fraction of ammonia

%output: entropy of mixing %kJ/kmol K

function [entropy\_m] = entropy\_mix(y)

%constants

R=8.314472; %kJ/kmolK

if(y==0||y==1)

entropy\_m=0; %kJ/kmol K

else

entropy\_m=-R\*(y\*log(y)+(1-y)\*log(1-y)); %kJ/kmol K

end% entropy\_m=entropy\_mmolar/(18.01528\*(1-y)+17.0306\*y);%kJ/kgK

end

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: entropy of the mixture (in gaseous phase) kJ/kmol K (mix)

function [entropymix\_g] = entropy\_mixture\_g(T,P,y)

%constants

ga=entropy\_ga(T,P);

gw=entropy\_gw(T,P);

gmix=entropy\_mix(y);

entropymix\_g=y\*ga+(1-y)\*gw+gmix;

end%kJ/kmol K (mix)

%input: pressure (bar) and temperature (K)

%output: pure ammonia vapor entropy %kJ/kmol K (ammonia)

function [entropyga] = entropy\_ga(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

sgroa=8.339026;

Troa=3.2252;

Proa=2.0;

Ca=[-1.049377\*10^(-2) -8.288224 -6.647257\*10^(2) -3.045352\*10^(3)];

Da=[3.673647 9.989629\*10^(-2) 3.617622\*10^(-2)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

if(Pr==0)

entropyga=0;

else

entropyga=-R\*(-sgroa-Da(1)\*log(Tr/Troa)+Da(2)\*(Troa-Tr)+Da(3)/2\*(Troa\*Troa-Tr\*Tr)+log(Pr/Proa)-3\*Ca(2)\*(Pr\*power(Tr,-4)-Proa\*power(Troa,-4))-11\*Ca(3)\*(Pr\*power(Tr,-12)-Proa\*power(Troa,-12))-11/3\*Ca(4)\*(power(Pr,3)\*power(Tr,-12)-power(Proa,3)\*power(Troa,-12))); %kJ/kmol K (ammonia)

end

end %entropyga=entropygamolar/17.0306; %kJ/kg K

%input: pressure (bar) and temperature (K)

%output: pure water vapor entropy %kJ/kmol K (water)

function [entropygw] = entropy\_gw(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

sgrow=13.453430;

Trow=5.0705;

Prow=3.0;

Cw=[2.136131\*10^(-2) -3.169291\*10^(1) -4.634611\*10^(4) 0.0];

Dw=[4.019170 -5.175550\*10^(-2) 1.951939\*10^(-2)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

if(Pr==0)

entropygw=0;

else

entropygw=-R\*(-sgrow-Dw(1)\*log(Tr/Trow)+Dw(2)\*(Trow-Tr)+Dw(3)/2\*(Trow\*Trow-Tr\*Tr)+log(Pr/Prow)-3\*Cw(2)\*(Pr\*power(Tr,-4)-Prow\*power(Trow,-4))-11\*Cw(3)\*(Pr\*power(Tr,-12)-Prow\*power(Trow,-12))-11/3\*Cw(4)\*(power(Pr,3)\*power(Tr,-12)-power(Prow,3)\*power(Trow,-12))); %kJ/kmol K (water)

end

end %entropygw=entropygwmolar/18.01528;

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: specific volume of the mixture (in liquid phase) m3/kmol (mix)

function [volumemix\_l] = volume\_mixture\_l(T,P,y)

%constants

la=volume\_la(T,P);

lw=volume\_lw(T,P);

lex=volumeex\_liquidm(T,y);

volumemix\_l=y\*la+(1-y)\*lw+lex;

end %m3/kmol (mix)

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: excess specific volume of the mixture (in liquid phase) m3/kmol

function [volumeex\_liquidmix] = volumeex\_liquidm(T,y)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

E=[-41.733398 0.02414 6.702285 -0.011475 63.608967 -62.490768 1.761064 0.008626 0.387983 -0.004772 4.648107 0.836376 -3.553627 0.000904 24.361723 -20.736547];

Tr=T/T\_B; %T in K

volumeex\_liquidmix=(R\*T\_B/P\_B\*(1-y)\*y\*(E(2)+E(4)\*Tr+(2\*y-1)\*(E(8)+E(10)\*Tr)+power((2\*y-1),2)\*E(14)))/100;%m3/kmol

end%volumeex\_liquidmix=volumeex\_liquidmixmolar/(100\*(18.01528\*(1-y)+17.0306\*y)%); %m3/kg

%input: pressure (bar) and temperature (K)

%output: pure liquid water specific volume m3/kmol (water)

function [volumelw] = volume\_lw(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

Aw=[2.748796\*10^(-2) -1.016665\*10^(-5) -4.452025\*10^(-3) 8.389246\*10^(-4)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

volumelw=(R\*T\_B/P\_B\*(Aw(1)+Aw(3)\*Tr+Aw(4)\*Tr\*Tr+Aw(2)\*Pr))/100; %m3/kmol (water)

end %volumelw=volumelwmolar/(18.01528\*100); %m3/kg (water)

%input: pressure (bar) and temperature (K)

%output: pure liquid ammonia specific volume m3/kmol (ammonia)

function [volumela] = volume\_la(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

Aa=[3.971423\*10^(-2) -1.790557\*10^(-5) -1.308905\*10^(-2) 3.752836\*10^(-3)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

volumela=(R\*T\_B/P\_B\*(Aa(1)+Aa(3)\*Tr+Aa(4)\*Tr\*Tr+Aa(2)\*Pr))/100; %m3/kmol (ammonia)

end %volumela=volumelamolar/(17.0306\*100); %m3/kg (ammonia)

%input: pressure (bar), temperature (K) and molar fraction of ammonia

%output: specific volume of the mixture (in gaseous phase) m3/kmol (mix)

function [volumemix\_g] = volume\_mixture\_g(T,P,y)

%constants

ga=volume\_ga(T,P);

gw=volume\_gw(T,P);

volumemix\_g=y\*ga+(1-y)\*gw;

end %m3/kmol (mix)

%input: pressure (bar) and temperature (K)

%output: pure ammonia vapor specific volume m3/kmol (ammonia)

function [volumega] = volume\_ga(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

Ca=[-1.049377\*10^(-2) -8.288224 -6.647257\*10^(2) -3.045352\*10^(3)];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

if(Pr==0)

volumega=0;

else

volumega=(R\*T\_B/P\_B\*(Tr/Pr+Ca(1)+Ca(2)\*power(Tr,-3)+Ca(3)\*power(Tr,-11)+Ca(4)\*power(Pr,2)\*power(Tr,-11)))/100; %m3/kmol (ammonia)

end

end %volumega=volumegamolar/(17.0306\*100); %m3/kg (ammonia)

%input: pressure (bar) and temperature (K)

%output: pure water vapor specific volume m3/kmol (water)

function [volumegw] = volume\_gw(T,P)

%constants

R=8.314472; %kJ/kmolK

T\_B=100; %K

P\_B=10; %bar

Cw=[2.136131\*10^(-2) -3.169291\*10^(1) -4.634611\*10^(4) 0.0];

Tr=T/T\_B;Pr=P/P\_B; %T and P are in K

if(Pr==0)

volumegw=0;

else

volumegw=(R\*T\_B/P\_B\*(Tr/Pr+Cw(1)+Cw(2)\*power(Tr,-3)+Cw(3)\*power(Tr,-11)+Cw(4)\*power(Pr,2)\*power(Tr,-11)))/100; %m3/kmol (water)

end

end %volumegw=volumegwmolar/(18.01528\*100); %m3/kg (water)

%input: Temperature (K) and mass fraction

%output: Bubble point pressure of the mixture (bar)

function [Pb] = Bubble\_P(T,x)

Pb=Criticalmix\_P(x);

Tb=1000;

incr=10;

while (abs(T-Tb)>.0001)

while (T-Tb<0)

Pb=Pb-incr;

while(Pb<=incr)

Pb=Pb+incr;

incr=incr/10;

end

Tb=Bubble\_T(Pb,x);

end

Pb=Pb+incr;

Tb=Bubble\_T(Pb,x);

incr=incr/10;

end

end

%input: Temperature (K) and mass fraction

%output: Dew point pressure of the mixture (bar)

function [Pd] = Dew\_P(T,x)

function [Pd] = Dew\_P(T,x)

Pd=Criticalmix\_P(x);

Td=1000;

incr=10;

while (abs(T-Td)>.0001)

while (T-Td<0)

Pd=Pd-incr;

while(Pd<=incr)

Pd=Pd+incr;

incr=incr/10;

end

Td=Dew\_T(Pd,x);

end

Pd=Pd+incr;

Td=Dew\_T(Pd,x);

incr=incr/10;

end

end