Plot

Initial Conditions -

%critical point for oxygen

Tc=154.6;

Pc=5.046e6;

R=8.314;

%vanderwall's constants

A=(27\*((R\*Tc)^2))/(64\*Pc);

B=(R\*Tc)/(8\*Pc);

%coefficients in constant pressure heat capacity

a = 28.167;

b = 0.630e-2;

c = -0.075e-5;

%reference state -

H\_ref = 0;

S\_ref = 0;

T\_ref = 298.15;

P\_ref = 1e5;

axes for plotting

T=[10 100 200 300 400 500 600]+273.15;

P=logspace(0,2,300)\*1e5;

enth = zeros(1, size(P, 2));

ent = zeros(1, size(P, 2));

nt = size(T, 2);

np = size(P, 2);

enthalpy plot (KJ/mol Vs Bar)-

hold on;

for t = 1:nt

for p = 1:np

enth(1, p) = 0.001\*enthalpy(T(1, t), P(1, p), [T\_ref, P\_ref, H\_ref], [A B], [a b c], R);

end

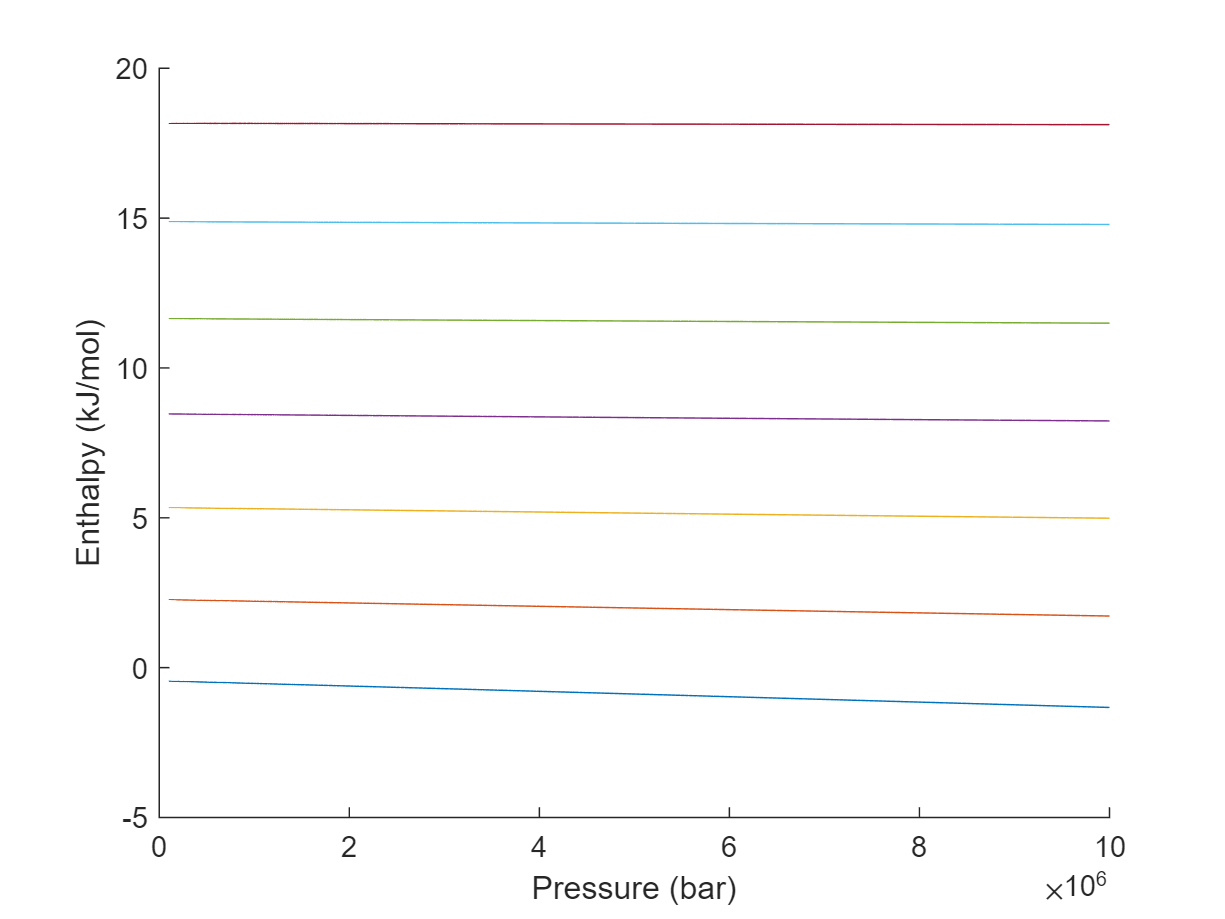
plot(P, enth);

end

xlabel("Pressure (bar)");

ylabel("Enthalpy (kJ/mol)");

hold off



entropy plot (J/K Vs Bar)-

figure;

hold on

for t = 1:nt

for p = 1:np

ent(1, p) = entropy(T(1, t), P(1, p), [T\_ref, P\_ref, S\_ref], [A B], [a b c], R);

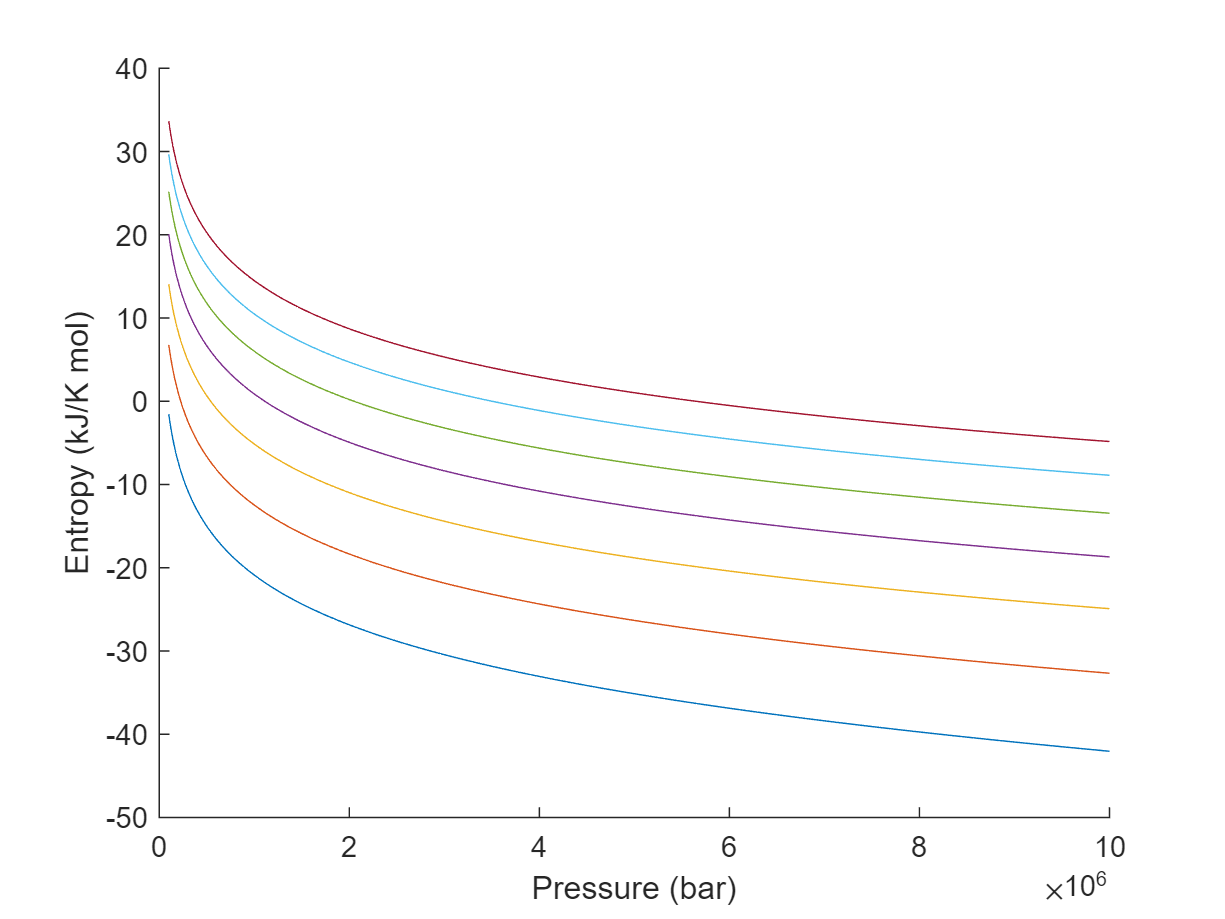
end

plot(P, ent);

end

xlabel("Pressure (bar)");

ylabel("Entropy (kJ/K mol)");



Correction – entropy has units J/K mol

Enthalpy

function y = enthalpy(T, P, referenceState, vdW\_consts, CpConsts, R)

vander walls constants -

A=vdW\_consts(1);

B=vdW\_consts(2);

coefficients in constant pressure heat capacity -

a = CpConsts(1);

b = CpConsts(2);

c = CpConsts(3);

reference state -

T\_ref = referenceState(1);

P\_ref = referenceState(2);

H\_ref = referenceState(3);

V\_ref = ((R\*T\_ref)/P\_ref)\*Z(T\_ref, P\_ref, [A B]);

V = (R\*T/P)\*Z(T, P, [A B]);

indivisual integrals -

H\_PV = R\*(T\_ref - T) + P\*V - P\_ref\*V\_ref;

H\_dPdT = A/V\_ref - A/V;

H\_Cp = a\*(T - T\_ref) + b\*(T^2 - T\_ref^2)/2 + c\*(T^3 - T\_ref^3)/3;

final enthalpy -

y = H\_PV + H\_dPdT + H\_Cp + H\_ref;

end

Entropy

function y = entropy(T, P, referenceState, vdW\_consts, CpConsts, R)

vanderwall's constants

A=vdW\_consts(1);

B=vdW\_consts(2);

coefficients in constant pressure heat capacity

a = CpConsts(1);

b = CpConsts(2);

c = CpConsts(3);

reference state -

T\_ref = referenceState(1);

P\_ref = referenceState(2);

S\_ref = referenceState(3);

V\_ref = ((R\*T\_ref)/P\_ref)\*Z(T\_ref, P\_ref, [A B]);

V = (R\*T/P)\*Z(T, P, [A B]);

indivisual integrals -

S\_Cp = (a-R)\*log(T/T\_ref) + b\*(T-T\_ref) + c\*(T^2 - T\_ref^2)/2;

S\_dpdT = R\*log((V-B)/(V\_ref-B));

final entropy -

y = S\_Cp + S\_dpdT + S\_ref;

end

Derivation of Functions Of Enthalpy and entropy -

