Semester Long Internship Report

On

Modelling and Simulation in OpenModelica and DWSIM

Submitted by

Naik Yutika Niralkumar

Under the guidance of

Prof. Kannan Moudgalya

Chemical Engineering Department

IIT Bombay

July 24, 2021

Acknowledgement

I wish to express my deepest gratitude to my internship guide Dr.Kannan M.Moudgalya, Professor, Department of Chemical Engineering, IIT Bombay for his continuous support and supervision throughout the internship.I have reaped benefits from his wisdom, guidance and patience.I would also like to extend my gratitude to Priyam Nayak and Malapati Sree Harsha of the department of Chemical Engineering,IIT Bombay, FOSSEE Team for their help and guidance.

Contents

1 Introduction to OpenModelica

OpenModelica is a free and open-source modelling environment that uses "Modelica" modelling language. It follows equation oriented approach. OpenModelica can be used for modelling, simulation, optimization and analysis of complex steady state and dynamic systems. Modelica modelling language allows users to express a system in the form of equations. OpenModelica complies expressions, equations, functions and algorithms into C code. The generated C code is combined with a library of utility functions, a run-time library, and a numerical Differential-Algebric Equation (DAE) solver. OpenModelica Connection Editor, called as OMEdit is the integrated Graphical User Interface (GUI) in OpenModelica for graphical modelling and editing. OMEdit consists of several libraries for various domains like Electrical, Magnetic, Math, Thermal, etc. It provides various user friendly features like representation of a model in the form of block diagrams. OMEdit can be used for creating custom models and for editing or drawing connections between the model interfaces. It also allows users to plot graphs between parameters of the model simulated.

2 Modelling in OpenModelica

2.1 SRK model

In 1972, Soave proposed an important modification to the RK EOS — or shall we say, a modification to vdW EOS. Between the time of vdW EOS and Redlich-Kwong's, a new concept for fluid characterization was being discussed. Pitzer had introduced the concept of acentric factor in 1955.

All modifications to the vdW EOS had focused on the temperature dependency of the attractive parameter. Soave expanded this by proposing a two-variable dependency for "a":

$$a = a(T, \omega) \tag{1}$$

It was the first time that "a" was expressed not only as a function of temperature, but also as a function of the shape (sphericity) of the molecules (through w, Pitzer's acentric factor). As we recall, Pitzer's acentric factor is a measure of the configuration and sphericity of the molecule. It can also be seen as a measure of the deformity of the molecule.

The Soave-Redlich-Kwong EOS is given by the expression:

$$(P + \alpha a\tilde{\nu}(\tilde{\nu} + b))(\tilde{\nu} - b) = RT \tag{2}$$

Like all cubic equations of state, the SRK EOS is also explicit in pressure. Notice, for example, how the SRK EOS readily becomes:

$$P = RT\tilde{\nu} - b\alpha a\tilde{\nu}(\tilde{\nu} + b) \tag{3}$$

where,

$$\alpha = 1 + (0.48508 + 1.55171\omega - 0.15613\omega^2)(1 - (Tr)^{1/2})^2) \tag{4}$$

The influence of acentric factor and temperature on the attractive term is introduced now through "a". What do we do next? We apply the criticality conditions to equation (3). Notice that expression (4) becomes unity at Tr=1, throughout the critical isotherm. We obtain:

$$a = 0.427480(R^2Tc^2/Pc) \tag{5}$$

$$b = 0.086640(RTc/Pc) \tag{6}$$

Now we show the cubic form (in compressibility factor) of Soave-Redlich-Kwong EOS. Defining,

$$A = (\alpha a P)/R^2T^2 \tag{7}$$

$$B = bP/RT \tag{8}$$

we are able to obtain:

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0 \tag{9}$$

For mixtures, Soave proposed a "little" modification to the mixing rules with which we have dealt with so far by introducing the use of "binary interaction parameters" (kij):

$$(\alpha a)m = \sum\sum yiyj(\alpha a)ij; (\alpha a)ij = ((\alpha a)i(\alpha a)j)^{1/2}(1 - kij) \tag{10}$$

$$bm = \sum yibi \tag{11}$$

The use of binary interaction parameters (kij) generated a lot of resistance upon their first introduction. This is because there is no analytical, science-based derivation that justifies their existence. Nowadays, they are regarded just as they are, empirical factors used to tune equations of state and make them match experimental data for mixtures. This has become the heuristic justification for their existence: with them, EOS can do a better job of matching experimental data. Heuristically speaking, they are a measure of interaction between a pair of dislike molecules. Based on this "definition," their value is zero for pairs of molecules that are alike. Actually, this is no more than a mathematical requirement in order for equation (10) to give$(\alpha a)ij = (\alpha a)i$when j=i. The determination of kij is based on experimental data from binary systems; "kij" results from the value that allows the given equation of state (through the expression in equation 10) to yield the closest match. These values are assumed to be constant (and so are used) when the same two components are part of a more complex multi-component mixture.

Code:

```
model SRK

//Soave - Redlich - Kwong Equation Of State
//=========================================================
//Naik Yutika Niralkumar
//Sardar Vallabhbhai National Institue of Technology, Surat
//=========================================================
//Parameter Section

parameter Real bip[Nc, Nc] = BIPSRK(Nc, C.CAS) "binary interaction
    parameter which characterizes the i-j pair";

parameter Real R(unit = "J/(mol K)") = 8.314 "Universal Gas
    Constants";

//Real MW[Nc](unit = "kg/kgmol")  "Molecular Weight";

//Real z[Nc]"Molar Composition of Feed";

//Real Tc1[Nc](unit = "K")  "Critical Temperature";

//Real Pc[Nc](unit = "Pa")  "Critical Pressure";

//Real omega[Nc]  "Acentric Factor";

Real uu = 1, ww = 0;

Real Cpres_p[Nc]  "residual specific heat";

Real Hres_p[Nc]  "residual enthalpy";

Real Sres_p[Nc]  "residual Entropy";

Real Pbubl(unit = "Pa", min = 0, start = Pmin) "Bubble point
    pressure";

Real gma_c[Nc], gmabubl_c[Nc], gmadew_c[Nc] "Excess Energy
    Properties";

Real philiqbubl_c[Nc]  "Fugacity Coefficient in Liquid Phase at
    bubble point", phivapdew_c[Nc]  "Fugacity Coefficient in Liquid
    Phase at dew point", Pvap_c[Nc]  "Vapour pressure of compound i";

//==========
//Variable Section
```

```
40
41
42
43 Real a[Nc](each start = 1) "SRK EOS Constants";
44 Real b[Nc](each start = 0) "SRK EOS Constants";
45
46 Real aml2[Nc], bml2[Nc], amv2[Nc], bmv2[Nc];
47 Real aml "SRK EOS Constant for Liquid Mixture";
48 Real bml "SRK EOS Constant for Liquid Mixture";
49
50 Real amv "SRK EOS Constant for Vapour Mixture";
51 Real bmv "SRK EOS Constant for Vapour Mixture";
52
53 Real Al "SRK EOS Constant for Liquid Mixture";
54 Real Bl "SRK EOS Constant for Liquid Mixture";
55
56 Real Av "SRK EOS Constant for Vapour Mixture";
57 Real Bv "SRK EOS Constant for Vapour Mixture";
58
59 Real Zl(start = 0) "Compressibility Factor of Liquid";
60 Real Zv(start = 1) "Compressibility Factor of Vapour";
61
62 //Real x[Nc](each start = 1, each min = 0, each max = 1) "Mole
       Fraction in Liquid Phase";
63 //Real y[Nc](each start = 1, each min = 0, each max = 1) "Mole
       Fraction in Vapour Phase";
64
65 Real r[Nc];
66 Real s[Nc];
67
68 Real t1[Nc], t2, t3[Nc], t4, t5;
69 Real u1[Nc], u2, u3[Nc], u4, u5;
70
71 //Real beta(start = 0) "Mole Fraction of Feed Vapourized";
72
73 Real phil[Nc](each start = 1) "Fugacity Coefficient in Liquid Phase"
       ;
74 Real phiv[Nc](each start = 1) "Fugacity Coefficient in Vapour Phase"
       ;
75
76 Real K_c[Nc](each start = 1) "Equilibrium Constant";
77
78 Real c[Nc] " Compound i" ;
79 Real a1, al, av, dadT[2], al2[Nc], av2[Nc];
80 Real AMWl(unit = "kg/kgmol") "Average Molecular Weight of Liquid
       Mixture";
```

```
Real AMWv(unit = "kg/kgmol") "Average Molecular Weight of Vapour
    Mixture";
Real mDHres[2](unit = "kJ/kmol") "Residual Molar Enthalpy";
Real mDSres[2](unit = "kJ/(kmol K)") "Residual Molar Entropy";
Real DHres[2](unit = "kJ/kg") "Residual Specific Enthalpy";
Real DSres[2](unit = "kJ/(kg K)") "Residual Specific Entropy";
Real DAres[2](unit = "kJ/kmol") "Residual Specific Helmoltz Free
    Energy";

//==========
//Equation Section

equation

//Calculation of equation of state constants

Cpres_p[:] = zeros(Nc);

Hres_p[:] = zeros(Nc);

Sres_p[:] = zeros(Nc);

for i in 1:Nc loop
      Pvap_c[i] = Simulator.Files.ThermodynamicFunctions.Psat(C[i].
    VP, T);
      gmadew_c[i] = 1;
      gmabubl_c[i] = 1;
      philiqbubl_c[i] = 1;
      phivapdew_c[i] = 1;
      gma_c[i] = 1;
end for;
//Calculation of SRK EOS Constants for Liquid and Vapour Phases

  aml = sum(aml2);
  bml = sum(bml2);

  Al = (aml*P)/((R*T)^2);
  Bl = (bml*P)/(R*T);

  (Zl^3)-(Zl^2)+((Al-Bl-(Bl^2))*Zl)-(Al*Bl) = 0;  //Compressibility
    Factor of Liquid Mixture

  amv = sum(amv2);
  bmv = sum(bmv2);

  Av = (amv*P)/((R*T)^2);
```

```
123   Bv = (bmv*P)/(R*T);
124
125   (Zv^3)-(Zv^2)+((Av-Bv-(Bv^2))*Zv)-(Av*Bv) = 0;  //Compressibility
       Factor of Vapour Mixture
126
127   t2 = -log(Zl-Bl);
128   t4 = log((Zl+Bl)/Zl);
129   t5 = Bl;
130
131   u2 = -log(Zv-Bv);
132   u4 = log((Zv+Bv)/Zv);
133   u5 = Bv;
134
135 for i in 1:Nc loop
136   t1[i] = b[i]*(Zl-1)/bml;
137   t3[i] = Al*((2*r[i]/aml)-(b[i]/bml));
138
139
140   u1[i] = b[i]*(Zv-1)/bmv;
141   u3[i] = Av*((2*s[i]/amv)-(b[i]/bmv));
142
143
144 //Calculation of Fugacity Coefficients of Components in Liquid and
       Vapour Phases
145
146   phil[i] = exp(t1[i]+t2-(t3[i]*t4/t5));
147   phiv[i] = exp(u1[i]+u2-(u3[i]*u4/u5));
148
149 //Calculation of Equilibrium Constants
150
151   K_c[i] = phil[i]/phiv[i];
152
153 //Calculation of SRK EOS Constants of Components
154
155   a[i] = ((1+((0.48+(1.574*C[i].AF)-(0.176*(C[i].AF^2)))*(1-((T/C[i
       ].Tc)^0.5))))^2)*((0.42747*(R*R*C[i].Tc*C[i].Tc))/C[i].Pc);
156   b[i] = 0.08664*R*C[i].Tc/C[i].Pc;
157
158   aml2[i] = sum(x_pc[2,i].*x_pc[2,:].*((a[i].*a[:]).^0.5)*(1-bip[Nc,
        Nc]));
159   bml2[i] = (x_pc[2,i]*b[i]);
160
161   amv2[i] = sum(x_pc[3,i]*x_pc[3,:].*((a[i]*a[:]).^0.5)*(1-bip[Nc,
       Nc]));
162   bmv2[i] = (x_pc[3,i]*b[i]);
163
```

```
164   r[i] = sum(x_pc[2,:].*((a[:].*a[i]).^0.5));
165   s[i] = sum(x_pc[3,:].*((a[:].*a[i]).^0.5));
166
167   c[i] = 0.48 + 1.574 * C[i].AF - 0.176 * C[i].AF ^ 2;
168   av2[i] = sum(x_pc[3,i].*x_pc[3,:].*(c[:].*(a[i].*C[i].Tc./C[i].Pc)
        .^0.5+c[i].*(a[:].*C[i].Tc./C[i].Pc).^0.5));
169   al2[i] = sum(x_pc[2,i].*x_pc[2,:].*(c[:].*(a[i].*C[i].Tc./C[i].Pc)
        .^0.5+c[i].*(a[:].*C[i].Tc./C[i].Pc).^0.5));
170 end for;
171
172 //Calculation of Average Molecular Weights of Liquid and Vapour
      Phases
173
174   AMWv = sum(x_pc[3,:].*C.MW);
175   AMWl = sum(x_pc[2,:].*C.MW);
176
177 //Calculation of Intermediate Values
178
179 a1 = -R / 2 * (0.42748 / T) ^ 0.5;
180
181 al = sum(al2);
182 av = sum(av2);
183
184 dadT[1] = a1*al;
185 dadT[2] = a1*av;
186
187 //Calculation of Residual Properties of Liquid Phase
188
189   DAres[1] = aml/(bml*(uu^2-4*ww)^0.5)*log((2*Zl+Bl*(uu-(uu^2-4*ww)
        ^0.5))/(2*Zl+Bl*(uu+(uu^2-4*ww)^0.5)))-R*T*log((Zl-Bl)/Zl)-R*T*
        log(Zl);
190   mDSres[1] = R*log((Zl-Bl)/Zl)+R*log(Zl)-uu/((uu^2-4*ww)^0.5*bml)*
        dadT[1]*log((2*Zl+Bl*(uu-(uu^2-4*ww)^0.5))/(2*Zl+Bl*(uu+(uu^2-4*
        ww)^0.5)));
191   mDHres[1] = DAres[1]+T*mDSres[1]+R*T*(Zl-1);
192   DHres[1] = mDHres[1]/AMWl;
193   DSres[1] = mDSres[1]/AMWl;
194
195 //Calculation of Residual Properties of Vapour Phases
196
197   DAres[2] = amv/bmv*log((2*Zv+Bv*(uu-(uu^2-4*ww)^0.5))/(2*Zv+Bv*(uu
        +(uu^2-4*ww)^0.5)))-R*T*log((Zv-Bv)/Zv)-R*T*log(Zv);
198   mDSres[2] = R*log((Zv-Bv)/Zv)+R*log(Zv)-uu/((uu^2-4*ww)^0.5*bmv)*
        dadT[2]*log((2*Zv+Bv*(uu-(uu^2-4*ww)^0.5))/(2*Zv+Bv*(uu+(uu^2-4*
        ww)^0.5)));
199   mDHres[2] = DAres[2]+T*mDSres[2]+R*T*(Zv-1);
```

```
200   DHres[2] = mDHres[2]/AMWv;
201   DSres[2] = mDSres[2]/AMWv;
202
203
204 //=======================================================
205
206
207 end SRK;
```

2.2 BIPSRK function

Binary Interaction Parameters for SRK
This function is used to get binary interaction parameters as output for the given components.

[Detailed information on binary interaction parameters is provided in the previous section.]

Code:

```
function BIPSRK

input Integer Nc;
input String CAS[Nc];
output Real BIP[Nc, Nc];
protected
constant String Us = "_";
String c_cc[Nc, Nc];
String d_cc[Nc, Nc];

constant String CAS_CAS[204] = {"74-98-6_115-07-1","106-97-8_75-28-5
    ","106-97-8_106-98-9","75-28-5_115-11-7","110-54-3_592-41-6","
    7727-37-9_7783-06-4","630-08-0_7783-06-4","124-38-9_7783-06-4","
    74-82-8_7783-06-4","74-84-0_7783-06-4","74-98-6_7783-06-4","
    106-97-8_7783-06-4","75-28-5_7783-06-4","109-66-0_7783-06-4","
    78-78-4_7783-06-4","463-82-1_7783-06-4","110-54-3_7783-06-4","
    142-82-5_7783-06-4","111-84-2_7783-06-4","124-18-5_7783-06-4","
    110-82-7_7783-06-4","108-87-2_7783-06-4","1678-91-7_7783-06-4","
    2207-04-7_7783-06-4","696-29-7_7783-06-4","71-43-2_7783-06-4","
    108-88-3_7783-06-4","108-38-3_7783-06-4","7783-06-4_7727-37-9","
    630-08-0_7727-37-9","124-38-9_7727-37-9","1333-74-0_7727-37-9","
    74-82-8_7727-37-9","74-84-0_7727-37-9","74-98-6_7727-37-9","
    106-97-8_7727-37-9","75-28-5_7727-37-9","109-66-0_7727-37-9","
    78-78-4_7727-37-9","110-54-3_7727-37-9","124-18-5_7727-37-9","
    108-87-2_7727-37-9","1678-91-7_7727-37-9","74-85-1_7727-37-9","
    115-07-1_7727-37-9","71-43-2_7727-37-9","108-88-3_7727-37-9","
    108-38-3_7727-37-9","108-67-8_7727-37-9","119-64-2_7727-37-9","
    7783-06-4_630-08-0","7727-37-9_630-08-0","124-38-9_630-08-0","
    1333-74-0_630-08-0","74-82-8_630-08-0","74-98-6_630-08-0","
    111-65-9_630-08-0","124-18-5_630-08-0","544-76-3_630-08-0","
    71-43-2_630-08-0","7783-06-4_124-38-9","7727-37-9_124-38-9","
    630-08-0_124-38-9","1333-74-0_124-38-9","74-82-8_124-38-9","
    74-84-0_124-38-9","74-98-6_124-38-9","106-97-8_124-38-9","75-28-5
    _124-38-9","109-66-0_124-38-9","78-78-4_124-38-9","463-82-1_124
    -38-9","110-54-3_124-38-9","142-82-5_124-38-9","111-65-9_124-38-9
    ","111-84-2_124-38-9","124-18-5_124-38-9","544-76-3_124-38-9","
    630-02-4_124-38-9","75-19-4_124-38-9","287-92-3_124-38-9","
    110-82-7_124-38-9","108-87-2_124-38-9","1678-91-7_124-38-9","
    74-85-1_124-38-9","115-07-1_124-38-9","106-98-9_124-38-9","
    71-43-2_124-38-9","108-88-3_124-38-9","108-38-3_124-38-9","
    106-42-3_124-38-9","100-41-4_124-38-9","100-42-5_124-38-9","
    103-65-1_124-38-9","98-82-8_124-38-9","98-83-9_124-38-9","95-63-6
    _124-38-9","108-67-8_124-38-9","101-81-5_124-38-9","90-12-0_124
    -38-9","119-64-2_124-38-9","85-01-8_124-38-9","7727-37-9_1333
    -74-0","630-08-0_1333-74-0","124-38-9_1333-74-0","74-82-8_1333
```

```
    -74-0","74-84-0_1333-74-0","74-98-6_1333-74-0","106-97-8_1333
    -74-0","109-66-0_1333-74-0","110-54-3_1333-74-0","142-82-5_1333
    -74-0","111-65-9_1333-74-0","540-84-1_1333-74-0","124-18-5_1333
    -74-0","544-76-3_1333-74-0","630-02-4_1333-74-0","110-82-7_1333
    -74-0","108-87-2_1333-74-0","74-85-1_1333-74-0","115-07-1_1333
    -74-0","71-43-2_1333-74-0","108-38-3_1333-74-0","100-18-5_1333
    -74-0","99-87-6_1333-74-0","101-81-5_1333-74-0","90-12-0_1333
    -74-0","119-64-2_1333-74-0","85-01-8_1333-74-0","776-35-2_1333
    -74-0","7783-06-4_74-82-8","7727-37-9_74-82-8","630-08-0_74-82-8"
    ,"124-38-9_74-82-8","1333-74-0_74-82-8","74-84-0_74-82-8","
    109-66-0_74-82-8","110-54-3_74-82-8","142-82-5_74-82-8","111-65-9
    _74-82-8","124-18-5_74-82-8","544-76-3_74-82-8","110-82-7_74-82-8
    ","1678-91-7_74-82-8","71-43-2_74-82-8","108-88-3_74-82-8","
    108-38-3_74-82-8","108-67-8_74-82-8","101-81-5_74-82-8","90-12-0
    _74-82-8","119-64-2_74-82-8","85-01-8_74-82-8","776-35-2_74-82-8"
    ,"106-97-8_67-56-1","75-28-5_67-56-1","109-66-0_67-56-1","
    110-54-3_67-56-1","79-29-8_67-56-1","107-83-5_67-56-1","96-14-0
    _67-56-1","111-65-9_67-56-1","540-84-1_67-56-1","96-37-7_67-56-1"
    ,"110-82-7_67-56-1","108-87-2_67-56-1","592-41-6_67-56-1","
    592-76-7_67-56-1","625-65-0_67-56-1","111-66-0_67-56-1","110-83-8
    _67-56-1","71-43-2_67-56-1","108-88-3_67-56-1","108-38-3_67-56-1"
    ,"100-41-4_67-56-1","106-97-8_64-17-5","142-82-5_64-17-5","
    111-65-9_64-17-5","540-84-1_64-17-5","111-84-2_64-17-5","
    1120-21-4_64-17-5","96-37-7_64-17-5","110-82-7_64-17-5","108-87-2
    _64-17-5","71-43-2_64-17-5","108-88-3_64-17-5","106-42-3_64-17-5"
    ,"100-41-4_64-17-5","106-97-8_1634-04-4","78-78-4_1634-04-4","
    111-65-9_1634-04-4","540-84-1_1634-04-4","108-87-2_1634-04-4","
    106-98-9_1634-04-4","115-11-7_1634-04-4","592-76-7_1634-04-4","
    106-99-0_1634-04-4","71-43-2_1634-04-4","108-88-3_1634-04-4","
    67-56-1_1634-04-4","142-82-5_108-20-3","110-82-7_108-20-3","
    71-43-2_108-20-3","108-88-3_108-20-3","100-41-4_108-20-3"};
12
13 constant Real BIPdb[204] =
14 {0.0073,-0.0047,0.0042,0.0024,0.003,0.148,0.070,0.109,0.091,0.085,0.087,0.056,
15 0.055,0.066,0.080,0.042,0.068,0.019,0.054,0.003,0.079,0.078,0.055,0.036,0.042,
16 0.009,0.014,0.022,0.148,0.011,-0.046,0.009,0.040,0.020,0.086,0.060,0.085,0.092,
17 0.107,0.155,0.124,0.090,0.092,0.044,0.085,0.170,0.219,0.230,0.225,0.304,0.070,
18 0.011,-0.082,0.004,0.015,0.040,0.190,0.629,0.256,0.072,0.109,-0.046,-0.082,
19 -0.046,0.097,0.132,0.130,0.134,0.129,0.145,0.137,0.111,0.117,0.121,0.123,0.099
20 ,0.134,0.147,0.106,0.110,0.136,0.083,0.103,0.096,0.057,0.069,0.061,0.096,0.096
```

```
,0.076,0.096,0.126,0.067,0.070,0.090,0.090,0.076,0.058,0.134,0.116,0.155,0.230
,0.009,0.004,-0.046,0.002,0.032,0.135,0.194,0.202,0.211,0.505,1.000,0.634,0.853
,0.044,-0.041,0.361,0.604,0.076,0.178,0.530,0.906,0.327,0.610,0.767,0.740,0.898
,1.000,0.784,0.091,0.040,0.015,0.097,0.002,0.003,0.018,0.026,0.015,0.054,0.042,
0.033,0.036,0.002,0.039,0.061,0.042,0.044,0.114,0.088,0.171,0.253,0.129,0.2015,
0.2411,0.1746,0.0932,0.0777,0.1432,0.1144,0.0786,0.0616,0.098,0.1374,0.0716,0.0
759,0.0707,0.0454,0.0675,0.1122,0.1147,0.133,0.0997,0.0976,0.0709,0.0759,0.096,
0.0399,0.0863,0.0356,0.0852,0.11,0.0774,0.1108,0.1145,0.1413,0.1284,0.0183,0.01
63,0.0172,0.0236,0.0293,0.001,-0.0169,-0.0008,-0.0052,-0.0009,-0.0009,-0.034,0.
0077,-0.0112,-0.0154,-0.011,-0.0088};


algorithm
for i in 1:Nc loop
  for j in 1:Nc loop
    for k in 1:2 loop
      BIP[i, j] := 0;
    end for;
  end for;
end for;
for i in 1:Nc loop
 for j in 1:Nc loop
    c_cc[i, j] := CAS[i] + Us + CAS[j];
    d_cc[i, j] := CAS[j] + Us + CAS[i];
    for k in 1:204 loop
      if c_cc[i, j] == CAS_CAS[k] then
        BIP[i, j] := BIPdb[k];
        BIP[j, i] := BIPdb[k];
        BIP[i, j] := BIPdb[k];
        BIP[j, i] := BIPdb[k];
      end if;
      if d_cc[i, j] == CAS_CAS[k] then
        BIP[j, i] := BIPdb[k];
        BIP[i, j] := BIPdb[k];
        BIP[i, j] := BIPdb[k];
        BIP[j, i] := BIPdb[k];
```

```
57        end if;
58      end for;
59    end for;
60  end for;
61
62  end BIPSRK;
```

3 Flowsheets in OpenModelica

3.1 Hydrogen Production

Background and Description:
Water Gas Shift reaction is one of the most important ways of producing pure hydrogen in chemical industry as it provides a cheap and effective way for industrial uses like ammonia synthesis. The future is focused on the idea of Hydrogen Economy; hence producing pure hydrogen from WGSR is beneficial. WSGR also helps in increasing the battery of fuel cells with hydrogen production and reducing the concentrations of carbon monoxide. It involves the reaction of Carbon Monoxide with steam to form carbon dioxide and hydrogen. It is an equilibrium reaction with conversion rate of approximately 80 percent. The initial amount of carbon monoxide and steam are 15.278 mol/s and 19.444 mol/s. Both CO and H2O are mixed and sent to an conversion reactor where they are reacted in vapour phase. After reaction, the vapour phase products are passed through a condenser/cooler where the vapour phase mol fraction dropped to 0.36. The outlet stream is passed to a separator where the vapour stream contains 0.9745 mole fraction of hydrogen and liquid stream is let out. The hydrogen stream is again passed through a cooler which is liquefies the pure hydrogen. Approximately 12.1818 mol/s of liquid hydrogen are formed.

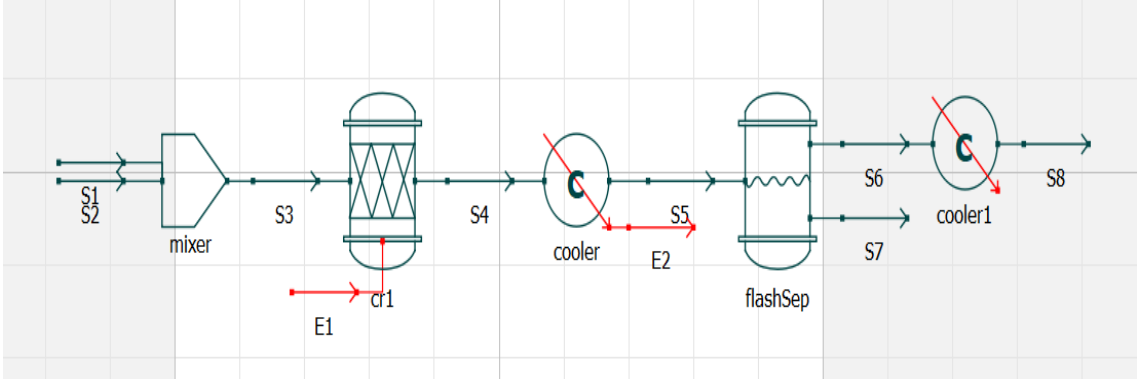
System of unit:
The system of units taken in this flowsheet are SI.

Thermodynamic package:
Raoult's law

Reaction:

$CO + H2O \leftrightarrow CO2 + H2$ (ΔH at 298 ℃ = -41.1 kJ /mol)

Flowsheet:



Results:

Object	S1	S2	S3	S4	S5	S6	S7	S8
Pressure (Pa)	101320	101325	101322	101322	101322	101322	101322	101322
Mass Flow (kg/s)	427.937	350.284	778.221	778.221	778.221	33.479	744.746	33.479
Molar Flow (mol/s)	15.278	19.444	34.722	34.722	34.722	12.5004	22.2216	12.5004
Mole fraction(Hydrogen)	0	0	0	0.352254	0.352254	0.9745	0.00221	0.9745

3.2 Refrigeration Cycle

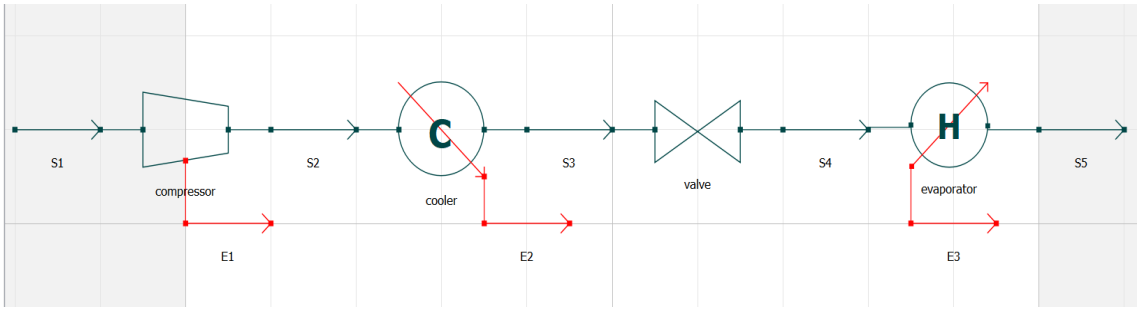
Background and Description:
Vapor Compression Refrigeration system is one in which the refrigerant undergoes phase changes, is one of the many refrigeration cycles and it is widely used method for air conditioning and in automobiles. It is also used in domestic and commercial refrigerators, large-scale warehouses for chilled or frozen storage of foods and meats, refrigerated trucks and railroad cars, and host of other commercial and industrial services. Oil refineries, petrochemical and chemical processing plants and natural gas processing plants are among the many industrial plants that often utilize large vapor-compression refrigeration systems.In very basic terms, refrigeration systems are used to remove heat from one area and transfer it into another area.
The vapor compression system simulated here uses propane as the liquid refrigerant medium because of its favorable properties.Circulating refrigerant enters the adiabatic compressor in the thermodynamic state known as saturated vapor, the compressor increases it pressure and temperature and propane leaves the compressor in the super-heated vapor state.This super-heated vapor now enters the condenser which converts it to a saturated liquid at the same pressure. Now this saturated liquid is at a high pressure hence it is throttled with the help of a valve and a vapor-liquid mixture at atmospheric pressure is sent to an evaporator which converts the mixture to saturated vapor and the outlet stream from the evaporator is recycled and sent as the input to the adiabatic compressor

System of unit:
The system of units taken in this flowsheet are SI.

Thermodynamic package:

Raoult's Law

Flowsheet:



Results:

Object	S1	S2	S3	S4	S5
Pressure (Pa)	101325	960000	960000	101325	101325
Temperature(K)	230.945	447.519	298.149	298.149	230.945
Molar Flow (mol/s)	22.68	22.68	22.68	22.68	22.68
Mole fraction(Propane)	1	1	1	1	1

4 Introduction to DWSIM

DWSIM is an open-source CAPE-OPEN compliant chemical process simulator for Windows, Linux and macOS. DWSIM is built on top of the Microsoft .NET and Mono Platforms and features a Graphical User Interface (GUI), advanced thermodynamics calculations, reactions support and petroleum characterization / hypothetical component generation tools.
DWSIM is able to simulate steady-state, vapor–liquid, vapor–liquid-liquid, solid–liquid and aqueous electrolyte equilibrium processes.

5 Characterization of Petroleum in DWSIM

The characterization of petroleum fractions requires several measurable laboratory properties:
1) Specific gravity (SG)
2) Boiling point curve (ASTM or true boiling point (TBP distillation)
3) Kinematic viscosity at 37.8 C (100 F) and 98.9 C (210 F) (n100, n210)
4) Refractive index (n)
5) Molecular weight (M)

With the exception of TBP distillation and molecular weight, these properties can be readily measured in any petroleum characterization laboratory.

The Google Sheet link for Petroleum Characterization in DWSIM: Characterization of Petroleum

6 Flowsheets in DWSIM

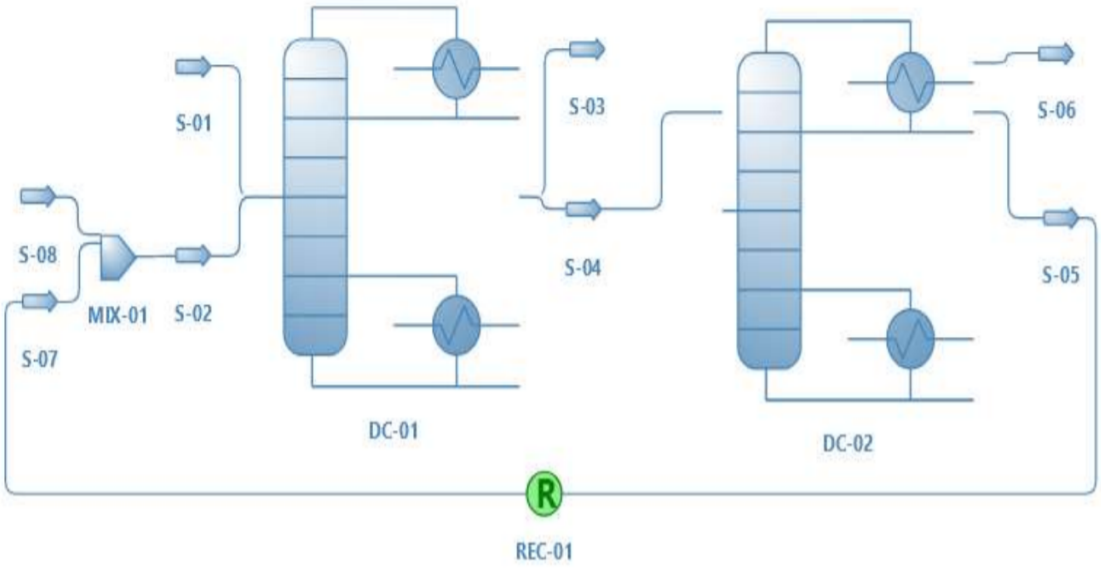
6.1 Heptane-Toluene Separation

Background and Description:
When the two components in a binary mixture have very close normal boiling points, their relative volatility is likely to be small if they do not form an azeotrope. For such cases, it may be more efficient to use extractive distillation with a solvent than normal distillation. In extractive distillation, a less volatile solvent is used to increase the relative volatilities of the original mixtures, allowing for easier separation. In this flowsheet, phenol is used as the solvent for the separation of n-heptane and toluene.
2 extractive distillation columns have been used with phenol as a solvent. After first distillation, n-heptane is a major component in top product with mole fraction of 0.987793 and as a bottom product, we get phenol (0.545804) and toluene (0.450301). To recover phenol, we add another column in which we take bottom product of previous column as a feed. After distillation in second column, phenol is recovered as a bottom product and used as a recycle stream along with a makeup stream of phenol.

System of Units:
Temperature : ℃,
Pressure : bar,
Molar flow : Kmol/h,
Mass flow : kg/h

Property Package:
UNIFAC

Flowsheet:



Results:

Object	Feed (S-01)	Solvent (S-02)	Top1 (S-03)	Bottom1 (S-04)	Bottom2 (S-05)	Top2 (S-06)	Recycle (S-07)	Make-up (S-08)
Pressure(bar)	1	1	1	1	1	1	1	1.01325
Temperature(C)	100.732	180.359	98.147	123.875	180.830	109.884	180.83	25
Mole fraction of n-heptane	0.5	9.16E-15	0.987793	0.003895	9.19E-09	0.00856	9.19E-15	0
Mole fraction of toluene	0.5	8.24E-08	0.009159	0.450301	8.27E-08	0.99049	8.28E-08	0
Mole fraction of phenol	0	1	0.003047	0.545804	1	0.00094	1	1

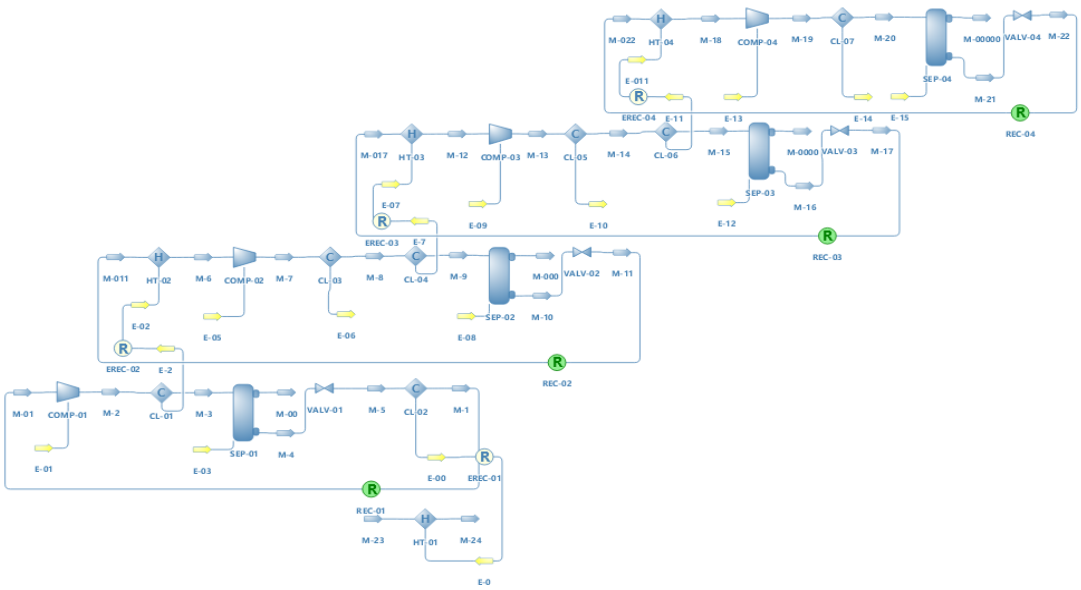
6.2 4-Step Refrigeration Cycle

Background and Description:
Compression refrigeration is widely used in chemical processes to cool process streams to below-ambient temperatures. A single stage (one evaporator, one compressor, one condenser and one expansion valve) can be used down to temperatures of about 40 ℃ using several refrigerants such as R134A, ammonia and propylene. Lower temperatures require multiple stages using progressively lower-boiling refrigerants in each stage.
In this flowsheet, there are four refrigeration cycles having Nitrogen, Methane, Ethylene and Propylene as refrigerants respectively. In the first cycle, temperature goes down to -195 C; in second cycle, temperature goes down to -173.296 ℃; in third cycle, temperature goes down to -106.465 ℃ , in fourth cycle temperature goes down to -25.5859 ℃.

System of Units:
Temperature : ℃,
Pressure : bar,
Molar flow : Kmol/h,
Mass flow : kg/h

Property Package:
UNIQUAC

Flowsheet:



Results:

Object	M-23	M-022	M-017	M-011	M-01	
Temperature	-190	-25.5859	-106.465	-173.296	-195	C
Pressure	1.92022	2.5	0.863	0.34	1.12468	bar
Molar Flow	636	3464	2562	2122	1268	kmol/h
Molar Fraction (Mixture) / Ethylene	0	0	1	0	0	
Molar Fraction (Mixture) / Propylene	0	1	0	0	0	
Molar Fraction (Mixture) / Nitrogen	1	0	0	0	1	
Molar Fraction (Mixture) / Methane	0	0	0	1	0	

Object	E-7	E-2	E-11	E-00	
Energy Flow	5165.11	4724.71	8846.36	891.466	kW

6.3 Kalina Cycle

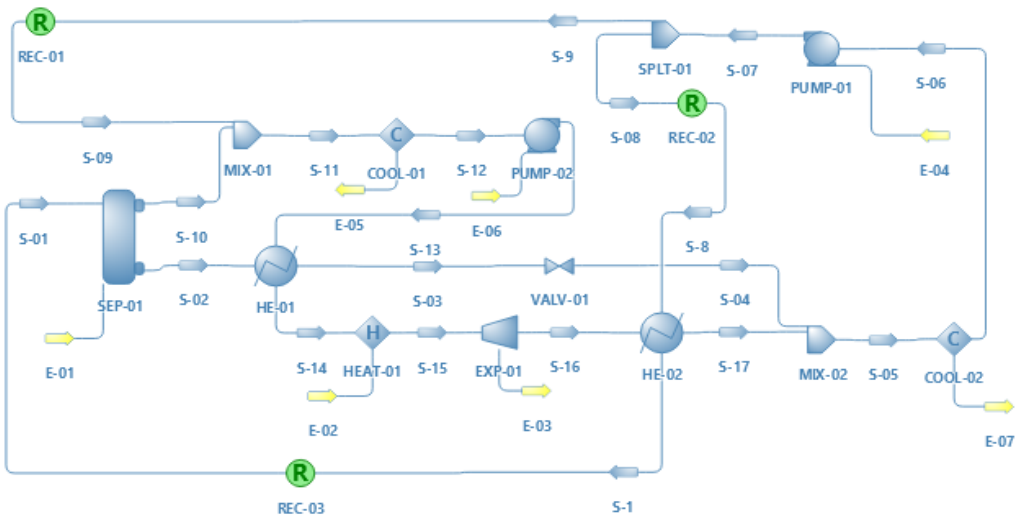
Background and Description:
A Kalina cycle consist of: absorber, condenser, gas-liquid separator, heat exchangers, valves, pumps and one or more turbine for producing power. Because of high performance and acceptable efficiency of the Kalina cycles, these cycles are very developed and investigated in recent years.
In this power generation cycle, ammonia-water mixture is used as the working fluid. Stream S-01 at 74.3565 °C, 3.5 bar and 0.3116 M fraction of NH3 with 3600 kg/h mass flow rate, enters gas-liquid separator in order to divide to rich vapor of the ammonia (S-10) and poor solution of the ammonia (S-02). Stream S-10 enters MIX-01 to mix with the stream S-09 and stream S-02 is sent to HE-01 heat exchanger to preheat the stream S-13. S-14 at 55.113°C, is sent to the HEAT-01 in order to absorb the solar thermal energy. Outlet stream of the HEAT-01 (S-15) at 300 °C and 80 bar, enters EXP-01 turbine to generate electricity. Stream S-16 leaves the turbine at 85.1638 °C and 1.29 bar and enters HE-02 heat exchanger. Temperature of stream S-17 is reduced to 49.821 °C and with stream S-04 is sent to the MIX-02 mixer. The outlet stream of MIX-02 (S-05) at 49.5955 °C enters COOL-02 absorber. In COOL-02, temperature of ammonia-water mixture reaches to 25 °C, by exchanging heat with water stream. S-06 stream at 25 °C and 1.29 bar is sent to PUMP-01 pump and pressure of it reaches to 3.5 bar. S-07 stream at 3.5 bar and with 4500 kg/h mass flow rate, leaves PUMP-01 pump and enters SPLT-01 splitter to divide into two streams: S-9 and S-08. Stream S-09 with 900 kg/h mass flow rate mixes with stream S-10 that comes from the SEP-01 gas-liquid separator. Temperature of the outlet stream of MIX-01 mixer (S-11) reaches to 56.0799 °C. Next it enters COOL-01 condenser and is cooled with water stream. After cooling, temperature of stream (S-12) reaches to

24.2 °C and next is sent to PUMP-02 pump. Pressure of the outlet stream (S-13) increases to 80 bar and then for preheating enters HE-01 heat exchanger. Stream S-03 at 62.1734 °C and 3.5 bar enters VALV-01 valve. After passing through the VALV-01, pressure of the stream reaches to 1.29 bar and mixes with stream S-17. Stream S-8 with 3600 kg/h mass flow rate is sent to HE-02 and after exchanging heat, at 74.3565 °C enters SEP-01 gas-liquid separator.

System of Units:
Temperature : ℃,
Pressure : bar,
Molar flow : Kmol/h,
Mass flow : kg/h

Property Package:
Cape Open (Predictive-SRK model)

Flowsheet:



Results:

Object	S-09	S-08	S-07	S-06	S-05	S-04	S-03	S-02	S-01	
Temperature	25.0037	25.0037	25.0037	25	49.5955	49.5026	62.1734	75	74.3565	C
Pressure	3.5	3.5	3.5	1.29	1.29	1.29	3.5	3.5	3.5	bar
Mass Flow	900	3600	4500	4500	4500	3192.1	3192.1	3192.1	3600	kg/h
Molar Flow	50.8232	203.293	254.116	254.116	254.116	179.452	179.452	179.452	203.293	kmol/h
Molar Fraction (Mixture) / Ammonia	0.311574	0.311574	0.311574	0.311574	0.311574	0.230824	0.230824	0.230824	0.311574	
Molar Fraction (Mixture) / Water	0.688426	0.688426	0.688426	0.688426	0.688426	0.769176	0.769176	0.769176	0.688426	

Object	S-17	S-16	S-15	S-14	S-13	S-12	S-11	S-10	
Temperature	49.821	85.1638	300	55.113	-24.6606	24.2	56.0799	75	C
Pressure	1.29	1.29	80	80	80	3.5	3.5	3.5	bar
Mass Flow	1307.9	1307.9	1307.9	1307.9	1307.9	1307.9	1307.9	407.904	kg/h
Molar Flow	74.6634	74.6634	74.6634	74.6634	74.6634	74.6634	74.6634	23.8402	kmol/h
Molar Fraction (Mixture) / Ammonia	0.505655	0.505655	0.505655	0.505655	0.505655	0.505655	0.505655	0.919402	
Molar Fraction (Mixture) / Water	0.494345	0.494345	0.494345	0.494345	0.494345	0.494345	0.494345	0.0805981	

6.4 Ethylene Glycol Production

Background and Description:
Monoethylene glycol (MEG) is an important raw material for industrial applications. MEG is used in the manufacture of polyester resins, antifreezes, and solvents, etc. MEG is commonly produced by the hydration of ethylene oxide (EtO). During the reaction, diethylene glycol (DEG) and triethylene glycol (TEG) are also produced as byproduct. Both DEG and TEG are also used for the manufacture of many chemicals, especially in the production of various of polymers.
EtO can be hydrolyzed either non-catalytically or catalytically. Non-catalytic hydration of EtO for the production of MEG is a well-known process in which a large amount of water is required. This increases the purification cost of products. Furthermore, the reaction has to be carried out at high temperature to increase the reaction rate appreciably, which causes high energy consumption.
In this flowsheet, water and ethylene oxide are given as a feed at 170 C and 35 bar pressure to the plug flow reactor. After reaction in PFR, monoethylene glycol, diethylene glycol, triethylene glycol and tetraethylene glycol are formed as product.
They are separated by simple distillation process using 8 distillation columns. The water separated is used as recycle.

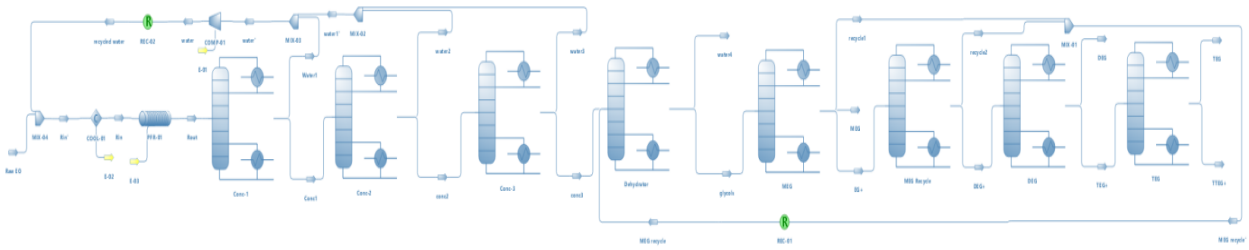
System of Units:
Temperature : ℃,
Pressure : bar,
Molar flow : Kmol/h,
Mass flow : kg/h

Property Package:
Soave-Redlich-Kwong (SRK)

Reactions:
Water + Ethylene Oxide $\xrightarrow{k1}$ Monoethylene Glycol
(k1/[L/(mol.min)] = exp(13.62-8220/T))
Ethylene Glycol + Ethylene Oxide $\xrightarrow{k2}$ Diethylene Glycol
(k2/[L/(mol.min)] = exp(15.57-8700/T))
Diethylene Glycol + Ethylene Oxide $\xrightarrow{k3}$ Triethylene Glycol
(k3/[L/(mol.min)] = exp(16.06-8900/T))
Triethylene Glycol + Ethylene Oxide $\xrightarrow{k4}$ Tetraethylene Glycol
(k4/[L/(mol.min)] = exp(16.30-9000/T))

Dimension of Plug Flow Reactor:
Length: 10 m
Diameter: 4.999 m

Flowsheet:



Results:

Object	Rin	Rout	Conc1	Conc2	Conc3	glycols	EG+	DEG+	TEG+	TTEG+
Temperature(C)	170	211.83	196.65	178.22	152.0	135.21	152.21	220.45	174.88	173.61
Pressure(bar)	35	33.96	14	9	4	0.17	0.22	0.12	0.025	0.015
Mass flow(kg/h)	550624	551093	385745	251464	110469	90904.6	21274.4	5474.9	245.06	13.82
Mass fraction (water)	0.91	0.87	0.82	0.72	0.37	0.003	1.1E-9	6.4E-23	0	0
Mass fraction (Ethylene Oxide)	0.09	1.3E-8	1E-10	3.1E-13	9.3E-17	0	0	0	0	0
Mass fraction (Ethylene glycol)	6.9E-6	0.12	0.17	0.25	0.58	0.93	0.74	2.8E-5	4.8E-12	6E-22
Mass fraction (Diethylene glycol)	6.2E-13	0.009	0.01	0.02	0.04	0.06	0.24	0.95	0.001	2.3E-9
Mass fraction (Triethylene glycol)	1.8E-13	0.0004	0.0006	0.0009	0.0022	0.003	0.011	0.045	0.965	0.473
Mass fraction (Tetraethylene glycol)	6.7E-15	1.5E-5	2.15E-5	3.3E-5	7.5E-5	9.1E-05	0.0004	0.0015	0.034	0.527

6.5 TAME Process

Background and Description:
Methanol recovery by distillation process uses water as an extractive agent in an extractive-distillation column to remove methanol from the distillate stream coming from the reactive-distillation column. A second column separates the methanol-water mixture coming from the base of the extraction column and recycles both methanol and water back to upstream units in the process.
Two Continues Stir Tank reactors each of 10 m3 volume are used for the reaction. The methanol-containing distillate D1 from the top of the reactive column is fed to stage 6 of a 12-stage extraction column. Water is fed on the top tray at a rate of 1046.88 kmol/h and a temperature of 48.85 ℃. Bottom product of this column is fed to third column of 33 stages. Water and methanol are separated as bottom and top products respectively so that they can be used again.

System of Units:
Temperature : ℃,
Pressure : bar,
Molar Flow : Kmol/h,
Mass Flow : kg/h

Property Package:
UNIFAC

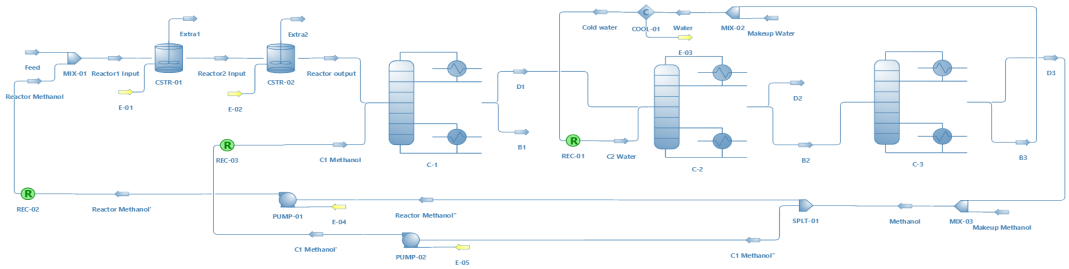
Reactions:

2M1B + Methanol ↔ TAME (Esterification)
2M2B + Methanol ↔ TAME (Esterification)
2M1B ↔ 2M2B

Reaction	Af1(kmol s^-1kg^-1)	Ef1(KJ/mol)	Ab1(kmol s^-1kg^-1)	Eb1(KJ/mol)
1	1.3263*10^8	76.1037	2.3535*10^11	110.5409
2	1.3718*10^11	98.2302	1.5414*10^14	124.9940
3	2.7187*10^10	96.5226	4.2933*10^10	104.1960

Volume of CSTR: 10 m3

Flowsheet:



Results:

Object	Feed	Reactor Methanol	Reactor Output	C1 Methanol	B1	Cold Water	B3	D3
Temperature: (℃)	69.85	77.3053	82.85	77.2094	138.569	48.85	115.51	78.736
Pressure: (bar)	10.1325	7.09275	6.0795	4.053	4.053	1.7225	1.722	1.722
Molar Flow: (kmol/h)	1040	313	1236.63	234.979	233.913	1046.8	1019.9	313.21
Mole Fraction(Water) :	0	5.7E-05	1.5E-05	5.7E-05	1.6E-09	0.9999	0.999	0.0001
Mole Fraction(Methanol) :	0	0.9999	0.15897	0.99994	0.00798	9.7E-05	0.0001	0.9999
Mole Fraction(2M1B) :	0.083	0	0.0262	0	5.8E-07	0	0	0
Mole Fraction(2M2B) :	0.16	1.2E-09	0.0841	1.2E-09	9.3E-06	1.4E-15	1.4E-15	2.1E-09
Mole Fraction(TAME) :	0	3.9E -15	0.0941	3.9E-15	0.992	2.9E-06	2.6E-06	6.7E-15