Function (S1)

```matlab
function Bootstrap


  global MER5212 MER678 %i5212 i678 aa bb cc TT obj1 obj2 CL


  global obj1


  i = 0;
  MER5212 = [];
  for func=4.3:0.2:4.5
    for OHV=obj1:1:obj1
%   for pp=861.1:1:861.1
      for Cp_spec=2.3:1:2.3
        MER5212(i+1,:) = [func,OHV,Cp_spec];
        i=i+1;
      end
    end
  end
  %i5212 = height(MER5212);
  MER5212;

  MER678 = [];
  interval = 0.25;
  max = 1.00;
  min = 0.00;
  limit = 0.50;
  i = 0;
  for hs=limit:interval:max
    for p=min:interval:limit
       for s=min:interval:limit
  %for p=0.01:interval:0.01
  %   for s=0.20:interval:0.20
  %     for hs=0.79:interval:0.79
          if hs+p+s == max
            MER678(i+1,:) = [p,s,hs];
            i=i+1;
          end
```

```matlab
        end
      end
    end
  %i678=height(MER678);


end

%The selection of the limits and intervals in the above defined variables
%is a task that requires expertise or educated guess from
%literature review, consultation and laboratory experimentation.
%Moreover, the limits and intervals is a great factor in the speed
%of the execution of the overall code
%and the accuracy of its result.

%Thus, focus on this matter may be very beneficial.
%The coder must look closely on narrowing limits,
%determining acceptable intervals,
%or prioritizing certain values.

%The convention of using the terms "coder-defined", "coder limited",
%or the like does not necessarily pertain to any claim by the code.
%Rather, it may pertain to variables defined or limited not by user-input
%through a user-interface, say a message box.
```

Function (S2)

```matlab
function Recipe


global mer NW0 NCO2 Totalm cat T0 Ts H0 NBp0 NBs0 NBt0 NBEt0 BA r0 V W_MW P_atm S TT Toluene_Cp

global E A h cp Ug Uf Ant_const vapHba Area VoverA Nc R RR Toluene Toluene_MW Toluene_MolarCp Boltz

global MER5212 MER678 i5212 i678


%efficiency of reactions
ef=1; %ef/Ef/eff/Eff = 'effective'/'reactive'


%Matrix of Isocyante & Polyol Properties (A & B Ingredients)---------------
%rows are only updated by MER512 & MER678 in Bootstrap
%           1       2       3       4       5    6    7    8    9    10
%           A       B1      B2      B3      B4   B5   B6   B7   B8   B9
mer=[   44.46    50       0       0       0    0    0    0    0     0; %1 Mass (g)
            0     0       0       0       0    0    0    0    0     0; %2 OHV of Bi
        369.9     0       0       0       0    0    0    0    0     0; %3 MW (g/mol)
            0     0       0       0       0    0    0    0    0     0; %4 Moles
          2.7     0       0       0       0    0    0    0    0     0; %5 Functionality
            0     0       0       0       0    0    0    0    0     0; %6 Xp of Bi
            0     0       0       0       0    0    0    0    0     0; %7 Xs of Bi
            0     0       0       0       0    0    0    0    0     0; %8 Xhs of Bi
            0     0       0       0       0    0    0    0    0     0; %9 Molar Cp (J/mol-K)
         1.23  1.08       0       0       0    0    0    0    0     0; %10 Density (g/cm^3)
            0     0       0       0       0    0    0    0    0     0; %11 Eq.Wt. (eq/g)
        1.799     0       0       0       0    0    0    0    0     0; %12 Specific Cp (J/g-K)
            0     0       0       0       0    0    0    0    0     0; %13 Volume (cm^3)
            0     0       0       0       0    0    0    0    0     0; %14 Moles p in Bi
            0     0       0       0       0    0    0    0    0     0; %15 Moles s in Bi
            0     0       0       0       0    0    0    0    0     0]; %16 Moles hs in Bi

mer(5,2)  = MER5212(i5212,1);          %Func. of B1 = Polyol Mix
mer(2,2)  = MER5212(i5212,2);          %OHV  of B1 = Polyol Mix
mer(12,2) = MER5212(i5212,3);          %Sp.Cp of B1 = Polyol Mix
```

```matlab
mer(6,2) = MER678(i678,1);                      %Xp  of B1 = Polyol Mix
mer(7,2) = MER678(i678,2);                      %Xs  of B1 = Polyol Mix
mer(8,2) = MER678(i678,3);                      %Xhs of B1 = Polyol Mix

for i=2:2   %up to 10
mer(3,i)=56100*mer(5,i)/mer(2,i);               %MW of Polyols
end

for i=1:2   %up to 10
mer(4,i)=mer(1,i)/mer(3,i)*ef;                  %Moles of Reactants
mer(9,i)=mer(12,i)*mer(3,i)/mer(5,i);           %Molar Cp of Reactants
mer(11,i)=mer(3,i)/mer(5,i);                    %Eq. Wt. of Reactants
mer(13,i)=mer(1,i)/mer(10,i);                   %Volume of Reactants
end

for i=2:2   %up to 10
mer(14,i)=mer(4,i)*mer(5,i)*mer(6,i);           %Moles p in Bi
mer(15,i)=mer(4,i)*mer(5,i)*mer(7,i);           %Moles s in Bi
mer(16,i)=mer(4,i)*mer(5,i)*mer(8,i);           %Moles hs in Bi
end
%---------------------------------------------------------------------


%Initial amount of c(13), c(14), c(15)    %up to 10
NBp0 = mer(14,2); %= sum(mer(14,2:10)) %Total Bp
NBs0 = mer(15,2); %= sum(mer(15,2:10)) %Total Bs
NBt0 = mer(16,2); %= sum(mer(16,2:10)) %Total Bhs

%Initial amount of c(11)
NBEt0 = 0; %mer(4,10)*mer(5,10)*mer(7,10); %Total Epoxy

%Initial amount of c(19)   %up to 10 (= sum(mer(4,2:10))/100)
NCO2 = (mer(4,2))/100; %Intrinsic CO2 in system


%CBA: Water
W_m=0;              %Mass (g)
W_M=W_m*ef;         %Eff. Mass (g)
W_MW=18;            %MW (g/mol)
nW0=(W_m/W_MW);     %Moles
NW0=nW0*ef;         %Eff. Moles (= W_M/W_MW)
```

```matlab
W_dens=1;            %Density (g/cm^3)
W_v=W_m/W_dens;      %Volume (cm^3)
W_V=W_v*ef;          %Eff. Volume (cm^3) (= W_M/W_dens)


%Matrix of PBA Properties (9 Entities)--------------------------------------
%         1        2         3         4         5         6         7         8         9
%         MF       n-Pen     iso-Pen   cyc-Pen   n-Hex     cyc-Hex   nButane   solstice  Forane
 BA = [    0        0         0         0         0         0         0         0         0;  %1
Mass (g)
          60.052   72.151    72.151    70.135    86.178    84.162    58.124    130.5     130.5;  %2
MW (g/mol)
           0        0         0         0         0         0         0         0         0;  %3
Moles
          0.98     0.626     0.616     0.751     0.6548    0.7781    0.551     1.27      1.27;  %4
Density (g/cm^3)
          129.3897 167.19    164.85    128       197.66    156       98.49     300       300;  %5
Heat capacity J/mol-K
          304.95   309.25    301       322.41    341.15    353.85    0         0         0;  %6
Boiling Point (K)
           0        0         0         0         0         0         0         0         0];  %7
Volume (cm^3)

for i=1:9
BA(3,i)= BA(1,i)/BA(2,i); %moles PBA
BA(7,i)= BA(1,i)/BA(4,i); %volume PBA
end
%---------------------------------------------------------------------------


%Matrix of Catalyst Mass & Eff. Catalyst Mass (11 Entities)----------------
%        1     2     3     4     5     6     7     8     9     10    11
%        cat5  cat8  UL-1  UL-6  UL-22 UL-29 UL-38 33-LV BL-17 Stan  SUL-4
cati=[ 0.12,    0,    0,    0,    0,    0,    0,    0,    0,    0,     0]; %cat mass (g)

cat = cati*ef; %eff. cat mass (g)
%---------------------------------------------------------------------------


%Other Ingredients Mass Input (g)
TCPPi=0;            %F.R.
```

```matlab
L6900i=0;        %Surf.
Toluenei=0;      %Solv.

%Other Ingredients Eff. Mass (g)
TCPP=TCPPi*ef;
L6900=L6900i*ef;
Toluene=Toluenei*ef;

%Toluene Properties
Toluene_dens = 0.86694; %g/cm3
Toluene_MW = 92.14; %g/mol
Toluene_MolarCp = 155.96; %J/mol-K
Toluene_Cp=(Toluene/Toluene_MW)*Toluene_MolarCp; %J/K (eff.)
Toluene_v = Toluenei/Toluene_dens; %cm^3 (volume)
Toluene_V = Toluene/Toluene_dens; %cm^3 (eff. volume)


%Total (Initial) Mass of Mixture    %up to 10 (use: sum(mer(1,1:10))
Totalm=sum(mer(1,1:2))+W_m+sum(BA(1,1:9))+sum(cati(1,1:11))+TCPPi+L6900i+Toluenei; %(g)


%Total (Initial) Volume of Mixture   %up to 10 (use: sum(mer(13,1:10))
%dens of cati(1:11), TCPPi, L6900i approx. 1 g/cm^3
V=sum(mer(13,1:2))+W_v+sum(BA(7,1:9))+sum(cati(1,1:11))+TCPPi+L6900i+Toluene_v; %(cm^3)


%Inital Temp. of Reactions (K)
Tr=TT;        %room temp.
T0=Tr+273.15;  %inital temp. of reactants
Ts=Tr+273.15;  %temp. of surr.


%Initial Height of Mixture (cm)
H0=1.5;


%Surfactant & Cell Structure Consideration*********************************

Csurf = (L6900/Totalm) + 2.1E-5;        %eff. concentration of surfactant (in total mixture)  %in w/w >>
why add 2.1E-5?
```

```
st = (21.046-(1.4378*log(Csurf)))/1000; %surface tension (original comment says unit is in N/m) >> formula
in the Publication is in dyn/cm, 1 dyn/cm = 10^-3 N/m
                                        % >> Publication: Modeling the Impact of Surfactants on
Polyurethane Foam Polymerization (2015)

r0 = 3.4E-3;                            %initial bubble radius (in cm; if in m = 3.4E-5 m or 0.000034 m)


WW = 0.05;                              %energy introduced by mixing (in J) >> assumed equal to Kanner's
Study: 10 seconds mixing, 1200 rpm >> review, if time permits
                                        % >> Publication: Urethane Foam Formation—Role of the Silicone
Surfactant (1969)

Nc = WW/(4*pi*st*((r0/100)^2));         %no. of nucleation sites or Nc=W/(4*pi*st*(r0/100)^2)
                                        % [dimensional analysis: J/((N/m)*(m^2)) = J/(N-m) = N-m/(N-m) >>
dimensionally correct, dimensionless overall]

R = 82.05736;                           %gas constant in atm-cm^3/mol-K (with 5 decimal places)


RR = 8.31446;                           %gas constant in J/mol-K (with 5 decimal places)
```

Function (S3)

```matlab
function Database


global E A h cp Ug Uf Ant_const vapHba

Press=1;

% ptot=1;

%Antoine equation constants, Pc, and Tc of BAs------------------------------
%          A         B        C          D        Pc     Tc
Ant_const=[-6.99601  0.89328  -2.52294  -3.16636  60    487.2;    %BA 1: Methyl Formate
           -7.28936  1.53679  -3.08367  -1.02456  33.7  469.7;    %BA 2: n-Pentane
           -7.12727  1.38996  -2.54302  -2.45657  33.9  460.4;    %BA 3: iso-Pentane (2-methyl butane)
           -6.51809  0.38442  -1.11706  -4.50275  45.1  511.7;    %BA 4: cyclo-Pentane
           -7.46765  1.44211  -3.28222  -2.50941  30.1  507.5;    %BA 5: n-Hexane
           -6.96009  1.31328  -2.75683  -2.45491  40.7  553.5;    %BA 6: cyclo-Hexane
           -6.88709  1.15157  -1.99873  -3.13003  38    425.2;    %BA 7: n-Butane
           -3.70105  -5.6665   3.99824  -0.02625  35    450  ;    %BA 8: Sol
           -4.77394  -2.7714  -0.78228  -0.02772  35    450  ];   %BA 9: Forane
%------------------------------------------------------------------------

%Latent Heat of vaporization of BAs (J/mol)[Using Giacalone Equation]------------------------------------
%          1           2           3           4           5           6           7           8        9
%          MF          n-Pen       iso-P       cyc-P       n-H         cyc-H       n-But       Sol      For
vapHba=[27648.6,    26363.35,   25372.42,   26378.7,    29543.300,  30108.864,  22473.6,    25317,
25225.65];
%------------------------------------------------------------------------------------------------------


%**********************************************************************


%Kinetics Consideration************************************************

%Arrhenious Constant for 13 reaction groups, uncatalyzed + catalyzed (with 11 kinds of catalyst)------
```

```
% >> used for calculating the Rate Constant, k, for each Reaction using the Arrhenius Equation: k =
A*(e^(E/(RT)))
% >> in the same units as k: [(mol/V)^(1-a)]·s^-1, where a = the overall order of the reaction >>
(cm^3)/mol-s
%Rxn. Group:   1       2       3       4      5      6      7      8      9      10      11      12      13
%         P-A/Ap S-A/Ap HS-A/Ap  A-U   Ap-U   A-W   Ap-W  Ap-Am  A-Amp  Ap-Amp  A-Urp  Ap-Ur  Ap-Urp
A = [     0.38    0.13  0.0125  0.012  0.012  0.25   0.25   2.5    2.5    2.5     0      0      0;
%0 uncatalyzed
          80      100     15     0      0     600    600   6000   6000   6000     0      0      0;
%1  cat5
          500      58     42     0      0     540    540   5400   5400   5400     0      0      0;
%2  cat8
           0     8000    1300    0      0      0      0      0      0      0       0      0      0;
%3  UL-1
           0      300     65     0      0      0      0      0      0      0       0      0      0;
%4  UL-6
           0    10000    3000    0      0      0      0      0      0      0       0      0      0;
%5  UL-22
           0      270     60     0      0      0      0      0      0      0       0      0      0;
%6  UL-29
           0      600    150     0      0      0      0      0      0      0       0      0      0;
%7  UL-38
           0      250     70     0      0      0      0      0      0      0       0      0      0;
%8  33-LV
           0       60     20     0      0     240    240     0      0      0       0      0      0;
%9  BL-17
           0      500    150     0      0      0      0      0      0      0       0      0      0;
%10 Stan
           0     1200    550     0      0      0      0      0      0      0       0      0      0];
%11 SUL-4
%-------------------------------------------------------------------------------------------

%Activation Energy (Ea in J/mol) for 13 reaction groups, uncatalyzed + catalyzed (with 11 kinds of
catalyst)-----
%Rxn. Group:   1       2       3       4      5       6      7      8       9      10      11      12      13
%         P-A/Ap S-A/Ap HS-A/Ap  A-U   Ap-U    A-W   Ap-W  Ap-Am  A-Amp  Ap-Amp  A-Urp  Ap-Ur  Ap-Urp
E = [    40000   42000   54000    0      0    39000  39000  39000  39000   39000    0      0      0;
%0  uncatalyzed
         60000    3000     300    0      0    10000  10000  10000  10000   10000    0      0      0;
%1  cat5
```

```
         37000    40000    42000     0     0    35000 35000 35000    35000    35000    0    0    0;
%2   cat8
             0    40000    50000     0     0      0     0     0       0        0       0    0    0;
%3   UL-1
             0    40000    82000     0     0      0     0     0       0        0       0    0    0;
%4   UL-6
             0    40000    52000     0     0      0     0     0       0        0       0    0    0;
%5   UL-22
             0    40000    78000     0     0      0     0     0       0        0       0    0    0;
%6   UL-29
             0    40000    65000     0     0      0     0     0       0        0       0    0    0;
%7   UL-38
             0    38000    45000     0     0      0     0     0       0        0       0    0    0;
%8   33-LV
             0    38000    45000     0     0    35000 35000 32000     0        0       0    0    0;
%9   BL-17
             0    55000    60000     0     0      0     0     0       0        0       0    0    0;
%10 Stan
             0    32000    38000     0     0      0     0     0       0        0       0    0    0];
%11 SUL-4
%----------------------------------------------------------------------------------------
------
 
%Heats of Reactions (J/mol) (delta H)-------------------------------------
%     1      2      3      4      5       6       7
%    P-A    S-A    T-A    A-U    A-W    A-Am    A-Ur   %Monomer or on Polymer
h=[72800, 72800, 72800,    0, 60000,  30000,      0];
%-------------------------------------------------------------------------
 
%cp of Reactants (J/mol-K)-----------------------------------------------
 
%cp of A (J/mol-K)
cp_A = mer(9,1);
 
%cp_ave of B (Polyols) (J/mol-K)   %up to 10
cp_Bave=mer(9,2);%(mer(4,2)*mer(5,2)*mer(9,2));%+mer(4,3)*mer(5,3)*mer(9,3)+mer(4,4)*mer(5,4)*mer(9,4)+mer(
4,5)*mer(5,5)*mer(9,5))/(mer(4,2)*mer(5,2)+mer(4,3)*mer(5,3)+mer(4,4)*mer(5,4)+mer(4,5)*mer(5,5));
 
%cp of Urethane (J/mol-K)
cp_U=cp_A+cp_Bave;
```

```matlab
%cp Vector (J/mol-K)
%     1        2      3       4     5     6     7
%     A        B      U       W     Am    CO2   Ur
cp=[cp_A, cp_Bave, cp_U, 75.42, 128, 39.6, 361];


%------------------------------------------------------------------------


%Heat Transfer Considerations*********************************************


%Overall Heat Transfer Coefficient (to surroundings, in W/m^2-K)
Ug=3;     %gel in (plastic) cup
Uf=2.2;   %foam


%Area of Heat Transfer & V2H Conversion Factor

%wood box
%Area=0.0102+0.004*c(24)*c(25)/273;
%VoverA=22400/102;

%plastic cup
%Area=0.006+0.002*c(24)*c(25)/273;
Area=0.0078;
VoverA=22400/35;

%Harith's small box
% Area=0.0072+0.0024*c(17)*c(18)/273;
% VoverA=22400/36;

%************************************************************************


  end
```

Function (S4)

```matlab
function ReacSim (t,c)


global mer E A h cat Ts cp Ug dTdt V kk Area VoverA Nc Boltz RR W_MW gm vapHba BA Toluene_Cp


%-----------------------------------------------------------------------------
%                     Part A: Instantaneous Mixture Cp (J/K)
%-----------------------------------------------------------------------------

Cp_solv = Toluene_Cp;
Cp_A    = cp(1)*c(12);
Cp_B    = cp(2)*(c(13)+c(14)+c(15));

Cp_BA = 0;
for i = 1:9
    for j = 26:34
    Cp_BA = Cp_BA + (BA(5,i)*c(j));
    end
end

Cp_U        = cp(3)*c(16);
Cp_W        = cp(4)*c(17);
Cp_Am       = cp(5)*c(18);
Cp_CO2      = cp(6)*c(19);
Cp_Ur       = cp(7)*c(20);

Cp_all = Cp_solv + Cp_A + Cp_B + Cp_BA + Cp_W + Cp_U + Cp_CO2 + Cp_Am + Cp_Ur;

Cp = Cp_all*(1+(c(24)-300)/1000); %Cp_others: FR, surf, cat? Cp_solv = 0; Cp_cat?
%the (1+(c(24)-300)/1000) maybe some assumptions/heuristics or find literature!

%-----------------------------------------------------------------------------


%-----------------------------------------------------------------------------
%                     Part B. Instantaneous Moles of Polymer Resin
%-----------------------------------------------------------------------------

moles_AnPoll = sum(c(1:2));    %up to 10
moles_water = c(17);
moles_pdpd = c(21);
moles_BA = 0; %moles_others: FR, surf, cat, solv? moles_solv = 0; moles_surf, moles_cat, + moles_CO2?
moles_resin = moles_AnPoll + moles_water + moles_pdpd + moles_BA;
molres = moles_resin;
```

```matlab
%-----------------------------------------------------------------------


%-----------------------------------------------------------------------
%                         Part C: Kinetics Consideration
%-----------------------------------------------------------------------

%Rate Constant Calculation - - - - - - - - - - - - - - - - - - - - - - - -

for i = 1:13
        kuncat(i) =  V     *A(1,i)*exp(E(1,i)/RR*(1/298-1/c(24)));
        kcat5 (i) = cat(1)*A(2,i)*exp(E(2,i)/RR*(1/298-1/c(24)));
        K(i)=kuncat(i)+kcat5(i);
end

ktr(1)=1; ktr(2)=1; ktr(3)=1;

kp(1)=K(1)*ktr(1);
kp(2)=K(2)*ktr(2);
kp(3)=K(3)*ktr(3);

% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

%Mass Transfer (Coeff) of Water Vapor - - - - - - - - - - - - - - - - - -

gm=E1_Viscosity(c(1), c(2), c(21),c(24));    %up to 10

%gm treatment
if gm <= kk
    gm=kk;
else if gm <= 0
    gm=kk;
else if gm > 1.5e13
    gm=1.5E13;
    end
    end
end

%mass transfer coeff of water from bubbles to resin
wdz= 1.5E-24 *(W_MW^1/3);
kwm=(Boltz*c(24)/(6*pi*gm*wdz));

%updating kk in Main.m -> ReacSim.m for t(i+1)
kk=gm;

% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```matlab
%Rate Constant (column) vector - - - - - -- - - - - - - - - - - - - - - - -

k = [ K(1) ;    K(2) ;   K(3) ; % 1   2   3      %for A  & B1 reactions: B1p, B1s, B1t
      K(1) ;    K(2) ;   K(3) ; % 4   5   6      %for A  & B2 reactions: B2p, B2s, B2t
      K(1) ;    K(2) ;   K(3) ; % 7   8   9      %for A  & B3 reactions: B3p, B3s, B3t
     kp(1) ;  kp(2) ; kp(3) ; %10 11 12      %for A  & BP reactions: BpP, BsP, BtP
     kp(1) ;  kp(2) ; kp(3) ; %13 14 15      %for Ap & B1 reactions: B1p, B1s, B1t
     kp(1) ;  kp(2) ; kp(3) ; %16 17 18      %for Ap & B2 reactions: B2p, B2s, B2t
     kp(1) ;  kp(2) ; kp(3) ; %19 20 21      %for Ap & B3 reactions: B3p, B3s, B3t
     kp(1) ;  kp(2) ; kp(3) ; %22 23 24      %for Ap & BP reactions: BpP, BsP, BtP


      K(4) ;  %25   (4) for A-U(rethane) reaction
      K(5) ;  %26   (5) for Ap-U(rethane) reaction
      K(6) ;  %27   (6) for A-W(ater) reaction
      K(7) ;  %28   (7) for Ap-W(ater) reaction
      K(8) ;  %29   (8) for Ap-Am(ine) reaction
      K(9) ;  %30   (9) for A-Amp(Amine on Polymer) reaction
      K(10);  %31   (10)for Ap-Amp(Amine on Polymer) reaction
      K(11);  %32   (11)for A-Urp(Urea on Polymer)
      K(12);  %33   (12)for Ap-Ur(Urea) reaction
      K(13);  %34   (13)for Ap-Urp(Urea on Polymer) reaction

      %35 36 37 38 39 40 41 42 43 44   45   (k(45): mass transf. from bubbles to resin)
        0; 0; 0; 0; 0; 0; 0; 0; 0; 0; kwm];

% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


%Concentration of Moieties - - - - - - - - - - - - - - - - - - - - - - - -

%mer(j,i), c(i) where i = up to 10
AA=mer(5,1)*c(1);                %of iso moieties
Ap=c(12)-mer(5,1)*c(1);          %of iso moieties on polymer
B1p=mer(5,2)*mer(6,2)*c(2);   %of primary hydroxyl moieties in Polyol 1
B1s=mer(5,2)*mer(7,2)*c(2);   %of secondary hydroxyl moieties in Polyol 1
B1t=mer(5,2)*mer(8,2)*c(2);   %of tertiary hydroxyl moieties  in Polyol 1
B2p=mer(5,3)*mer(6,3)*c(3);   %of primary hydroxyl moieties in Polyol 2
B2s=mer(5,3)*mer(7,3)*c(3);   %of secondary hydroxyl moieties in Polyol 2
B2t=mer(5,3)*mer(8,3)*c(3);   %of tertiary hydroxyl moieties in Polyol 2
B3p=mer(5,4)*mer(6,4)*c(4);   %of primary hydroxyl moieties in Polyol 3
B3s=mer(5,4)*mer(7,4)*c(4);   %of secondary hydroxyl moieties in Polyol 3
B3t=mer(5,4)*mer(8,4)*c(4);   %of tertiary hydroxyl moieties in Polyol 3
%Bip=mer(5,i)*mer(6,i)*c(i);   %of primary hydroxyl moieties in Polyol i
%Bis=mer(5,i)*mer(7,i)*c(i);   %of secondary hydroxyl moieties in Polyol i
%Bit=mer(5,i)*mer(8,i)*c(i);   %of tertiary hydroxyl moieties in Polyol i
BpP=c(13)-(B1p+B2p+B3p);      %of primary hydroxyl moieties on polymer   -(+Bip)
BsP=c(14)-(B1s+B2s+B3s);      %of secondary hydroxyl moieties on polymer  -(+Bis)
```

```matlab
BtP=c(15)-(B1t+B2t+B3t);        %of tertiary hydroxyl moieties on polymer   -(+Bit)
Amine=2*c(18);                  %of amine moieties
AmineP=c(22)-Amine;             %of amine moieties on polymer
Urea=2*c(20);                   %of urea moieties
UreaP=c(23)-Urea;               %of urea moieties on polymer


% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

%Reaction Rate (column) vector (45 x 1) - - - - - - - - - - - - - - - - - -

      %PRIMARY              SECONDARY           H-SECONDARY
r=[k(1)*AA*B1p/V^2;  k(2)*AA*B1s/V^2;  k(3)*AA*B1t/V^2; %A and B1 reaction rate
   k(4)*AA*B2p/V^2;  k(5)*AA*B2s/V^2;  k(6)*AA*B2t/V^2; %A and B2 reaction rate
   k(7)*AA*B3p/V^2;  k(8)*AA*B3s/V^2;  k(9)*AA*B3t/V^2; %A and B3 reaction rate
   %          0;                 0;                 0;[A and Bi reaction rate]
   k(10)*AA*BpP/V^2; k(11)*AA*BsP/V^2; k(12)*AA*BtP/V^2; %A and BP reaction rate
   k(13)*Ap*B1p/V^2; k(14)*Ap*B1s/V^2; k(15)*Ap*B1t/V^2; %Ap and B1 reaction rate
   k(16)*Ap*B2p/V^2; k(17)*Ap*B2s/V^2; k(18)*Ap*B2t/V^2; %Ap and B2 reaction rate
   k(19)*Ap*B3p/V^2; k(20)*Ap*B3s/V^2; k(21)*Ap*B3t/V^2; %Ap and B3 reaction rate
   %          0;                 0;                 0;[Ap and Bi reaction rate]
   k(22)*Ap*BpP/V^2; k(23)*Ap*BsP/V^2; k(24)*Ap*BtP/V^2; %Ap and BP reaction rate

   k(25)*AA*c(16)/V^2;  %A and Urethane reaction rate
   k(26)*Ap*c(16)/V^2;  %Ap and Urethane reaction rate
   k(27)*AA*c(17)/V^2;  %A and W reaction rate
   k(28)*Ap*c(17)/V^2;  %Ap and W reaction rate
   k(29)*Ap*c(18)/V^2;  %Ap and Amine reaction rate
   k(30)*AA*AmineP/V^2; %A and AmineP reaction rate
   k(31)*Ap*AmineP/V^2; %Ap and AmineP reaction rate
   k(32)*AA*UreaP/V^2;  %A and UreaP reaction rate
   k(33)*Ap*Urea/V^2;   %Ap and Urea reaction rate
   k(34)*Ap*UreaP/V^2;  %Ap and UreaP reaction rate

   %35 36 37 38 39 40 41 42 43 44        45         %r(45) = water vap from bubbles to resin,
     0; 0; 0; 0; 0; 0; 0; 0; 0; 0; k(45)*c(35)]; % but input in c(35) is -r(45) = water vap from resin to bubbles

% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

%Degree of Polymerization Calculation - - - - - - - - - - - - - - - - - - -

DPx1=(mer(4,1)+mer(4,2))/(c(1)+c(2)+c(21)); %up to 10
%DP(1)=DP(1);
%DPx2=(DPx1^(-2/3));
%DPx2=0.36;
%DPx2=15*((c(2)+c(3)+c(4)));
%DP(2)=1/log(DP(1));
pow=2/3;
```

```matlab
%DPx2a=DPx1^pow;
%DPx2=1/(DPx2a);
%Y=2/DPx2;
Y=2*(DPx1^pow);


% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

%Stoichiometric Coefficient Matrix (23 x 45) - - - - - - - - - - - - - - - - -

    %1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
38 39 40 41 42 43 44 45   >> add more columns for every additional Bi reaction
sc = [ -1 -1 -1  0  0  0  0  0  0 -1 -1 -1  0  0  0  0  0  0  0  0  0  0  0  0  0 -1  0 -1  0  0 -1  0 -1  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%1 for the reactions of Monomer A   (Isocyanate) (with B, BP, U, W, Am/P, CO2, Ur/P)
       -1 -1 -1  0  0  0  0  0  0  0  0  0 -1 -1 -1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%2 for the reactions of Monomer B1 (G76-635) (with A and with Ap)
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%3 for the reactions of Monomer B2 (V360) (with A and with Ap)
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%4 for the reactions of Monomer B3 (R315x) (with A and with Ap)
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%5 for the reactions of Monomer B4 (M5020) (with A and with Ap)


    %1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
38 39 40 41 42 43 44 45
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%6 for the reactions of Monomer B5  ----- (with A and with Ap)
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%7 for the reactions of Monomer B6  ----- (with A and with Ap)
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%8 for the reactions of Monomer B7  ----- (with A and with Ap)
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%9 for the reactions of Monomer B8  ----- (with A and with Ap)


    %1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
38 39 40 41 42 43 44 45
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%10 for the reactions of Monomer B9/ESBO (with A and with Ap)
        0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 0  0  0  0  0  0  0  0  ;%11 for the reactions of Total Epoxy (with A and with Ap)


    %1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
38 39 40 41 42 43 44 45
       -1 -1 -1  0  0  0  0  0  0 -1 -1 -1 -1 -1 -1  0  0  0  0  0  0 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1  0  0  0
 0  0  0  0  0  0  0  0  ;%12 for the reactions of Total A  (Monomer A + A on Polymer) (with B, BP, U, W, Am/P, CO2,
Ur/P)
```

```
      -1  0  0  0  0  0  0  0  0 -1  0  0 -1  0  0  0  0  0  0  0  0  0 -1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%13 for the reactions of Total Bp (from Monomers B1, B2, B3... + Bp on Polymer (with A and
with Ap))
       0 -1  0  0  0  0  0  0  0  0 -1  0  0 -1  0  0  0  0  0  0  0  0  0 -1  0  0  0  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%14 for the reactions of Total Bs (from Monomers B1, B2, B3... + Bs on Polymer (with A and
with Ap))
       0  0 -1  0  0  0  0  0  0  0  0 -1  0  0 -1  0  0  0  0  0  0  0  0  0 -1  0  0  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%15 for the reactions of Total Bt (from Monomers B1, B2, B3... + Bt on Polymer (with A and
with Ap))

       %1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
38 39 40 41 42 43 44 45
       1  1  1  0  0  0  0  0  0  1  1  1  1  1  1  0  0  0  0  0  0  0  1  1  1 -1 -1  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%16 for the reactions of Urethane (from A/Ap + B/BP reactions, with A/Ap reactions to
Allophanate)
       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -1 -1  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  0  0  1  ;%17 for the reactions of Water (with A/Ap reactions to Amine + CO2 + mass transfer)
       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  1 -1  0  0  0  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%18 for the reactions of Amine (from A/Ap + W reactions, considering Ap-Am reaction only (to
Urea); excludes A & Ap reactions with AmP) BUT Urea formation accounts A & Ap reactions with AmP: sc(20,30-31) is = 1,
though sc(18,30-31) = 0 >> hmmm
       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  1  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%19 for the reactions of CO2 (from A/Ap + W reactions)
       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  1  1  0 -1  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%20 for the reactions of Urea (sc(20,30-31) is = 1, though sc(18,30-31) = 0 >> hmmm; Ap-Ur
reaction only (to Biuret); excludes A & Ap reactions with UrP)

       %1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37
38 39 40 41 42 43 44 45
       1  1  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 -Y -Y -Y  0 -Y  0  0  0  0 -Y  0  0 -Y  0  0  0
0  0  0  0  0  0  0  0  ;%21 for the reactions of P [= product/polymer/resin]
       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  1 -1 -1 -1  0  0  0  0  0  0
0  0  0  0  0  0  0  0  ;%22 for the reactions of Total Amine (from A/Ap + W, includes A & Ap reactions with AmP)
       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  1  1 -1 -1 -1  0  0  0  0  0  0
0  0  0  0  0  0  0  0 ];%23 for the reactions of Total Urea (from A/Ap + Am/AmP, includes A & Ap reactions with UrP)

% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

%Temperature Profile Calculation - - - - - - - - - - - - - - - - - - - - - - -

%----------------------------------------------------------------------------
%                        BA Consideration
%----------------------------------------------------------------------------

%dbaldt(i) = rate of mass transfer of BA(i) from bubbles to resin
%drdt       = rate of change of bubble radius
%dcondt(i) = rate of condensation of BA(i) in bubbles
```

```matlab
[dbaldt,drdt,dcondt]=E2_BA(c(19), c(21), c(24), c(26), c(27), c(28), c(29), c(30), c(31), c(32), c(33), c(34), molres,
c(36), c(37), c(38));

Tdbaldt = sum(dbaldt);                  %total mass transfer rate of [BAs] (amt/s) >> from bubbles to resin
Tdcondt = sum(dcondt);                  %total rate of [BAs] that condense in bubbles (amt/s)

for i=1:9
    Hvap(i) = dbaldt(i)*vapHba(i);      %heat released by the system in the mass transfer BA(i) (J/s) %from bubbles to
resin, row vector
    Hcond(i) =-dcondt(i)*vapHba(i);     %heat released by the system in the condensation a BA(i) in bubbles (J/s) %from
bubbles to resin, row vector
end

THvap  = sum(Hvap);                     %total heat released by the system in the mass transfer of BAs (J/s) >> review
THcond = sum(Hcond);                    %total heat released by the system in the condensation of BAs in bubbles (J/s)
>> review

%-------------------------------------------------------------------------

%-------------------------------------------------------------------------
%                          dTdt Expression
%-------------------------------------------------------------------------

dTdtn_h1 = h(1)*(r(1)+r(10)+r(13)+r(22));                        %from (P-A) reactions (J/s) (Monomer + on Polymer)
dTdtn_h2 = h(2)*(r(2)+r(11)+r(14)+r(23));                        %from (S-A) reactions (J/s) (Monomer + on Polymer)
dTdtn_h3 = h(3)*(r(3)+r(12)+r(15)+r(24));                        %from (T-A) reactions (J/s) (Monomer + on Polymer)
dTdtn_h4 = h(4)*(r(25)+r(26));                                   %from (A-U) reactions (J/s) (Monomer + on Polymer)
dTdtn_h5 = h(5)*(r(27)+r(28));                                   %from (A-W) reactions (J/s) (Monomer + on Polymer)
dTdtn_h6 = h(6)*(r(29)+r(30)+r(31));                             %from (A-Am) reactions (J/s) (Monomer + on Polymer)
dTdtn_h7 = h(7)*(r(32)+r(33)+r(34));                             %from (A-Ur) reactions (J/s) (Monomer + on Polymer)
dTdtn_OAHT = Ug*Area*(Ts-c(24));                                 %Overall Heat Transfer (J/s) %Ug, Area = const.
%THvap  = sum(Hvap(1:9));                                        %Total heat absorbed during vaporization of BAs
(J/s)
%THcond = sum(Hcond(1:9));                                       %Total heat released during condensation of BAs (in
bubbles) (J/s)
dTdtn = dTdtn_h1 + dTdtn_h2 + dTdtn_h3 + dTdtn_h4 + dTdtn_h5 + dTdtn_h6 + dTdtn_h7 + dTdtn_OAHT + THvap + THcond;
%(J/s)
dTdtd = Cp;          %(J/K)
dTdt = dTdtn/dTdtd; %(K/s)

%-------------------------------------------------------------------------

% - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

%-------------------------------------------------------------------------
```

```matlab
%-----------------------------------------------------------------------------
%                        Part D: Final Output of ReacSim
%-----------------------------------------------------------------------------


dCO2dt=(r(27)+r(28));

dydt=[sc*r;                             %c(1) to c(23) = Amt. of 23 entities (comments on sc)
      dTdt;                             %c(24) = Temperature
      VoverA*(dCO2dt+(-Tdbaldt));       %c(25) = Height
      dbaldt(1);                        %c(26) = Amt.of BA 1 (in liq. resin)
      dbaldt(2);                        %c(27) = Amt.of BA 2 (in liq. resin)
      dbaldt(3);                        %c(28) = Amt.of BA 3 (in liq. resin)
      dbaldt(4);                        %c(39) = Amt.of BA 4 (in liq. resin)
      dbaldt(5);                        %c(30) = Amt.of BA 5 (in liq. resin)
      dbaldt(6);                        %c(31) = Amt.of BA 6 (in liq. resin)
      dbaldt(7);                        %c(32) = Amt.of BA 7 (in liq. resin)
      dbaldt(8);                        %c(33) = Amt.of BA 8 (in liq. resin)
      dbaldt(9);                        %c(34) = Amt.of BA 9 (in liq. resin)
      (-r(45));                         %c(35) = Amt.of Water that vaporized %resin to bubbles
      dCO2dt/Nc;                        %c(36) = Amt.of CO2 that evolved into each bubble
      (-Tdbaldt)/Nc;                    %c(37) = Amt.of Total BA that vaporized into each bubble %resin to bubbles
      drdt;                             %c(38) = Bubble Diameter  >> f(c(36, c(37), c(24), c(38), c(21)] in bafn
      Tdcondt];                         %c(39) = Amt.of Total BAs that condensed in bubbles

%-----------------------------------------------------------------------------

%-----------------------------------------------------------------------------
%          Part E: Safety Nets from Complex Number Calculations
%-----------------------------------------------------------------------------


if t > 20
    if c(21) < 0
    %     if t > 20
            dydt(21)=0; %c(21) = pdp
    %     end
    end
end


%-----------------------------------------------------------------------------

End
```

Function (S5)

```matlab
function Main

%profile on;
%diary on;
clear;
clc;
close all;
clear title;


global aa bb cc MER5212 MER678 combon zz i5212 i678 NBEt0 NBp0 NBs0 NBt0 NCO2 T0 H0 BA NW0 r0

global Matrix_Matches Matrix_MaxPoints Matrix_TempProfile Matrix_ViscoProfile Matrix_HeightProfile trange_min t_int
trange_max mer

global xx y1 y2 y3 y4 y5 y6 matrices_height imax kk CL imax2


%note that B1 = BM or Bmix
%update Ac & Bc of B1, verify for A


B_UserInput
clear title;
lowerCL = (100-CL)/100;
upperCL = (100+CL)/100;


format bank


Bootstrap
rr1 = height(MER5212);
rr2 = height(MER678);
run_size = rr1*rr2;
fprintf('\nMER5212 (Functionality, OH#, Cp) Combinations = %d\n', rr1);
fprintf('\nMER678 (xp, xs, xhs) Combinations = %d\n', rr2);
fprintf('\nExpected runs = %d x %d = %d\n\n', rr1,rr2,run_size);
fprintf('Conditions for Match Finding: %.4f*Input Tmax <= Simulated Tmax <= %.4f*Input Tmax\n\n', lowerCL, upperCL)


combon = 1;
zz = 2;


for i5212 = 1:height(MER5212)
```

```matlab
%combon = 1;

for i678 = 1:1:height(MER678)

    %Solving ReacSim ----------------------------------------------------------------------
    ----------------------

    D_Database

    kk=1;

    trange_min = 0; t_int = 5; trange_max = cc*60;
    matrices_height = ((trange_max - trange_min)/t_int) + 1;

                                                    %1            2            3            4            5
6          7          8          9          10         11
                                                    %A           B1           B2           B3           B4
B5         B6         B7         B8         B9     T.Epoxy
    [t,c] = ode45( @E_ReacSim, trange_min:t_int:trange_max, [   mer(4,1);    mer(4,2);   mer(4,3); mer(4,4);
mer(4,5); mer(4,6); mer(4,7); mer(4,8); mer(4,9); mer(4,10);  NBEt0;

                                                    %12           13           14           15           16
17         18         19         20         21         22       23
                                                    %T.A          T.Bp         T.Bs         T.Bt         U
W          A          CO2        Ur         T.P        T.Am     T.Ur
                                      mer(4,1)*mer(5,1); NBp0;        NBs0;        NBt0;        0;
0;         0;         NCO2;      0;         0;         0;       0;

                                                    %24           25           26           27           28
29         30         31         32         33         34
                                                    %Temp         Ht.          BA 1         BA 2         BA 3
BA 4       BA 5       BA 6       BA 7       BA 8       BA 9
                                         T0;          H0;       BA(3,1);   BA(3,2);
BA(3,3);   BA(3,4);   BA(3,5);   BA(3,6);   BA(3,7);   BA(3,8);    BA(3,9);

                                                    %35           36           37           38           39
                                                    %Vap. W    CO2 in Bubb.    T.BA       Bubb.r
Cond.BA
                                         NW0;         6.95E-12;     0;         r0;
0]);

    %--------------------------------------------------------------------------------------------
    ----------------------

    %Unnested Viscosity Calculation--------------------------------------------------------------
    ----------------------
```

```matlab
        pdpnk=(mer(4,1)+mer(4,2))-(c(:,1)+c(:,2)); %up to 10 %arithmetic ops = element-wise %row vector
        pdpdk=c(:,21); %row vector

        TS = (mer(4,1)+mer(4,2))-(c(1,1)+c(1,2)); %up to 10 %treshold

        %pdpk calculation, where pdpk = column vector
        for i=1:matrices_height
            if pdpnk(i)<=TS %treshold
                pdpk(i,1)=2;
            else
                pdpk(i,1)=pdpnk(i)/pdpdk(i);
            end
        end

        MWpro=318.*pdpk+700; %column vector
        Denpro=1.116;

        %values of group contributions to Parameters A & B of some groups
                %1       2       3     4     5       6      7      8       9      10      11      12
        %   carbon    -CH<    >C<   AR   Ortho   Meta   Para   -OH    -O-    -N=C=O  C-O-C  SugarRing
        AGC=[-0.21   -0.15   -1.20  0    -0.12   0.05   -0.01  -2.14  -0.38  -4.83   -0.73    0.42];
        BGC=[88        35      400  20    100    -34     -5    1218    140    2176    210    -1408];

        %Parameter A
                                   %A                                                      %B1              %up to 10
        Ac=[(-6.53+AGC(1)*1)+AGC(4)*2+AGC(5)*2+AGC(10)*2+AGC(11)*2,      (-6.53+AGC(1)*6)+AGC(8)*3+AGC(11)*3];%   (-
6.53+AGC(1)*12)+AGC(8)*5+AGC(11)*9+AGC(12)*1,   (-6.53+AGC(1)*13)+AGC(8)*3+AGC(11)*7];
        Acpro=-0.9.*pdpk-21.43; %product %column vector

        %Parameter B
                                   %A                                                      %B1              %up to 10
        Bc=[  (263+BGC(1)*1)+BGC(4)*2+BGC(5)*2+BGC(10)*2+BGC(11)*2,         (263+BGC(1)*6)+BGC(8)*3+BGC(11)*3];%
(263+BGC(1)*12)+BGC(8)*5+BGC(11)*9+BGC(12)*1,     (263+BGC(1)*13)+BGC(8)*3+BGC(11)*7];
        Bcpro=500.*pdpk+7085; %product %column vector

        %Pure Component Vicosity   %up to 10 + 1
                                    %A                                                     %B1
%Product
        g3=[mer(10,1)*mer(3,1)*exp(Ac(1)+(Bc(1)./c(:,24))),    mer(10,2)*mer(3,2)*exp(Ac(2)+(Bc(2)./c(:,24))),
Denpro.*MWpro(:,1).*exp(Acpro(:,1)+(Bcpro(:,1)./c(:,24)))];  %arithmetic ops = element-wise
        %mer(10,3)*mer(3,3)*exp(Ac(3)+(Bc(3)./c(:,24))),    mer(10,4)*mer(3,4)*exp(Ac(4)+(Bc(4)./c(:,24)))

        %Mass Fractions   %up to 10 + 1
        x1=((c(:,1)*mer(3,1)))./((c(:,1)*mer(3,1))+(c(:,2)*mer(3,2))+(c(:,21).*MWpro))); %arithmetic ops = element-wise
        x2=((c(:,2)*mer(3,2)))./((c(:,1)*mer(3,1))+(c(:,2)*mer(3,2))+(c(:,21).*MWpro))); %arithmetic ops = element-wise
        x5=( (c(:,21).*MWpro)./((c(:,1)*mer(3,1))+(c(:,2)*mer(3,2))+(c(:,21).*MWpro))); %arithmetic ops = element-wise
```

```matlab
        %Mixture Viscosity %up to 10 + 1
        gm3=exp((x1.*log(g3(:,1)))+(x2.*log(g3(:,2)))+(x5.*log(g3(:,3))));
        %+(x3.*log(g3(:,3)))+(x4.*log(g3(:,4)))

        %------------------------------------------------------------------------------------
---------------------

        %Variable Assignment-----------------------------------------------------------------
---------------------

        xx = t;                             %x values for the Profiles
        y1 = c(:,24)- 273.15;               %y1 = y values for the Temperature Profile (in deg. C)
        y2 = gm3(:,1);                      %y2 = y values for the Viscosity Profile
        y3 = c(:,25);                       %y3 = y values for the Height Profile
        %y4 = c(:,13);                        %y4 = y values for the Bp Profile
        %y5 = c(:,16);                        %y5 = y values for the Urethane Profile
        %y6 = c(:,21);                         %y6 = y values for the pdp Profile

        %------------------------------------------------------------------------------------
---------------------

        %For Finding Properties at Maximum----------------------------------------------------
---------------------

        imax = find(max(y1) == y1);    %the ith row of y1 for which y1 is max
        imax2 = find(max(y2) == y2);   %the ith row of y2 for which y1 is max

        %------------------------------------------------------------------------------------
---------------------

        %Validation---------------------------------------------------------------------------
---------------------


        fprintf('Combo %d [i5212: %d, i678: %d | ', combon, i5212, i678);

        %validity criteria for match-finding
        if lowerCL*aa <= y1(imax) && y1(imax) <= upperCL*aa %&& lowerCL*bb <= xx(imax) && xx(imax) <= upperCL*bb

            fprintf('%.2f %.2f %.2f , %.2f %.2f %.2f | %.2f %.2f, %.2f %.2f] MATCH!\n',
mer(5,2),mer(2,2),mer(12,2),mer(6,2),mer(7,2),mer(8,2),aa,y1(imax),bb,xx(imax));

            beep on; beep;

            %populating match matrices if match is found
            F_Simulate_MatchMatrices
```

```matlab
            %simulating plots if match is found
            G_Simulate_Plot1
            %G_Simulate_Plot2

            %updating zz if match is found
            zz = zz + 1;

        else

            fprintf('%.2f %.2f %.2f , %.2f %.2f %.2f | %.2f %.2f, %.2f %.2f]
Mismatch\n',mer(5,2),mer(2,2),mer(12,2),mer(6,2),mer(7,2),mer(8,2),aa,y1(imax),bb,xx(imax));

        end

        %------------------------------------------------------------------------------------------------
----------------------

    combon = combon + 1;

    end

    %combon = combon + 1;

end
```

Function (S6)

```matlab
function FoamSim


global combon xx y1 imax2 trange_max Matrix_Matches

%ensure legend is shown
legend show

%legend for curve
zeys = combon;
text = ['Combo ',num2str(zeys)];

%plot T vs. t curve
%figure
%plot_1 = plot(xx,y1,'DisplayName',text);
plot(xx,y1,'DisplayName',text);
title('Temperature Profile of Matching Runs')
xlabel('Time (s)')
ylabel('Temperature (deg. C)')
axis([0, trange_max, 0, 500-273.15])

%hold plot to superimpose gel point on curve
hold on


%legend for gel point
max_text = ['T_m_a_x of C',num2str(zeys)];

%plot for gel point >> inaccurate imax, use imax of max(y2) instead
plot(xx(imax2),y1(imax2),'^r','DisplayName',max_text);


%hold plot to superimpose plot for next combon
hold on


end

prompt = {'Enter desired max. temp. (in deg. C):','Enter corresponding time for max. temp. (in s):', 'Enter time range
for profile (in min):', 'Enter Confidence (in %):'};
  title = 'Inputs';
  dims = [1 48];
  definput = {'145','470', '10', '5'};
  answer = inputdlg(prompt,title,dims,definput);
  aa = str2double(answer{1}); %round(str2double(answer{1}),2);
```

```matlab
    bb = str2double(answer{2}); %round(str2double(answer{2}),2);
    cc = str2double(answer{3}); %round(str2double(answer{3}),2);
    CL = str2double(answer{4}); %round(str2double(answer{4}),2);

    prompt = {'Enter room temp. (in deg. C):'};
    title = 'Inputs';
    dims = [1 48];
    definput = {'33'};
    answer = inputdlg(prompt,title,dims,definput);
    TT = str2double(answer{1}); %round(str2double(answer{1}),2);


nmatches = height(Matrix_Matches);
if nmatches == 0
    fprintf('\nNo match has been found throughout whole run.\n\n');
else if nmatches == 1
    fprintf('\nThere is %d match.\n\n',nmatches);
else
    fprintf('\nThere are %d matches.\n\n',nmatches);
    end
end



end
```