Modeling of Toluene Sulfonic Acid Catalyzed Oxide Addition Reaction for Soy-Based Polyol

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Supporting information: Component variables and component rate expressions.

Component Variable	**Concentration of-**	**Initial Condition**	**Component Rate Expression**
C_{ESBO}	Monomer epoxy	C_{ESBO0}	$\sum_{i=1}^{4} -r_i$
M_{EPOXY}	Total functional groups of epoxy	$f_{ESBO}C_{ESBO0}$	$\sum_{i=1}^{8} -r_i$
$M_{Alcohol}$	Total functional groups of Alcohol	$f_{Alcohol}C_{Alcohol0}$	$-r_4 - r_8$
C_{EG}	Monomer EG	C_{EG0}	$-r_1 - r_5$
C_{DEG}	Monomer DEG	C_{DEG0}	$-r_2 - r_6$
C_{TEG}	Monomer TEG	C_{TEG0}	$-r_3 - r_7$
P	Polyol	0	$\sum_{i=1}^{3} r_i - (\frac{1}{DP})r_8$

Supporting document for

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MATLAB CODE

Script

```
clear;clc;close all;
global esbo0 eg0 deg0 teg0 fesbo water0 r
constants
[t,c]=ode45(@polyol,[0:1200:8400],[esbo0;esbo0*fesbo;eg0;deg0;teg0;0;water0;
0]);
DPP=(esbo0+eg0+deg0+teg0)./(c(:,1)+c(:,3)+c(:,4)+c(:,5)+c(:,6))
```

Constants

```
function constants
global h A E esbo0 eg0 deg0 teg0 cat Cpesbo Cpeg Cpdeg Cpteg U area
Nalcohol0 fesbo feg fdeg fteg T0 Tin Nwater0 water0 fwater
esbo0=814.5/1000;%mol initial concentration of Epoxidized Soybean Oil
eg0=85.5/62.7;%mol initial concentration of Ethylene Glycol
deg0=0/106.12;%mol initial concentration of Diethylene Glycol
teg0=0/150.17;%mol initial concentration of Triethylene Glycol
water0=0*815.8/18;%mol initial concentration of water
cat=5;%g  mass of gel reaction catalyst
fesbo=7;
feg=2;
fdeg=2;
fteg=2;
fwater=2;
T0=125+273.15;
Tin=161+273.15;
Nalcohol0=feg*eg0+fdeg*deg0+fteg*teg0;
Nwater0=water0*fwater;
ee=1.4e5;
aa=5.5e17;
E(1)=ee;%J/mol  activation energy of ESBO and EG reaction
E(2)=ee;%J/mol  activation energy of ESBO and DEG reaction
E(3)=ee;%J/mol  activation energy of ESBO and TEG reaction
E(4)=ee;%J/mol  activation energy of ESBO and Alcohol reaction
E(5)=ee;%J/mol  activation energy of ESBOp and EG reaction
E(6)=ee;%J/mol  activation energy of ESBOp and DEG reaction
E(7)=ee;%J/mol  activation energy of ESBOp and TEG reaction
E(8)=ee;%J/mol  activation energy of ESBOp and Alcohol reaction
E(9)=ee;%J/mol  activation energy of ESBOp and Water reaction
E(10)=ee;%J/mol  activation energy of ESBOp and ACIDp reaction
E=[E(1),E(2),E(3),E(4),E(5),E(6),E(7),E(8),E(9),E(10)];
A(1)=aa;%ESBO and EG reaction rate constant at 298K
A(2)=aa;%ESBO and DEG reaction rate constant at 298K
A(3)=aa;%ESBO and TEG reaction rate constant at 298K
A(4)=aa;%ESBO and Alcohol on polyol reaction rate constant at 298K
A(5)=aa;%ESBOp and EG reaction rate constant at 298K
A(6)=aa;%ESBOp and DEGP reaction rate constant at 298K
A(7)=aa;%ESBOp and TEG reaction rate constant at 298K
```

```
A(8)=aa;%ESBOp and Alcohol reaction rate constant at 298K
A(9)=aa;%ESBOp and Water reaction rate constant at 298K
A(10)=aa;%ESBOp and ACIDp reaction rate constant at 298K
A=[A(1),A(2),A(3),A(4),A(5),A(6),A(7),A(8),A(9),A(10)];
```

Function

```
function dydt=polyol(t,c)
global fwater Nalcohol0 sc r A E esbo0 eg0 deg0 teg0 cat k V fesbo feg fdeg
fteg esbop T0 Tin TRXN DP water0
TRXN=(T0-273)+(Tin-T0+5)*t/(t+500); %Temperature
V=esbo0*fesbo*(1000/fesbo)/0.994+eg0*feg*31.35/1.11+deg0*fdeg*53.06/1.12+teg
0*fteg*75.085/1.10+cat/1.24+water0*18/1;
for i=1:10
    k(i)=cat*A(1,i)*exp(-E(1,i)/(8.3145*(TRXN+273)));
end
DP(1)=(esbo0+eg0+deg0+teg0)/(c(1)+c(3)+c(4)+c(5)+c(6));
DP(1)=DP(1)^5;
a=1;
esbop=c(2)-fesbo*c(1);
alcoholp=Nalcohol0-(feg*c(3)+fdeg*c(4)+fteg*c(5));
r=[k(1)*fesbo*c(1)*feg*c(3)/V^2;
   k(2)*fesbo*c(1)*fdeg*c(4)/V^2;
   k(3)*fesbo*c(1)*fteg*c(5)/V^2;
   k(4)*fesbo*c(1)*alcoholp/V^2;
   k(5)*esbop*feg*c(3)/V^2;
   k(6)*esbop*fdeg*c(4)/V^2;
   k(7)*esbop*fteg*c(5)/V^2;
   k(8)*alcoholp*esbop/V^2
   k(9)*esbop*fwater*c(7)/V^2;
   k(10)*esbop*c(8)/V^2];

   % 1   2   3   4   5   6   7      8      9   10
sc=[-1  -1  -1  -1   0   0   0      0      0   0; %1 monomer ESBO
    -a  -a  -a  -a  -a  -a  -a     -a     -a  -a; %2 total ESBO
    -1   0   0   0  -1   0   0      0      0   0; %3 monomer EG
     0  -1   0   0   0  -1   0      0      0   0; %4 monomer DEG
     0   0  -1   0   0   0  -1      0      0   0; %5 monomer TEG
     1   1   1   0   0   0   0  -1/DP(1)  1  -1; %6 Polymer
     0   0   0   0   0   0   0      0     -1   0; %7 Water
     0   0   0   0   0   0   0      0      1  -1];%8 Acid
  dydt=[sc*r];
```