DEHYDROGENATION REACTORS FOR STYRENE PRODUCTION

Reaction scheme:

Thermal reactions:

$$C_8H_{10} \leftrightarrow C_8H_8 + H_2 \qquad r_{t1} = k_{t1}\left(P_{EB} - \frac{P_{ST}P_{H_2}}{K_{eq}}\right)$$

$$C_8H_{10} \rightarrow C_6H_6 + C_2H_4 \qquad r_{t2} = k_{t2}P_{EB}$$

$$C_8H_{10} + H_2 \rightarrow C_7H_8 + CH_4 \qquad r_{t3} = k_{t3}P_{EB}$$

Catalytic reactions :

$$C_8H_{10} \leftrightarrow C_8H_8 + H_2 \qquad r_{c1} = \frac{k_1K_{EB}(P_{EB} - P_{ST}P_{H_2}/K_{eq})}{(1+K_{EB}P_{EB}+K_{H_2}P_{H_2}+K_{ST}P_{ST})^2}$$

$$C_8H_{10} \rightarrow C_6H_6 + C_2H_4 \qquad r_{c2} = \frac{k_2K_{EB}P_{EB}}{(1+K_{EB}P_{EB}+K_{H_2}P_{H_2}+K_{ST}P_{ST})^2}$$

$$C_8H_{10} + H_2 \rightarrow C_7H_8 + CH_4 \qquad r_{c3} = \frac{k_3K_{EB}P_{EB}K_{H_2}P_{H_2}}{(1+K_{EB}P_{EB}+K_{H_2}P_{H_2}+K_{ST}P_{ST})^2}$$

$$C_8H_8 + 2H_2 \rightarrow C_7H_8 + CH_4 \qquad r_{c4} = \frac{k_3K_{EB}P_{EB}K_{H_2}P_{H_2}}{(1 + K_{EB}P_{EB} + K_{H_2}P_{H_2} + K}$$

Nomenclature:

Thermal reactions:

At1 The pre-exponential factor for the first thermal reaction. Unit: kmol / m^3hbar; At2 The pre-exponential factor for the

first thermal reaction. Unit: kmol $/m^3$hbar; At3 The pre-exponential factor for the first thermal reaction. Unit: kmol $/m^3$hbar;
Et1 The activation energy for the first thermal reaction. Unit: kJ/mol; Et2 The activation energy for the second thermal reaction. Unit: kJ/mol; Et3 The activation energy for the third thermal reaction. Unit: kJ/mol;
R Gas constant. Unit: SI; kt1 The rate coefficient of the first thermal reaction. Unit: kmol $/m^3$hbar; kt2 The rate coefficient of the second thermal reaction. Unit: kmol $/m^3$hbar;
kt3 The rate coefficient of the third thermal reaction. Unit: kmol $/m^3$hbar; rt1 The reaction rate of the first thermal reaction. Unit: kmol $/m^3$h; rt2 The reaction rate of the second thermal reaction. Unit: kmol $/m^3$h;
rt3 The reaction rate of the third thermal reaction. Unit: kmol $/m^3$h;

Catalytic reactions:
A1 The pre-exponential factor for the first catalytic reaction. Unit: kmol / kg – cat h; A2 The pre-exponential factor for the second catalytic reaction. Unit: kmol / kg – cat h; A1 The pre-exponential factor for the third catalytic reaction. Unit: kmol / kg – cat h;
E1 The activation energy for the first catalytic reaction. Unit: kJ/mol; Et2 The activation energy for the second catalytic reaction. Unit: kJ/mol; Et3 The activation energy for the third catalytic reaction. Unit: kJ/mol;
k1 The rate coefficient of the first catalytic reaction. Unit: kmol/kg-cat h; k2 The rate coefficient of the second catalytic reaction. Unit: kmol/kg-cat h; k3 The rate coefficient of the third catalytic reaction. Unit: kmol/kg-cat h;
k4 The rate coefficient of the fourth catalytic reaction. Unit: kmol/kg-cat h; Keq The kinetic equilibrium constant for the first reversible reaction.Unit:1/bar; rc1 The reaction rate of the first catalytic reaction. kmol/kg-cat h;
rc2 The reaction rate of the second catalytic reaction. kmol/kg-cat h; rc3 The reaction rate of the third catalytic reaction. kmol/kg-cat h; rc4 The reaction rate of the fourth catalytic reaction. kmol/kg-cat h;

Adsorption:
AEB The pre-exponential factor for ethylbenzene adsorption. Unit: bar^{-1}; AST The pre-exponential factor for styrene adsorption. Unit: bar^{-1}; AH2 The pre-exponential factor for hydrogen adsorption. Unit: kmol $/m^3$hbar;
ΔHaEB Adsorption enthalpy of ethylbenzene. Unit:kJ/mol; ΔHaST Adsorption enthalpy of styrene. Unit:kJ/mol; ΔHaH2 Adsorption enthalpy of hydrogen;
KEB The adsorption equilibrium constant of ethylbenzene. Unit:1/bar; KST The adsorption equilibrium constant of styrene. Unit:1/bar; KH2: The adsorption equilibrium constant of hydrogen. Unit:1/bar;

Partial pressures of components:
PEB The partial pressure of ethylbenzene. Unit:1/bar; PST The partial pressure of styrene. Unit:1/bar; PBZ The partial pressure of benzene. Unit:1/bar;
PH2 The partial pressure of hydrogen. Unit:1/bar; PETH The partial pressure of ethylene. Unit:1/bar; PTO he partial pressure of toluene. Unit:1/bar;
PH2O The partial pressure of water. Unit:1/bar; PMTH The partial pressure of methane. Unit:1/bar; PT Total pressure of gas mixtures within the first reactor. Unit: 1/bar;
P Total pressure of gas mixtures in the second reactor. Unit: 1/bar;

Concentration of components:
CEB The concentration of ethylbenzene. Unit: mol/ m^3 ; CST The concentration of styrene.

Unit: mol/ m^3 ; CBZ The concentration of benzene. Unit: mol/ m^3 ;
CH2 The concentration of hydrogen. Unit: mol/ m^3 ; CETH The concentration of ethylene.
Unit: mol/ m^3 ; CTO The concentration of toluene. Unit: mol/ m^3 ;
CH2O The concentration of water. Unit: mol/ m^3 ; CTO The concentration of toluene.
Unit: mol/ m^3 ; CH2O The concentration of water. Unit: mol/ m^3;
CMTH The concentration of methane. Unit: mol/ m^3 ;

Selectivity of products:
SST Selectivity of styrene; SBZ Selectivity of benzene;
STO Selectivity of toluene;
SH2 Selectivity of hydrogen;

Heat of reactions:
ΔH1 Reaction enthalpy of the first reaction. Unit: kJ/kmol; ΔH2 Reaction enthalpy of the second reaction. Unit: kJ/kmol; ΔH3 Reaction enthalpy of the third reaction. Unit: kJ/kmol;
ΔH4 Reaction enthalpy of the fourth reaction. Unit: kJ/kmol;

Heat capacity of components:
Cp1 Heat capacity of ethylbenzene. Unit: kJ/kgK; Cp2 Heat capacity of styrene. Unit: kJ/kgK; Cp3 Heat capacity of benzene. Unit: kJ/kgK;
Cp4 Heat capacity of toluene. Unit:kJ/kgK; Cp5 Heat capacity of hydrogen. Unit: kJ/kgK; Cp6 Heat capacity of water. Unit: kJ/kgK;

Physical properties of the catalyst:
dp Catalyst equivalent pellet diameter. Unit: m; ρb Catalyst bulk diamter. Unit: kg-cat/m^3; ρs Catalyst pellet density. Unit: kg-cat/m^3;
εs Catalyst interval void fraction. ; τ Tortuosity of the catalyst;
ϵ Void fraction of the beds. ;

Dimensions of reactors:
Dr Diameter of the reactors. Unit: cm; Di Diameter of the reactors. Unit: m;
z The height of the reactos. Unit: m;
Ac The cross section area of the reactors. Unit: m^2; L The total height of the reactors. Unit:m.

Physical properties of feed mixture:
μ The viscosity of the mixture. Unit: kg/ms; u The superficial velocity of the inlet feed stream. Unit: m/s; G The superficial velocity of inlet feed stream. Unit: kg/hm^2 ;
ρg Density of the gas mixture. Unit: kg/m^3 ;

The initial flow rates of components in the feed mixture:
FEB0 The initial molar flow rate of ethylbenzene. Unit: kmol/h; FST0 The initial molar flow rate of styrene. Unit: kmol/h; FBZ0 The initial molar flow rate of benzene. Unit: kmol/h;
FTO0 The initial molar flow rate of toluene. Unit: kmol/h; FH20 The initial molar flow rate of hydrogen. Unit: kmol/h; FCH40 The initial molar flow rate of methane. Unit: kmol/h;
FC2H40 The initial molar flow rate of ethylene. Unit: kmol/h; FH2O0 The initial molar flow rate of water. Unit: kmol/h; FT0 The initial total molar flow rate of the feed stream. Unit: kmol/h;

Conversions of reactants:
X1EB Conversion of ethylbenzene in the first reactor; X1BZ Conversion of benzene in the first reactor; X1TO Conversion of toluene in the first reactor;
X1H2 Conversion of hydrogen in the first reactor; X2EB Conversion of ethylbenzene in the second reactor; X2BZ Conversion of benzene in the second reactor;
X2TO Conversion of toluene in the second reactor; X2H2 Conversion of hydrogen in the

second reactor;

Temperature:
T Temperature of gas mixtures along the reactors. Unit: K;

Calculation of key variable profiles

Concentration profiles

For the first reactor (r101), excluding water (or steam):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO,
   S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

  (*Construct the models for the thermal reactions*)
  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
  kt3 = At3*Exp[(-Et3*10^3)/(R*T[z])];


  (*Thermal reaction rates of three reactions*)
  rt1 = kt1*(PEB - (PST*PH2)/Keq); (**kmol/m3h**)
  rt2 = kt2*PEB;
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rt3 = kt3 * PEB;


(*Construct the models for the catalytic reactions*)
A1 = 4.594 * 10^9;  (**kmol/kg-cath**)
A2 = 1.060 * 10^15;
A3 = 1.246 * 10^26;
A4 = 8.024 * 10^10;
E1 = 175.38; (**kJ/mol**)
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;
k1 = A1 * Exp[(-E1 * 10^3)/(R * T[z])]; (**kmol/kg-cath**)
k2 = A2 * Exp[(-E2 * 10^3)/(R * T[z])];
k3 = A3 * Exp[(-E3 * 10^3)/(R * T[z])];
k4 = A4 * Exp[(-E4 * 10^3)/(R * T[z])];


(*Catalytic reaction rates of four reactions*)
rc1 = (k1 * KEB * (PEB - (PST * PH2)/Keq))/(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2; (**kmol/kg-cath**)
rc2 = (k2 * KEB * PEB)/(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2;
rc3 = (k3 * KEB * PEB * KH2 * PH2)/(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2;
rc4 = (k4 * KST * PST * KH2 * PH2)/(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2;


(*Construct the models for the thermodynamic equilibriums*)
AEB = 1.014 * 10^-5;  (**1/bar**)
AST = 2.678 * 10^-5;
AH2 = 4.519 * 10^-7;
ΔHaEB = -102.22; (**kJ/mol**)
ΔHaST = -104.56;
ΔHaH2 = -117.95;
```

$$KEB = AEB*Exp\left[\frac{-\Delta HaEB*10^3}{R*T[z]}\right]; (**1/bar**)$$

$$KST = AST*Exp\left[\frac{-\Delta HaST*10^3}{R*T[z]}\right];$$

$$KH2 = AH2*Exp\left[\frac{-\Delta HaH2*10^3}{R*T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267*T[z] - 0.002194*T[z]*T[z])}{R*T[z]}\right]; (**1/bar**)$$

```
(*(**The initial molar flowrates of components**)*)
FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 1080*3.6;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;
```

(*Partial pressure of components*)

$$PEB = PT[z]*\frac{\frac{FEB0}{FT0}(1-(X1EB[z]-X1BZ[z]-X1TO[z])-X1BZ[z]-X1TO[z])}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

(**1/bar**)

$$PST = PT[z]*\frac{\frac{FST0}{FT0}+\frac{FEB0}{FT0}*(X1EB[z]-X1BZ[z]-X1TO[z])}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PBZ = PT[z]*\frac{\frac{FBZ0}{FT0}+\frac{FEB0}{FT0}*X1BZ[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PH2 = PT[z]*\frac{\frac{FH20}{FT0}+\frac{FEB0}{FT0}*X1H2[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PETH = PT[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X1BZ[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PTO = PT[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X1TO[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PH2O = PT[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PMTH = PT[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X1EB[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB*10^5}{R*T[z]};$$

$$C1ST = \frac{PST*10^5}{R*T[z]};$$

$$C1BZ = \frac{PBZ*10^5}{R*T[z]};$$

$$C1H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C1ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C1TO = \frac{PTO*10^5}{R*T[z]};$$

$$C1H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C1MTH = \frac{PMTH*10^5}{R*T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z]-X1BZ[z]-X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99*(T[z]-298.15) + \frac{-8.2026*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) +$$

$$\frac{6.499*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-2.311*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2=105\,510+12.986*(T[z]-298.15)+\frac{-7.67*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{9.592*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-4.125*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H3=-54\,680+10.86*(T[z]-298.15)+\frac{-15.1844*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{23.04*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-9.9955*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H4=-172\,370+(-31.13)*(T[z]-298.15)+\frac{-6.9818*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{16.54*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-7.685*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

(*Heat capacities of components*)

$Cp1=-0.43426+6.0671*10^{-3}*T[z]-3.8625*10^{-6}*T[z]*T[z]+9.1282*10^{-10}*(T[z])^3;$ (**kJ/kgK**)

$Cp2=-0.26436+5.564*10^{-3}*T[z]-3.0018*10^{-6}*T[z]*T[z]+5.3317*10^{-10}*(T[z])^3;$

$Cp3=-0.40599+6.6616*10^{-3}*T[z]-4.5318*10^{-6}*T[z]*T[z]+12.255*10^{-10}*(T[z])^3;$

$Cp4=-0.27127+5.9142*10^{-3}*T[z]-3.8631*10^{-6}*T[z]*T[z]+9.54*10^{-10}*(T[z])^3;$

$Cp5=13.57+4.637*10^{-3}*T[z]-6.905*10^{-6}*T[z]*T[z]+38.23*10^{-10}*(T[z])^3;$

$Cp6=1.7911+0.1069*10^{-3}*T[z]+0.58611*10^{-6}*T[z]*T[z]-1.998*10^{-10}*(T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

$\rho b = 1422;$

$\epsilon = 0.4312;$

(*Dimensions of the reactor*)

L = 10;

$Di=\frac{Dr}{100};$

$Ac=\frac{\pi}{4}*(Di)^2;$

(*The important properties of the gas mixture*)

$\mu=(-10.035+0.25191*T[z]-0.000037932*T[z]*T[z])*3.6*10^{-4};$ (**kg/ms**)

u = 22.003/Ac;

G = 89 520.109/Ac;

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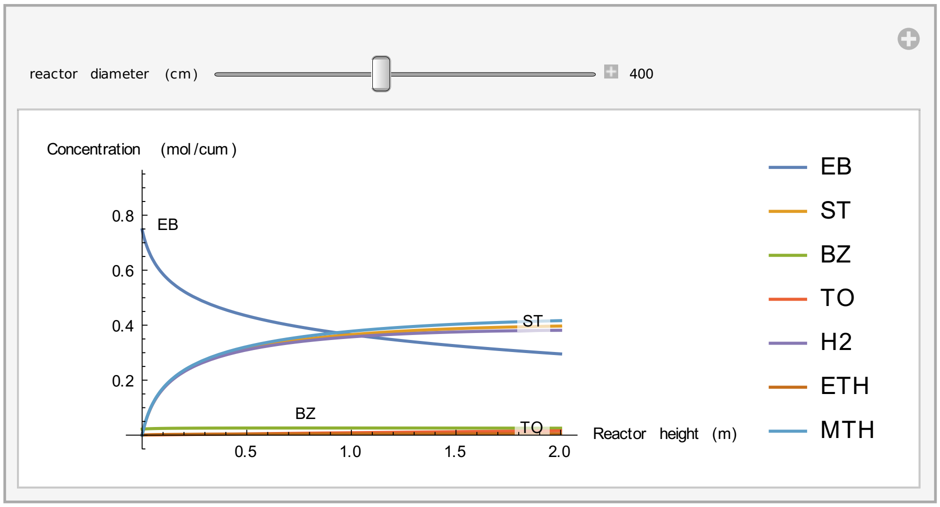
ρg = (10^5*10^-3)/(R*T[z]) *(PEB*106.168 + PST*104.15 + PBZ*78.114 +
    PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r101 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2* ϵ/ρb)* (Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3* ϵ/ρb)* (Ac*ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3 *(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) *10^-5 * (Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0 *(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
      (FEB0*(-ΔH1*(rc1 + rt1* ϵ/ρb) - ΔH2*(rc2 + rt2* ϵ/ρb) - ΔH3*(rc3 + rt3* ϵ/ρb) - ΔH4*rc4)),
    X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 886},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB,  C1ST,  C1BZ,  C1TO,
    C1H2,  C1ETH,  C1H2O, C1MTH}, {z, 0, 2}];
Figure1 = Plot[{C1EB /. r101, C1ST /. r101, C1BZ /. r101, C1TO /. r101,
    C1H2 /. r101,  C1ETH /. r101,  C1MTH /. r101}, {z, 0, 2},
   PlotRange→ All, AxesLabel → {"Reactor height (m)", "Concentration (mol/cum)"},
   PlotLegends → {"EB", "ST", "BZ", "TO", "H2", "ETH", "MTH"},
   PlotLabels→ Placed[{"EB", "ST", "BZ", "TO"}, Above]], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



For the second reactor (r202), excluding water (or steam):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
   S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},

  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
```

$$kt1 = At1*Exp\left[\frac{-Et1*10^3}{R*T[z]}\right]; \text{(**kmol/m3hbar**)}$$

$$kt2 = At2*Exp\left[\frac{-Et2*10^3}{R*T[z]}\right];$$

$$kt3 = At3*Exp\left[\frac{-Et3*10^3}{R*T[z]}\right];$$

```
  A1 = 4.594*10^9; (**kmol/kg-cath**)
  A2 = 1.060*10^15;
  A3 = 1.246*10^26;
```

A4 = 8.024 * 10^{10};
E1 = 175.38; (**kJ/mol**)
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;

$$k1 = A1 * \mathrm{Exp}\left[\frac{-E1 * 10^3}{R * T[z]}\right]; \ (**\mathrm{kmol/kg-cath}**)$$

$$k2 = A2 * \mathrm{Exp}\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * \mathrm{Exp}\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * \mathrm{Exp}\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

AEB = 1.014 * 10^{-5}; (**1/bar**)
AST = 2.678 * 10^{-5};
AH2 = 4.519 * 10^{-7};
ΔHaEB = −102.22; (**kJ/mol**)
ΔHaST = −104.56;
ΔHaH2 = −117.95;

$$KEB = AEB * \mathrm{Exp}\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; \ (**1/\mathrm{bar}**)$$

$$KST = AST * \mathrm{Exp}\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * \mathrm{Exp}\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = \mathrm{Exp}\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \ (**1/\mathrm{bar}**)$$

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \ (**\mathrm{kmol/m3h}**)$$

rt2 = kt2 * PEB;
rt3 = kt3 * PEB;

$$C2EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C2ST = \frac{PST * 10^5}{R * T[z]};$$

$$C2BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C2H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C2ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C2TO = \frac{PTO*10^5}{R*T[z]};$$

$$C2H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C2MTH = \frac{PMTH*10^5}{R*T[z]};$$

$$S2ST = \frac{X2EB[z] - X2BZ[z] - X2TO[z]}{X2EB[z]};$$

$$S2BZ = \frac{X2BZ[z]}{X2EB[z]};$$

$$S2TO = \frac{X2TO[z]}{X2EB[z]};$$

$$S2H2 = \frac{X2H2[z]}{X2EB[z]};$$

FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 3954.696;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

$$PEB = P[z]*\frac{\frac{FEB0}{FT0}(1 - (X2EB[z] - X2BZ[z] - X2TO[z]) - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

(**1/bar**)

$$PST = P[z]*\frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0}*(X2EB[z] - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PBZ = P[z]*\frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0}*X2BZ[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2 = P[z]*\frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0}*X2H2[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PETH = P[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X2BZ[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PTO = P[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X2TO[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PH2O = P[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PMTH = P[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X2EB[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$rc1 = \frac{k1*KEB*\left(PEB-\frac{PST*PH2}{Keq}\right)}{(1+KEB*PEB+KH2*PH2+KST*PST)^2}; \text{ (**kmol/kg−cath**)}$$

$$rc2 = \frac{k2*KEB*PEB}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$rc3 = \frac{k3*KEB*PEB*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$rc4 = \frac{k4*KST*PST*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$\Delta H1 = 117\,690+41.99*(T[z]-298.15)+\frac{-8.2026*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{6.499*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-2.311*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510+12.986*(T[z]-298.15)+\frac{-7.67*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{9.592*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-4.125*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H3 = -54\,680+10.86*(T[z]-298.15)+\frac{-15.1844*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{23.04*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-9.9955*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

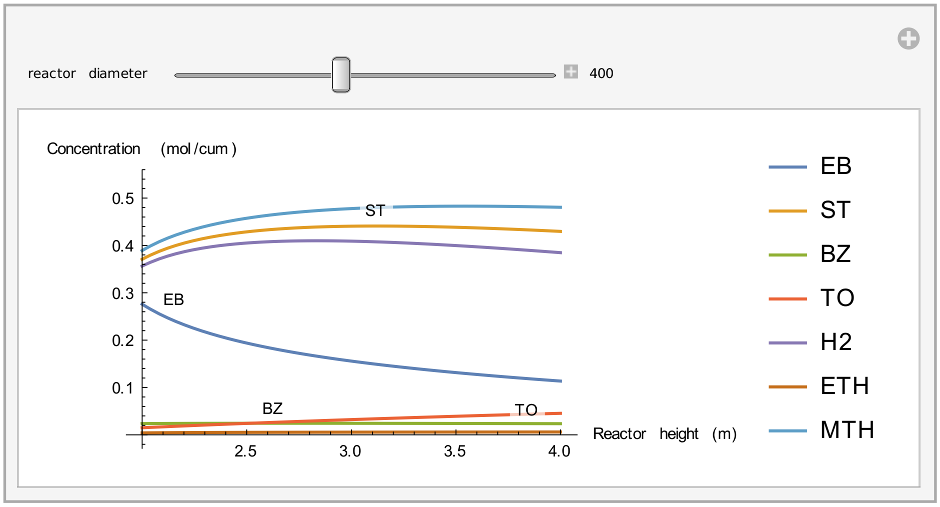
$$\Delta H4 = -172\,370+(-31.13)*(T[z]-298.15)+\frac{-6.9818*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{16.54*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-7.685*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$Cp1 = -0.43426+6.0671*10^{-3}*T[z]-3.8625*10^{-6}*T[z]*T[z]+9.1282*10^{-10}*(T[z])^3; \text{ (**kJ/kgK**)}$$

```
Cp2 = -0.26436 + 5.564*10^-3 *T[z] - 3.0018*10^-6 *T[z]*T[z] + 5.3317*10^-10 *(T[z])^3;
Cp3 = -0.40599 + 6.6616*10^-3 *T[z] - 4.5318*10^-6 *T[z]*T[z] + 12.255*10^-10 *(T[z])^3;
Cp4 = -0.27127 + 5.9142*10^-3 *T[z] - 3.8631*10^-6 *T[z]*T[z] + 9.54*10^-10 *(T[z])^3;
Cp5 = 13.57 + 4.637*10^-3 *T[z] - 6.905*10^-6 *T[z]*T[z] + 38.23*10^-10 *(T[z])^3;
Cp6 = 1.7911 + 0.1069*10^-3 *T[z] + 0.58611*10^-6 *T[z]*T[z] - 1.998*10^-10 *(T[z])^3;

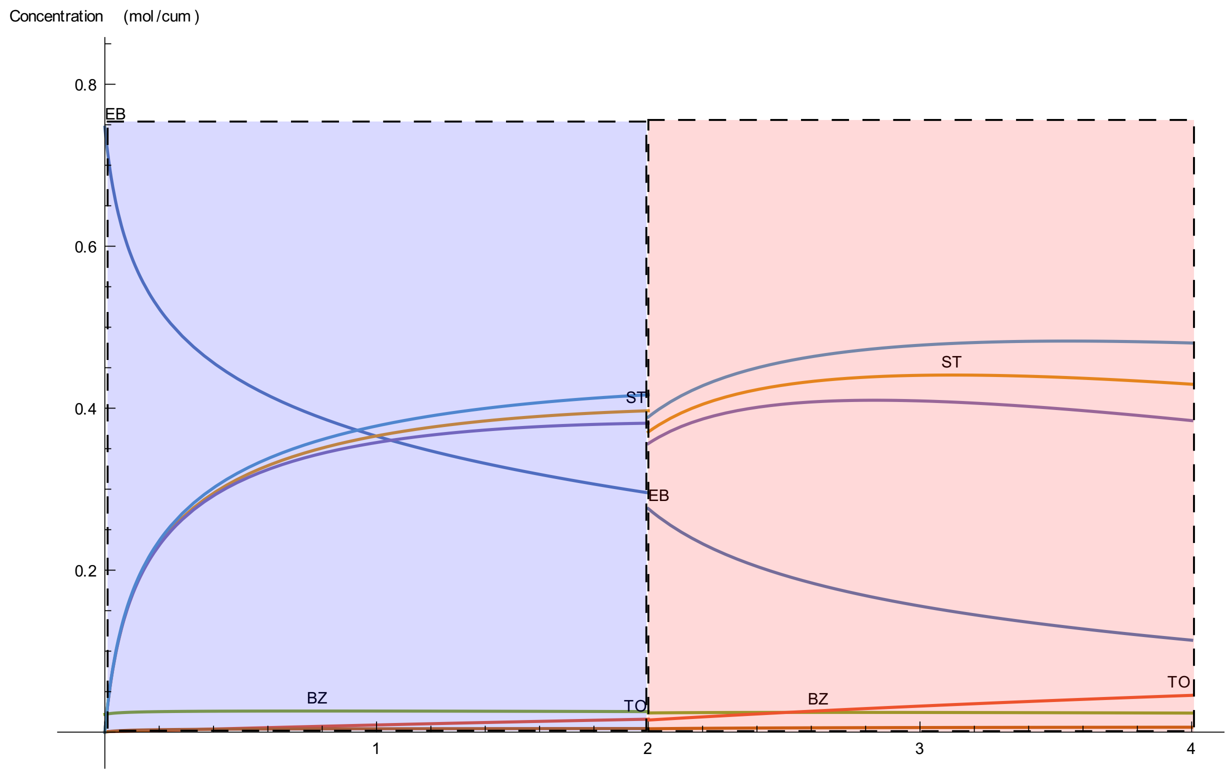
L = 10;
Di = Dr/100;
Ac = π/4 *(Di)^2;
dp = 5.5/1000; (**m**)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;
ρb = 1422;
ϵ = 0.4312; (**void fraction of bed**)
ρg = (10^5*10^-3)/(R*T[z]) *(PEB*106.168 + PST*104.15 + PBZ*78.114 +
      PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r202 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
      X2BZ'[z] == (rc2 + rt2 * ϵ/ρb)* (Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3 * ϵ/ρb)* (Ac*ρb)/FEB0,
      X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
      P'[z] == -(1 - ϵ)/ϵ^3 *(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) *10^-5 * (Ac*ρb)/FEB0,
      T'[z] == (Ac*ρb)/FEB0 *(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
            104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
            78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
            2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
         (FEB0*(-ΔH1*(rc1 + rt1 * ϵ/ρb) - ΔH2*(rc2 + rt2 * ϵ/ρb) - ΔH3*(rc3 + rt3 * ϵ/ρb) - ΔH4*rc4)),
      X2EB[2] == X1EB[2] /. r101, X2BZ[2] == X1BZ[2] /. r101, X2TO[2] == X1TO[2] /. r101,
      X2H2[2] == X1H2[2] /. r101, P[2] == PT[2] /. r101, T[2] == 870},
    {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB,  C2ST,  C2BZ,  C2TO,
      C2H2,  C2ETH,  C2H2O, C2MTH}, {z, 2, 4}];
Figure2 = Plot[{C2EB /. r202, C2ST /. r202, C2BZ /. r202, C2TO /. r202, C2H2 /. r202,  C2ETH /. r202,
      C2MTH /. r202}, {z, 2, 4}, AxesLabel → {"Reactor height (m)", "Concentration (mol/cum)"},
    PlotLabels → Placed[{"EB", "ST", "BZ", "TO"}, Above],
```

```
    PlotLegends → {"EB", "ST", "BZ", "TO", "H2", "ETH", "MTH"}, PlotRange → All]], Column[{
  Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



Concentrations of each components (excluding water) within these two reactors

```
Legended [Show [Figure1 , Figure2 ],
  SwatchLegend [{Blue , Red}, {"1st reactor ", "2nd reactor "}]]
```



Concentrations of each component with water (or steam) included for reactor r101

Manipulate[

Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST, AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0, FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4, PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO, S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

(*Construct the models for the thermal reactions*)

At1 = $2.2215*10^{16}$; (kmol/m3hbar**)**

At2 = $2.4217*10^{20}$;

At3 = $3.8224*10^{17}$;

Et1 = 272.23; (kJ/mol**)**

Et2 = 352.79;

Et3 = 313.06;

R = 8.314;

kt1 = At1*Exp$\left[\dfrac{-Et1*10^3}{R*T[z]}\right]$; (kmol/m3hbar**)**

$$kt2 = At2 * Exp\left[\frac{-Et2 * 10^3}{R * T[z]}\right];$$

$$kt3 = At3 * Exp\left[\frac{-Et3 * 10^3}{R * T[z]}\right];$$

(*Thermal reaction rates of three reactions*)

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right);$$ **(**kmol/m3h**)**

rt2 = kt2 * PEB;

rt3 = kt3 * PEB;

(*Construct the models for the catalytic reactions*)

$A1 = 4.594 * 10^9$; **(**kmol/kg−cath**)**

$A2 = 1.060 * 10^{15}$;

$A3 = 1.246 * 10^{26}$;

$A4 = 8.024 * 10^{10}$;

E1 = 175.38; (kJ/mol**)**

E2 = 296.29;

E3 = 474.76;

E4 = 213.78;

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right];$$ **(**kmol/kg−cath**)**

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

(*Catalytic reaction rates of four reactions*)

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$ **(**kmol/kg−cath**)**

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

(*Construct the models for the thermodynamic equilibriums*)

$AEB = 1.014 * 10^{-5};$ (**1/bar**)

$AST = 2.678 * 10^{-5};$

$AH2 = 4.519 * 10^{-7};$

$\Delta HaEB = -102.22;$ (**kJ/mol**)

$\Delta HaST = -104.56;$

$\Delta HaH2 = -117.95;$

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right];$$ (**1/bar**)

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right];$$ (**1/bar**)

(*(**The initial molar flowrates of components**)*)

FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)

FST0 = 0.00332919*3.6;

FBZ0 = 1.464*3.6;

FTO0 = 0.0482245*3.6;

FH20 = 0;

FCH40 = 0;

FC2H40 = 0;

FH2O0 = 1080*3.6;

FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

(*Partial pressure of components*)

$$PEB = PT[z] * \frac{\frac{FEB0}{FT0}(1 - (X1EB[z] - X1BZ[z] - X1TO[z]) - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(**1/bar**)

$$PST = PT[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (X1EB[z] - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PBZ = PT[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2 = PT[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X1H2[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PETH = PT[z] * \frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PTO = PT[z] * \frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0} * X1TO[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2O = PT[z] * \frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PMTH = PT[z] * \frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0} * X1EB[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C1ST = \frac{PST * 10^5}{R * T[z]};$$

$$C1BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C1H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C1ETH = \frac{PETH * 10^5}{R * T[z]};$$

$$C1TO = \frac{PTO * 10^5}{R * T[z]};$$

$$C1H2O = \frac{PH2O * 10^5}{R * T[z]};$$

$$C1MTH = \frac{PMTH * 10^5}{R * T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

ρb = 1422;

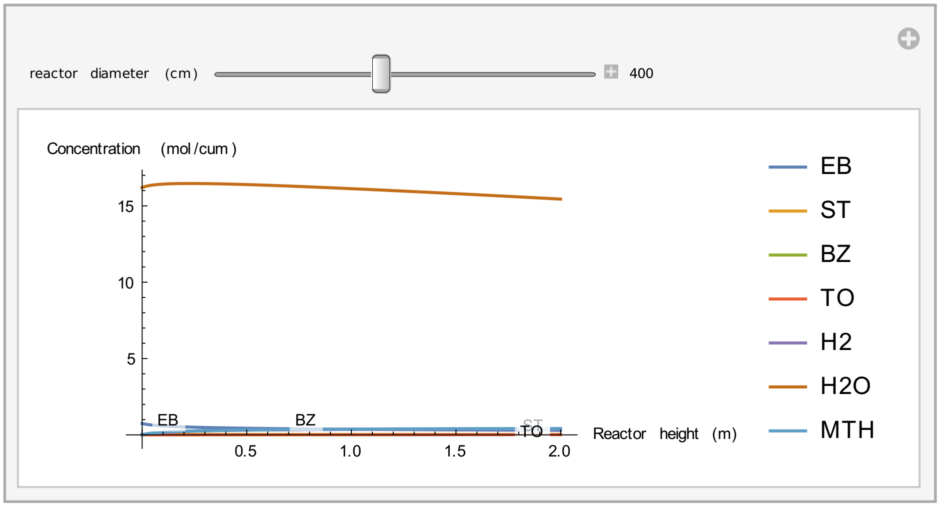
```
ϵ = 0.4312;


(*Dimensions of the reactor*)
L = 10;
Di = Dr/100;
Ac = π/4 * (Di)^2;

(*The important properties of the gas mixture*)
μ = (-10.035 + 0.25191 * T[z] - 0.000037932 * T[z] * T[z]) * 3.6 * 10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;

ρg = (10^5 * 10^-3)/(R * T[z]) * (PEB * 106.168 + PST * 104.15 + PBZ * 78.114 +
    PTO * 92.141 + PH2O * 18.020 + PH2 * 2.010 + PMTH * 16.043 + PETH * 28.054);
r102 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3) * ϵ/ρb) * (Ac * ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2 * ϵ/ρb) * (Ac * ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3 * ϵ/ρb) * (Ac * ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * ϵ/ρb) * (Ac * ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458 * (1 - ϵ))/((ρg * dp * u)/μ)) * 7.7160 * 10^-8 * (u * G * FEB0)/(ρb * dp * Ac) * 10^-5 * (Ac * ρb)/FEB0,
    T'[z] == (Ac * ρb)/FEB0 * (1/(106.168 * FEB0 * (1 - X1EB[z]) * Cp1 +
          104.15 * (FST0 + FEB0 * (X1EB[z] - X1BZ[z] - X1TO[z])) * Cp2 +
          78.114 * (FBZ0 + FEB0 * X1BZ[z]) * Cp3 + 92.141 * (FTO0 + FEB0 * X1TO[z]) * Cp4 +
          2.010 * (FH20 + FEB0 * X1H2[z]) * Cp5 + 18.020 * FH2O0 * Cp6)) *
      (FEB0 * (-ΔH1 * (rc1 + rt1 * ϵ/ρb) - ΔH2 * (rc2 + rt2 * ϵ/ρb) - ΔH3 * (rc3 + rt3 * ϵ/ρb) - ΔH4 * rc4)),
    X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 886},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
    C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];
Figure3 = Plot[{C1EB /. r102, C1ST /. r102, C1BZ /. r102, C1TO /. r102,
   C1H2 /. r102, C1H2O /. r102, C1MTH /. r102}, {z, 0, 2},
  PlotRange → All, AxesLabel → {"Reactor height (m)", "Concentration (mol/cum)"},
  PlotLegends → {"EB", "ST", "BZ", "TO", "H2", "H2O", "MTH"},
```

```
    PlotLabels → Placed[{"EB", "ST", "BZ", "TO"}, Above]], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



Concentrations of each components with water (or steam) included for reactor r202

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
   S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},

  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
```

$$kt1 = At1 * Exp\left[\frac{-Et1 * 10^{3}}{R * T[z]}\right]; \text{ (**kmol/m3hbar**)}$$

$$kt2 = At2 * Exp\left[\frac{-Et2 * 10^{3}}{R * T[z]}\right];$$

$$kt3 = At3 * Exp\left[\frac{-Et3 * 10^{3}}{R * T[z]}\right];$$

```
  A1 = 4.594*10^9; (**kmol/kg-cath**)
```

$$A2 = 1.060 * 10^{15};$$
$$A3 = 1.246 * 10^{26};$$
$$A4 = 8.024 * 10^{10};$$
$$E1 = 175.38; \text{ (**kJ/mol**)}$$
$$E2 = 296.29;$$
$$E3 = 474.76;$$
$$E4 = 213.78;$$
$$k1 = A1 * \mathrm{Exp}\left[\frac{-E1 * 10^3}{R * T[z]}\right]; \text{ (**kmol/kg-cath**)}$$
$$k2 = A2 * \mathrm{Exp}\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$
$$k3 = A3 * \mathrm{Exp}\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$
$$k4 = A4 * \mathrm{Exp}\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$
$$AEB = 1.014 * 10^{-5}; \text{ (**1/bar**)}$$
$$AST = 2.678 * 10^{-5};$$
$$AH2 = 4.519 * 10^{-7};$$
$$\Delta HaEB = -102.22; \text{ (**kJ/mol**)}$$
$$\Delta HaST = -104.56;$$
$$\Delta HaH2 = -117.95;$$
$$KEB = AEB * \mathrm{Exp}\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; \text{ (**1/bar**)}$$
$$KST = AST * \mathrm{Exp}\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$
$$KH2 = AH2 * \mathrm{Exp}\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$
$$Keq = \mathrm{Exp}\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \text{ (**1/bar**)}$$

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \text{ (**kmol/m3h**)}$$
$$rt2 = kt2 * PEB;$$
$$rt3 = kt3 * PEB;$$

$$C2EB = \frac{PEB * 10^5}{R * T[z]};$$
$$C2ST = \frac{PST * 10^5}{R * T[z]};$$
$$C2BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C2H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C2ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C2TO = \frac{PTO*10^5}{R*T[z]};$$

$$C2H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C2MTH = \frac{PMTH*10^5}{R*T[z]};$$

$$S2ST = \frac{X2EB[z] - X2BZ[z] - X2TO[z]}{X2EB[z]};$$

$$S2BZ = \frac{X2BZ[z]}{X2EB[z]};$$

$$S2TO = \frac{X2TO[z]}{X2EB[z]};$$

$$S2H2 = \frac{X2H2[z]}{X2EB[z]};$$

FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 3954.696;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

$$PEB = P[z]*\frac{\frac{FEB0}{FT0}(1 - (X2EB[z] - X2BZ[z] - X2TO[z]) - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

(**1/bar**)

$$PST = P[z]*\frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0}*(X2EB[z] - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PBZ = P[z]*\frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0}*X2BZ[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2 = P[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X2H2[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PETH = P[z] * \frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0} * X2BZ[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PTO = P[z] * \frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0} * X2TO[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2O = P[z] * \frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PMTH = P[z] * \frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0} * X2EB[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2}; \text{(**kmol/kg-cath**)}$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) +$$

$$\frac{16.54*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-7.685*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$Cp1 = -0.43426 + 6.0671*10^{-3}*T[z] - 3.8625*10^{-6}*T[z]*T[z] + 9.1282*10^{-10}*(T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564*10^{-3}*T[z] - 3.0018*10^{-6}*T[z]*T[z] + 5.3317*10^{-10}*(T[z])^3;$

$Cp3 = -0.40599 + 6.6616*10^{-3}*T[z] - 4.5318*10^{-6}*T[z]*T[z] + 12.255*10^{-10}*(T[z])^3;$

$Cp4 = -0.27127 + 5.9142*10^{-3}*T[z] - 3.8631*10^{-6}*T[z]*T[z] + 9.54*10^{-10}*(T[z])^3;$

$Cp5 = 13.57 + 4.637*10^{-3}*T[z] - 6.905*10^{-6}*T[z]*T[z] + 38.23*10^{-10}*(T[z])^3;$

$Cp6 = 1.7911 + 0.1069*10^{-3}*T[z] + 0.58611*10^{-6}*T[z]*T[z] - 1.998*10^{-10}*(T[z])^3;$

$L = 10;$

$Di = \frac{Dr}{100};$

$Ac = \frac{\pi}{4}*(Di)^2;$

dp = 5.5/1000; (**m**)

$\mu = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^{-4};$ (**kg/ms**)

u = 22.003/Ac;

G = 89 520.109/Ac;

$\rho b = 1422;$

$\epsilon = 0.4312;$ (**void fraction of bed**)

$$\rho g = \frac{10^5*10^{-3}}{R*T[z]}*(PEB*106.168 + PST*104.15 + PBZ*78.114 + PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);$$

$$r201 = \text{Quiet}@\text{NDSolve}\Big[\Big\{X2EB'[z] == \left(rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$

$$X2BZ'[z] == \left(rc2 + rt2*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},\ X2TO'[z] == \left(rc3 + rc4 + rt3*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$

$$X2H2'[z] == \left(rc1 - rc3 - 2\,rc4 + (rt1 - rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$

$$P'[z] == -\frac{1-\epsilon}{\epsilon^3}*\left(1.28 + \frac{458*(1-\epsilon)}{\frac{\rho g*dp*u}{\mu}}\right)*7.7160*10^{-8}*\frac{u*G*FEB0}{\rho b*dp*Ac}*10^{-5}*\frac{Ac*\rho b}{FEB0},$$

$$T'[z] == \frac{Ac*\rho b}{FEB0}*(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 + 104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 + 78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 + 2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*$$

$$\left(FEB0*\left(-\Delta H1*\left(rc1 + rt1*\frac{\epsilon}{\rho b}\right) - \Delta H2*\left(rc2 + rt2*\frac{\epsilon}{\rho b}\right) - \Delta H3*\left(rc3 + rt3*\frac{\epsilon}{\rho b}\right) - \Delta H4*rc4\right)\right),$$

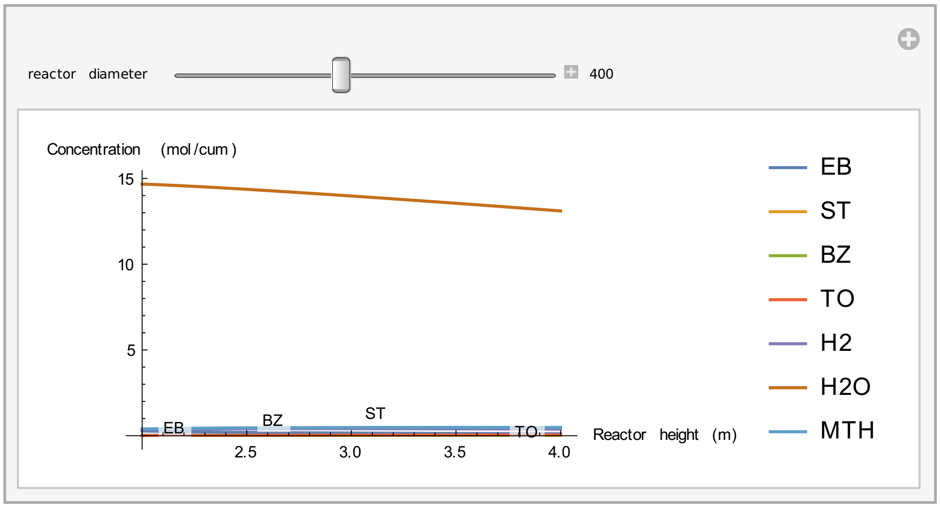
X2EB[2] == X1EB[2] /. r102, X2BZ[2] == X1BZ[2] /. r102, X2TO[2] == X1TO[2] /. r102,

X2H2[2] == X1H2[2] /. r102, P[2] == PT[2] /. r102, T[2] == 870},

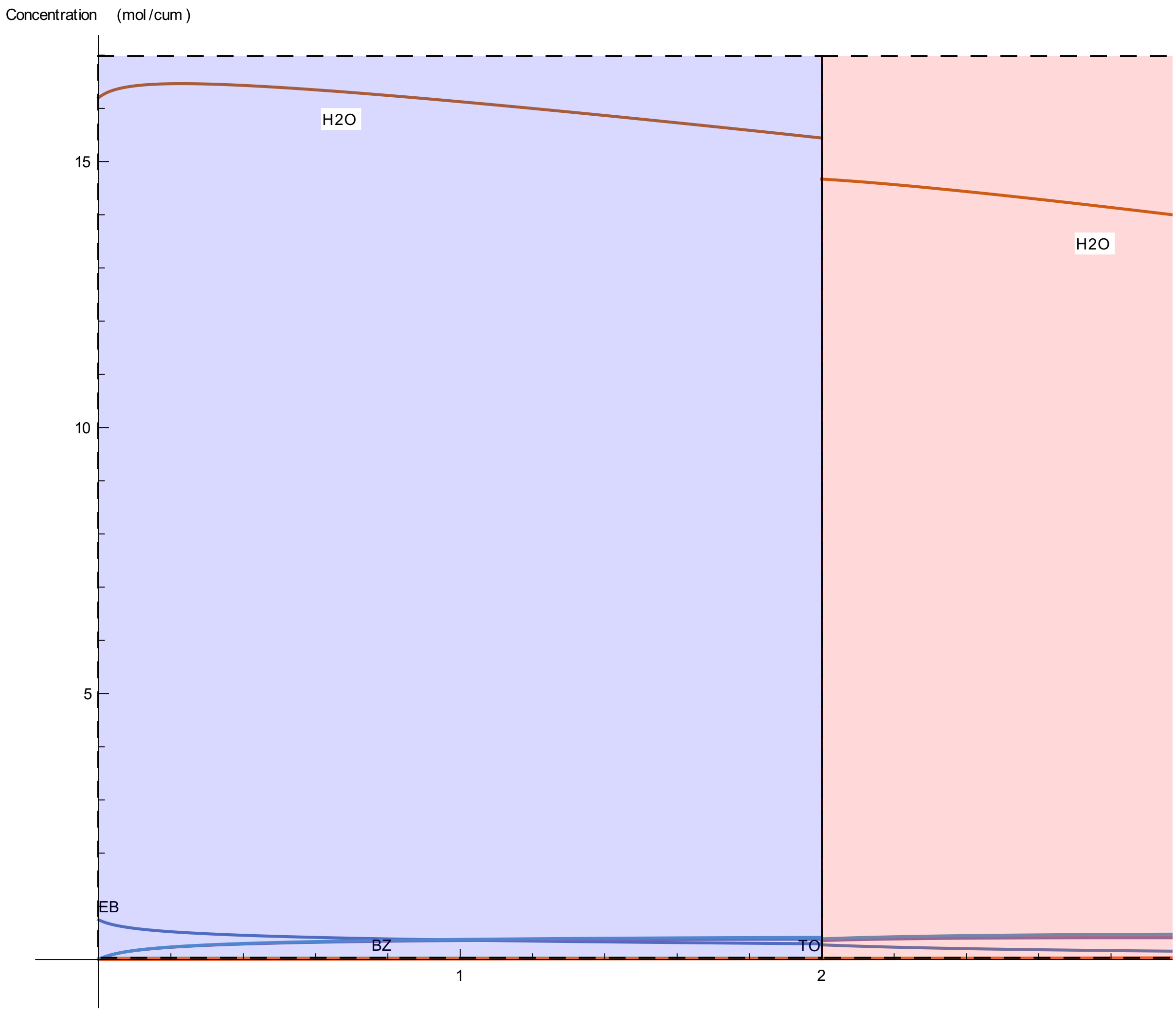
{P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,

C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];

```
Figure4 = Plot[{C2EB /. r201, C2ST /. r201, C2BZ /. r201, C2TO /. r201, C2H2 /. r201, C2H2O /. r201,
    C2MTH /. r201}, {z, 2, 4}, AxesLabel → {"Reactor height (m)", "Concentration (mol/cum)"},
  PlotLabels → Placed[{"EB", "ST", "BZ", "TO"}, Above],
  PlotLegends → {"EB", "ST", "BZ", "TO", "H2", "H2O", "MTH"}, PlotRange → All], Column[{
 Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```




```
Legended [Show[Figure3 , Figure4 ],
 SwatchLegend [{Blue , Red}, {"1st reactor ", "2nd reactor "}]]
```



Temperature profiles:

For the first reactor (r101):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO,
   S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

  (*Construct the models for the thermal reactions*)
```

```
At1 = 2.2215*10^16;  (**kmol/m3hbar**)
At2 = 2.4217*10^20;
At3 = 3.8224*10^17;
Et1 = 272.23;  (**kJ/mol**)
Et2 = 352.79;
Et3 = 313.06;
R = 8.314;
kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
kt3 = At3*Exp[(-Et3*10^3)/(R*T[z])];


(*Thermal reaction rates of three reactions*)
rt1 = kt1*(PEB - (PST*PH2)/Keq); (**kmol/m3h**)
rt2 = kt2*PEB;
rt3 = kt3*PEB;


(*Construct the models for the catalytic reactions*)
A1 = 4.594*10^9;  (**kmol/kg-cath**)
A2 = 1.060*10^15;
A3 = 1.246*10^26;
A4 = 8.024*10^10;
E1 = 175.38; (**kJ/mol**)
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;
k1 = A1*Exp[(-E1*10^3)/(R*T[z])]; (**kmol/kg-cath**)
k2 = A2*Exp[(-E2*10^3)/(R*T[z])];
k3 = A3*Exp[(-E3*10^3)/(R*T[z])];
k4 = A4*Exp[(-E4*10^3)/(R*T[z])];
```

```
(*Catalytic reaction rates of four reactions*)
```

$$rc1 = \frac{k1*KEB*\left(PEB - \frac{PST*PH2}{Keq}\right)}{(1 + KEB*PEB + KH2*PH2 + KST*PST)^2}; \text{ (**kmol/kg-cath**)}$$

$$rc2 = \frac{k2*KEB*PEB}{(1 + KEB*PEB + KH2*PH2 + KST*PST)^2};$$

$$rc3 = \frac{k3*KEB*PEB*KH2*PH2}{(1 + KEB*PEB + KH2*PH2 + KST*PST)^2};$$

$$rc4 = \frac{k4*KST*PST*KH2*PH2}{(1 + KEB*PEB + KH2*PH2 + KST*PST)^2};$$

```
(*Construct the models for the thermodynamic equilibriums*)
```

$AEB = 1.014*10^{-5};$ (**1/bar**)

$AST = 2.678*10^{-5};$

$AH2 = 4.519*10^{-7};$

$\Delta HaEB = -102.22;$ (**kJ/mol**)

$\Delta HaST = -104.56;$

$\Delta HaH2 = -117.95;$

$$KEB = AEB*Exp\left[\frac{-\Delta HaEB*10^3}{R*T[z]}\right]; \text{ (**1/bar**)}$$

$$KST = AST*Exp\left[\frac{-\Delta HaST*10^3}{R*T[z]}\right];$$

$$KH2 = AH2*Exp\left[\frac{-\Delta HaH2*10^3}{R*T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267*T[z] - 0.002194*T[z]*T[z])}{R*T[z]}\right]; \text{ (**1/bar**)}$$

```
(*(**The initial molar flowrates of components**)*)
FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 1080*3.6;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;
```

(*Partial pressure of components*)

$$PEB = PT[z]*\frac{\frac{FEB0}{FT0}(1-(X1EB[z]-X1BZ[z]-X1TO[z])-X1BZ[z]-X1TO[z])}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

(**1/bar**)

$$PST = PT[z]*\frac{\frac{FST0}{FT0}+\frac{FEB0}{FT0}*(X1EB[z]-X1BZ[z]-X1TO[z])}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PBZ = PT[z]*\frac{\frac{FBZ0}{FT0}+\frac{FEB0}{FT0}*X1BZ[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PH2 = PT[z]*\frac{\frac{FH20}{FT0}+\frac{FEB0}{FT0}*X1H2[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PETH = PT[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X1BZ[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PTO = PT[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X1TO[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PH2O = PT[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PMTH = PT[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X1EB[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB*10^5}{R*T[z]};$$

$$C1ST = \frac{PST*10^5}{R*T[z]};$$

$$C1BZ = \frac{PBZ*10^5}{R*T[z]};$$

$$C1H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C1ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C1TO = \frac{PTO*10^5}{R*T[z]};$$

$$C1H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C1MTH = \frac{PMTH*10^5}{R*T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99*(T[z] - 298.15) + \frac{-8.2026*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{6.499*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986*(T[z] - 298.15) + \frac{-7.67*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{9.592*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86*(T[z] - 298.15) + \frac{-15.1844*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{23.04*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13)*(T[z] - 298.15) + \frac{-6.9818*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{16.54*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$$Cp1 = -0.43426 + 6.0671*10^{-3}*T[z] - 3.8625*10^{-6}*T[z]*T[z] + 9.1282*10^{-10}*(T[z])^3;$$ (**kJ/kgK**)

$$Cp2 = -0.26436 + 5.564*10^{-3}*T[z] - 3.0018*10^{-6}*T[z]*T[z] + 5.3317*10^{-10}*(T[z])^3;$$

$$Cp3 = -0.40599 + 6.6616*10^{-3}*T[z] - 4.5318*10^{-6}*T[z]*T[z] + 12.255*10^{-10}*(T[z])^3;$$

$$Cp4 = -0.27127 + 5.9142*10^{-3}*T[z] - 3.8631*10^{-6}*T[z]*T[z] + 9.54*10^{-10}*(T[z])^3;$$

$$\mathrm{Cp5} = 13.57 + 4.637 * 10^{-3} * \mathrm{T[z]} - 6.905 * 10^{-6} * \mathrm{T[z]} * \mathrm{T[z]} + 38.23 * 10^{-10} * (\mathrm{T[z]})^3;$$

$$\mathrm{Cp6} = 1.7911 + 0.1069 * 10^{-3} * \mathrm{T[z]} + 0.58611 * 10^{-6} * \mathrm{T[z]} * \mathrm{T[z]} - 1.998 * 10^{-10} * (\mathrm{T[z]})^3;$$

(*Physical properties of the catalyst*)

$$\mathrm{dp} = 5.5/1000; \ (*\mathrm{m}*)$$

$$\rho\mathrm{b} = 1422;$$

$$\epsilon = 0.4312;$$

(*Dimensions of the reactor*)

$$\mathrm{L} = 10;$$

$$\mathrm{Di} = \frac{\mathrm{Dr}}{100};$$

$$\mathrm{Ac} = \frac{\pi}{4} * (\mathrm{Di})^2;$$

(*The important properties of the gas mixture*)

$$\mu = (-10.035 + 0.25191 * \mathrm{T[z]} - 0.000037932 * \mathrm{T[z]} * \mathrm{T[z]}) * 3.6 * 10^{-4}; \ (**\mathrm{kg/ms}**)$$

$$\mathrm{u} = 22.003/\mathrm{Ac};$$

$$\mathrm{G} = 89\,520.109/\mathrm{Ac};$$

$$\rho\mathrm{g} = \frac{10^5 * 10^{-3}}{\mathrm{R} * \mathrm{T[z]}} * (\mathrm{PEB} * 106.168 + \mathrm{PST} * 104.15 + \mathrm{PBZ} * 78.114 + \mathrm{PTO} * 92.141 + \mathrm{PH2O} * 18.020 + \mathrm{PH2} * 2.010 + \mathrm{PMTH} * 16.043 + \mathrm{PETH} * 28.054);$$

$$\mathrm{r103} = \mathrm{Quiet} @ \mathrm{NDSolve}\Big[\Big\{\mathrm{X1EB'[z]} == \left(\mathrm{rc1} + \mathrm{rc2} + \mathrm{rc3} + (\mathrm{rt1} + \mathrm{rt2} + \mathrm{rt3}) * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{X1BZ'[z]} == \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}}, \ \mathrm{X1TO'[z]} == \left(\mathrm{rc3} + \mathrm{rc4} + \mathrm{rt3} * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{X1H2'[z]} == \left(\mathrm{rc1} - \mathrm{rc3} - 2\,\mathrm{rc4} + (\mathrm{rt1} - \mathrm{rt3}) * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{PT'[z]} == -\frac{1 - \epsilon}{\epsilon^3} * \left(1.28 + \frac{458 * (1 - \epsilon)}{\frac{\rho\mathrm{g} * \mathrm{dp} * \mathrm{u}}{\mu}}\right) * 7.7160 * 10^{-8} * \frac{\mathrm{u} * \mathrm{G} * \mathrm{FEB0}}{\rho\mathrm{b} * \mathrm{dp} * \mathrm{Ac}} * 10^{-5} * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{T'[z]} == \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}} * (1/(106.168 * \mathrm{FEB0} * (1 - \mathrm{X1EB[z]}) * \mathrm{Cp1} + 104.15 * (\mathrm{FST0} + \mathrm{FEB0} * (\mathrm{X1EB[z]} - \mathrm{X1BZ[z]} - \mathrm{X1TO[z]})) * \mathrm{Cp2} + 78.114 * (\mathrm{FBZ0} + \mathrm{FEB0} * \mathrm{X1BZ[z]}) * \mathrm{Cp3} + 92.141 * (\mathrm{FTO0} + \mathrm{FEB0} * \mathrm{X1TO[z]}) * \mathrm{Cp4} + 2.010 * (\mathrm{FH20} + \mathrm{FEB0} * \mathrm{X1H2[z]}) * \mathrm{Cp5} + 18.020 * \mathrm{FH2O0} * \mathrm{Cp6})) *$$

$$\left(\mathrm{FEB0} * \left(-\Delta\mathrm{H1} * \left(\mathrm{rc1} + \mathrm{rt1} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H2} * \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H3} * \left(\mathrm{rc3} + \mathrm{rt3} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H4} * \mathrm{rc4}\right)\right),$$

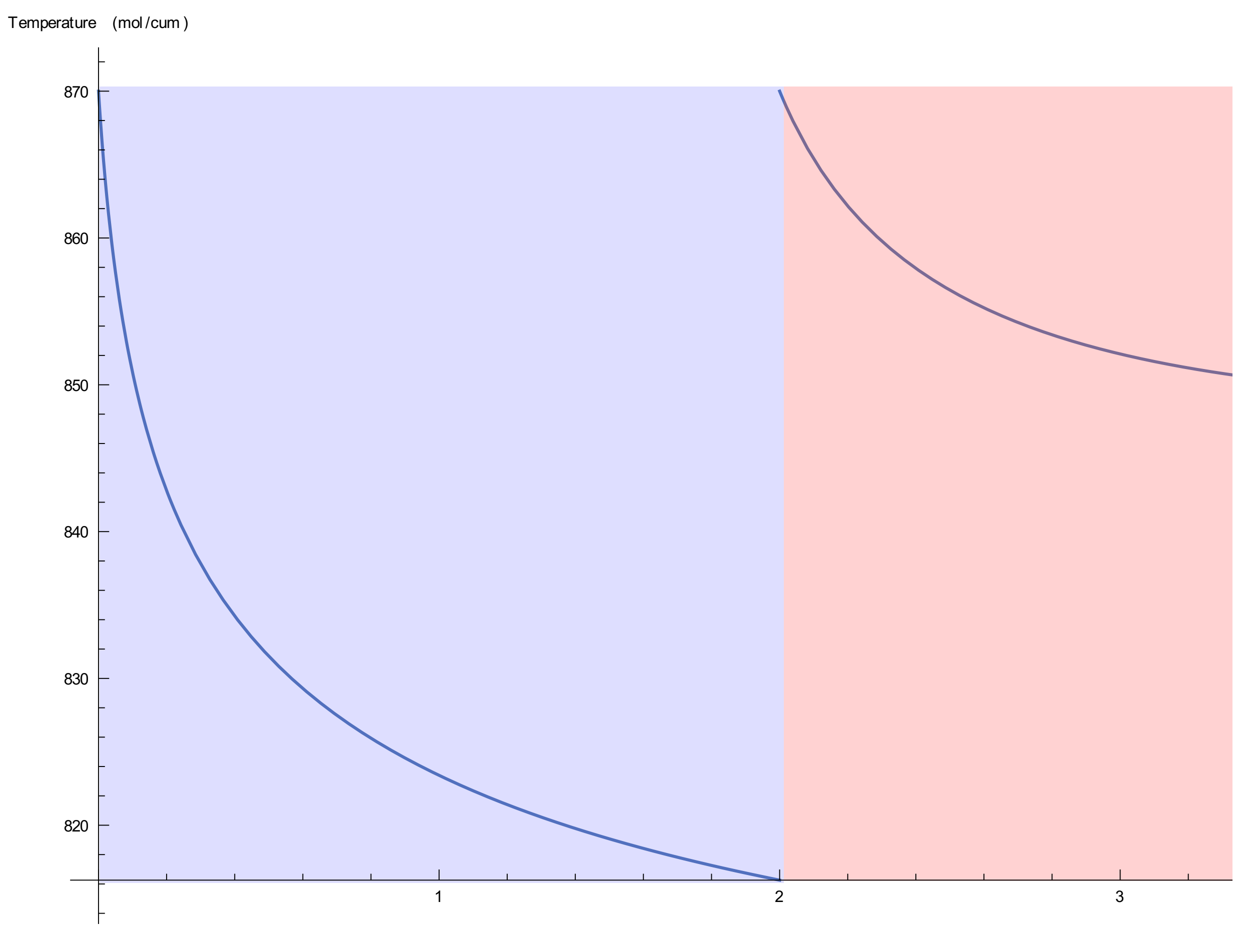
$$\mathrm{X1EB[0]} == 0, \ \mathrm{X1BZ[0]} == 0, \ \mathrm{X1TO[0]} == 0, \ \mathrm{X1H2[0]} == 0, \ \mathrm{PT[0]} == 1.25, \ \mathrm{T[0]} == 870\Big\},$$

```
{PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
   C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];
Figure5 = Plot[{T[z] /. r103}, {z, 0, 2}, PlotRange→ All,
    AxesLabel → {"Reactor height (m)", "Temperature (K)"}], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```

For the second reactor (r202):

Temperature profiles for these two reactors:

```
Legended [Show[Figure5 , Figure6 ],
 SwatchLegend [{Blue , Red}, {"1st  reactor ", "2nd  reactor "}]]
```



Pressure Profiles

For the first reactor (r101):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO,
   S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

  (*Construct the models for the thermal reactions*)
  At1 = 2.2215*10^16;  (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23;  (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
  kt3 = At3*Exp[(-Et3*10^3)/(R*T[z])];


  (*Thermal reaction rates of three reactions*)
  rt1 = kt1*(PEB - (PST*PH2)/Keq); (**kmol/m3h**)
  rt2 = kt2*PEB;
  rt3 = kt3*PEB;


  (*Construct the models for the catalytic reactions*)
  A1 = 4.594*10^9;  (**kmol/kg-cath**)
  A2 = 1.060*10^15;
  A3 = 1.246*10^26;
  A4 = 8.024*10^10;
  E1 = 175.38; (**kJ/mol**)
```

```
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;
```

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right]; \text{ (**kmol/kg-cath**)}$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

(*Catalytic reaction rates of four reactions*)

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2}; \text{ (**kmol/kg-cath**)}$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

(*Construct the models for the thermodynamic equilibriums*)

$AEB = 1.014 * 10^{-5};$ (**1/bar**)

$AST = 2.678 * 10^{-5};$

$AH2 = 4.519 * 10^{-7};$

```
ΔHaEB = -102.22; (**kJ/mol**)
ΔHaST = -104.56;
ΔHaH2 = -117.95;
```

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; \text{ (**1/bar**)}$$

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \text{ (**1/bar**)}$$

(*(The initial molar flowrates of components**)*)**

```
FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 1080*3.6;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;
```

(*Partial pressure of components*)

$$\mathrm{PEB} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FEB0}}{\mathrm{FT0}}\,(1 - (\mathrm{X1EB[z]} - \mathrm{X1BZ[z]} - \mathrm{X1TO[z]}) - \mathrm{X1BZ[z]} - \mathrm{X1TO[z]})}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

(1/bar**)**

$$\mathrm{PST} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FST0}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1EB[z]} - \mathrm{X1BZ[z]} - \mathrm{X1TO[z]})}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

$$\mathrm{PBZ} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FBZ0}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X1BZ[z]}}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

$$\mathrm{PH2} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FH20}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X1H2[z]}}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

$$\mathrm{PETH} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FC2H40}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X1BZ[z]}}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

$$\mathrm{PTO} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FTO0}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X1TO[z]}}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

$$\mathrm{PH2O} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FH2O0}}{\mathrm{FT0}}}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

$$\mathrm{PMTH} = \mathrm{PT[z]} * \frac{\frac{\mathrm{FCH40}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X1EB[z]}}{1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X1TO[z]} + \mathrm{X1BZ[z]} + \mathrm{X1H2[z]})};$$

(* Concentration of components*)

$$C1EB = \frac{PEB*10^5}{R*T[z]};$$

$$C1ST = \frac{PST*10^5}{R*T[z]};$$

$$C1BZ = \frac{PBZ*10^5}{R*T[z]};$$

$$C1H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C1ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C1TO = \frac{PTO*10^5}{R*T[z]};$$

$$C1H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C1MTH = \frac{PMTH*10^5}{R*T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99*(T[z] - 298.15) + \frac{-8.2026*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{6.499*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986*(T[z] - 298.15) + \frac{-7.67*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{9.592*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3; \quad (**kJ/kgK**)$$

$$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$$

$$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$$

$$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$$

$$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$$

$$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

ρb = 1422;

ϵ = 0.4312;

(*Dimensions of the reactor*)

L = 10;

$$Di = \frac{Dr}{100};$$

$$Ac = \frac{\pi}{4} * (Di)^2;$$

(*The important properties of the gas mixture*)

$$\mu = (-10.035 + 0.25191 * T[z] - 0.000037932 * T[z] * T[z]) * 3.6 * 10^{-4}; \quad (**kg/ms**)$$

u = 22.003/Ac;

G = 89 520.109/Ac;

$$\rho g = \frac{10^5 * 10^{-3}}{R * T[z]} * (PEB * 106.168 + PST * 104.15 + PBZ * 78.114 + PTO * 92.141 + PH2O * 18.020 + PH2 * 2.010 + PMTH * 16.043 + PETH * 28.054);$$

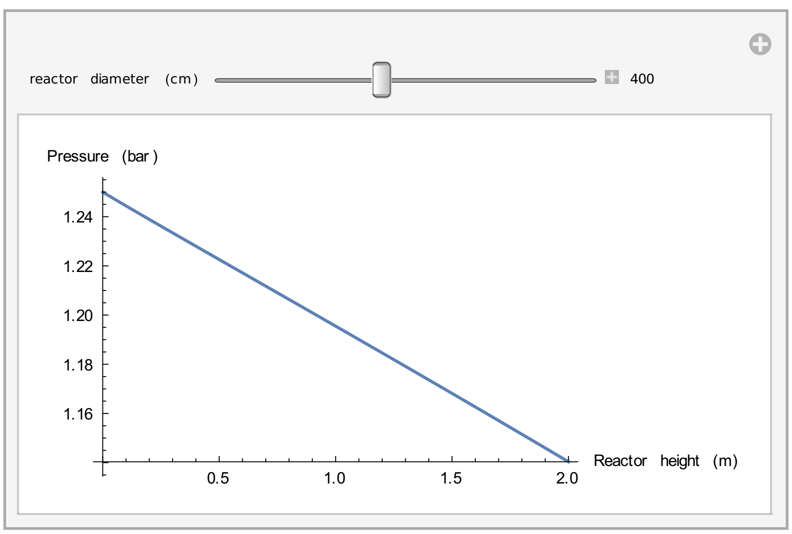
$$r104 = Quiet @ NDSolve\Big[\Big\{X1EB'[z] == \left(rc1 + rc2 + rc3 + (rt1 + rt2 + rt3) * \frac{\epsilon}{\rho b}\right) * \frac{Ac * \rho b}{FEB0},$$

$$X1BZ'[z] == \left(rc2 + rt2 * \frac{\epsilon}{\rho b}\right) * \frac{Ac * \rho b}{FEB0},\ X1TO'[z] == \left(rc3 + rc4 + rt3 * \frac{\epsilon}{\rho b}\right) * \frac{Ac * \rho b}{FEB0},$$

```
X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * ε/ρb) * (Ac*ρb)/FEB0,

PT'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5 * (Ac*ρb)/FEB0,

T'[z] == (Ac*ρb)/FEB0 * (1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
      104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
      78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
      2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
    (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
  X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 870},
 {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
  C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];
Figure7 = Plot[{PT[z] /. r104}, {z, 0, 2}, PlotRange→ All,
   AxesLabel → {"Reactor height (m)", "Pressure (bar)"}]], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



For the second reactor (r202):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
   S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},
```

$At1 = 2.2215*10^{16};$ (**kmol/m3hbar**)
$At2 = 2.4217*10^{20};$
$At3 = 3.8224*10^{17};$
$Et1 = 272.23;$ (**kJ/mol**)
$Et2 = 352.79;$
$Et3 = 313.06;$
$R = 8.314;$

$$kt1 = At1*Exp\left[\frac{-Et1*10^3}{R*T[z]}\right];$$ (**kmol/m3hbar**)

$$kt2 = At2*Exp\left[\frac{-Et2*10^3}{R*T[z]}\right];$$

$$kt3 = At3*Exp\left[\frac{-Et3*10^3}{R*T[z]}\right];$$

$A1 = 4.594*10^{9};$ (**kmol/kg−cath**)
$A2 = 1.060*10^{15};$
$A3 = 1.246*10^{26};$
$A4 = 8.024*10^{10};$
$E1 = 175.38;$ (**kJ/mol**)
$E2 = 296.29;$
$E3 = 474.76;$
$E4 = 213.78;$

$$k1 = A1*Exp\left[\frac{-E1*10^3}{R*T[z]}\right];$$ (**kmol/kg−cath**)

$$k2 = A2*Exp\left[\frac{-E2*10^3}{R*T[z]}\right];$$

$$k3 = A3*Exp\left[\frac{-E3*10^3}{R*T[z]}\right];$$

$$k4 = A4*Exp\left[\frac{-E4*10^3}{R*T[z]}\right];$$

$AEB = 1.014*10^{-5};$ (**1/bar**)
$AST = 2.678*10^{-5};$
$AH2 = 4.519*10^{-7};$
$\Delta HaEB = -102.22;$ (**kJ/mol**)
$\Delta HaST = -104.56;$
$\Delta HaH2 = -117.95;$

$$KEB = AEB*Exp\left[\frac{-\Delta HaEB*10^3}{R*T[z]}\right];$$ (**1/bar**)

$$KST = AST*Exp\left[\frac{-\Delta HaST*10^3}{R*T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \text{(**1/bar**)}$$

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \text{(**kmol/m3h**)}$$

rt2 = kt2 * PEB;
rt3 = kt3 * PEB;

$$C2EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C2ST = \frac{PST * 10^5}{R * T[z]};$$

$$C2BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C2H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C2ETH = \frac{PETH * 10^5}{R * T[z]};$$

$$C2TO = \frac{PTO * 10^5}{R * T[z]};$$

$$C2H2O = \frac{PH2O * 10^5}{R * T[z]};$$

$$C2MTH = \frac{PMTH * 10^5}{R * T[z]};$$

$$S2ST = \frac{X2EB[z] - X2BZ[z] - X2TO[z]}{X2EB[z]};$$

$$S2BZ = \frac{X2BZ[z]}{X2EB[z]};$$

$$S2TO = \frac{X2TO[z]}{X2EB[z]};$$

$$S2H2 = \frac{X2H2[z]}{X2EB[z]};$$

FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;

$$FTO0 = 0.0482245*3.6;$$
$$FH20 = 0;$$
$$FCH40 = 0;$$
$$FC2H40 = 0;$$
$$FH2O0 = 3954.696;$$
$$FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;$$
$$PEB = P[z]*\frac{\frac{FEB0}{FT0}(1-(X2EB[z]-X2BZ[z]-X2TO[z])-X2BZ[z]-X2TO[z])}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$
(**1/bar**)
$$PST = P[z]*\frac{\frac{FST0}{FT0}+\frac{FEB0}{FT0}*(X2EB[z]-X2BZ[z]-X2TO[z])}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$
$$PBZ = P[z]*\frac{\frac{FBZ0}{FT0}+\frac{FEB0}{FT0}*X2BZ[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$
$$PH2 = P[z]*\frac{\frac{FH20}{FT0}+\frac{FEB0}{FT0}*X2H2[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$
$$PETH = P[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X2BZ[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$
$$PTO = P[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X2TO[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$
$$PH2O = P[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$
$$PMTH = P[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X2EB[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$rc1 = \frac{k1*KEB*\left(PEB-\frac{PST*PH2}{Keq}\right)}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};\ (**kmol/kg-cath**)$$
$$rc2 = \frac{k2*KEB*PEB}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$
$$rc3 = \frac{k3*KEB*PEB*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$
$$rc4 = \frac{k4*KST*PST*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$\Delta H1 = 117\,690 + 41.99*(T[z] - 298.15) + \frac{-8.2026*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{6.499*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986*(T[z] - 298.15) + \frac{-7.67*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{9.592*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86*(T[z] - 298.15) + \frac{-15.1844*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{23.04*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13)*(T[z] - 298.15) + \frac{-6.9818*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{16.54*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$Cp1 = -0.43426 + 6.0671*10^{-3}*T[z] - 3.8625*10^{-6}*T[z]*T[z] + 9.1282*10^{-10}*(T[z])^3;\ (**kJ/kgK**)$$
$$Cp2 = -0.26436 + 5.564*10^{-3}*T[z] - 3.0018*10^{-6}*T[z]*T[z] + 5.3317*10^{-10}*(T[z])^3;$$
$$Cp3 = -0.40599 + 6.6616*10^{-3}*T[z] - 4.5318*10^{-6}*T[z]*T[z] + 12.255*10^{-10}*(T[z])^3;$$
$$Cp4 = -0.27127 + 5.9142*10^{-3}*T[z] - 3.8631*10^{-6}*T[z]*T[z] + 9.54*10^{-10}*(T[z])^3;$$
$$Cp5 = 13.57 + 4.637*10^{-3}*T[z] - 6.905*10^{-6}*T[z]*T[z] + 38.23*10^{-10}*(T[z])^3;$$
$$Cp6 = 1.7911 + 0.1069*10^{-3}*T[z] + 0.58611*10^{-6}*T[z]*T[z] - 1.998*10^{-10}*(T[z])^3;$$

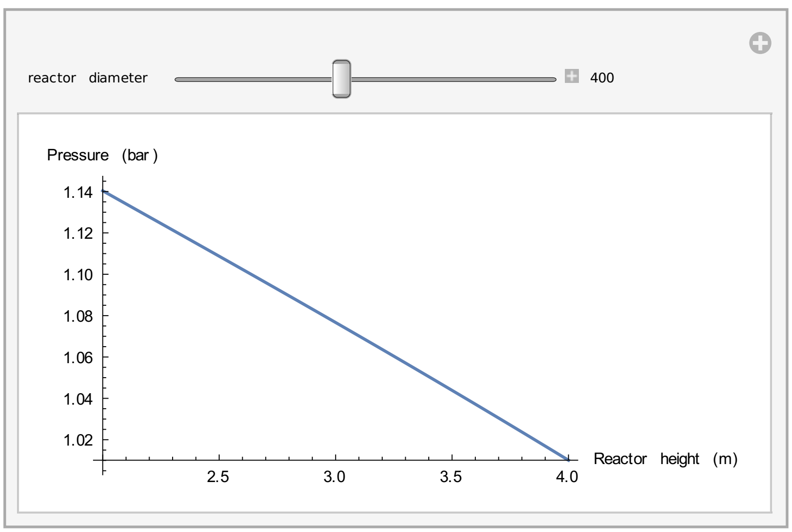
$$L = 10;$$
$$Di = \frac{Dr}{100};$$
$$Ac = \frac{\pi}{4}*(Di)^2;$$
$$dp = 5.5/1000;\ (**m**)$$
$$\mu = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^{-4};\ (**kg/ms**)$$
$$u = 22.003/Ac;$$
$$G = 89\,520.109/Ac;$$
$$\rho b = 1422;$$
$$\epsilon = 0.4312;\ (**void\ fraction\ of\ bed**)$$
$$\rho g = \frac{10^5*10^{-3}}{R*T[z]}*(PEB*106.168 + PST*104.15 + PBZ*78.114 + PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);$$

$$r204 = Quiet@NDSolve\Big[\Big\{X2EB'[z] == \left(rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$
$$X2BZ'[z] == \left(rc2 + rt2*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},\ X2TO'[z] == \left(rc3 + rc4 + rt3*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$

```
X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * ϵ/ρb) * (Ac * ρb)/FEB0,

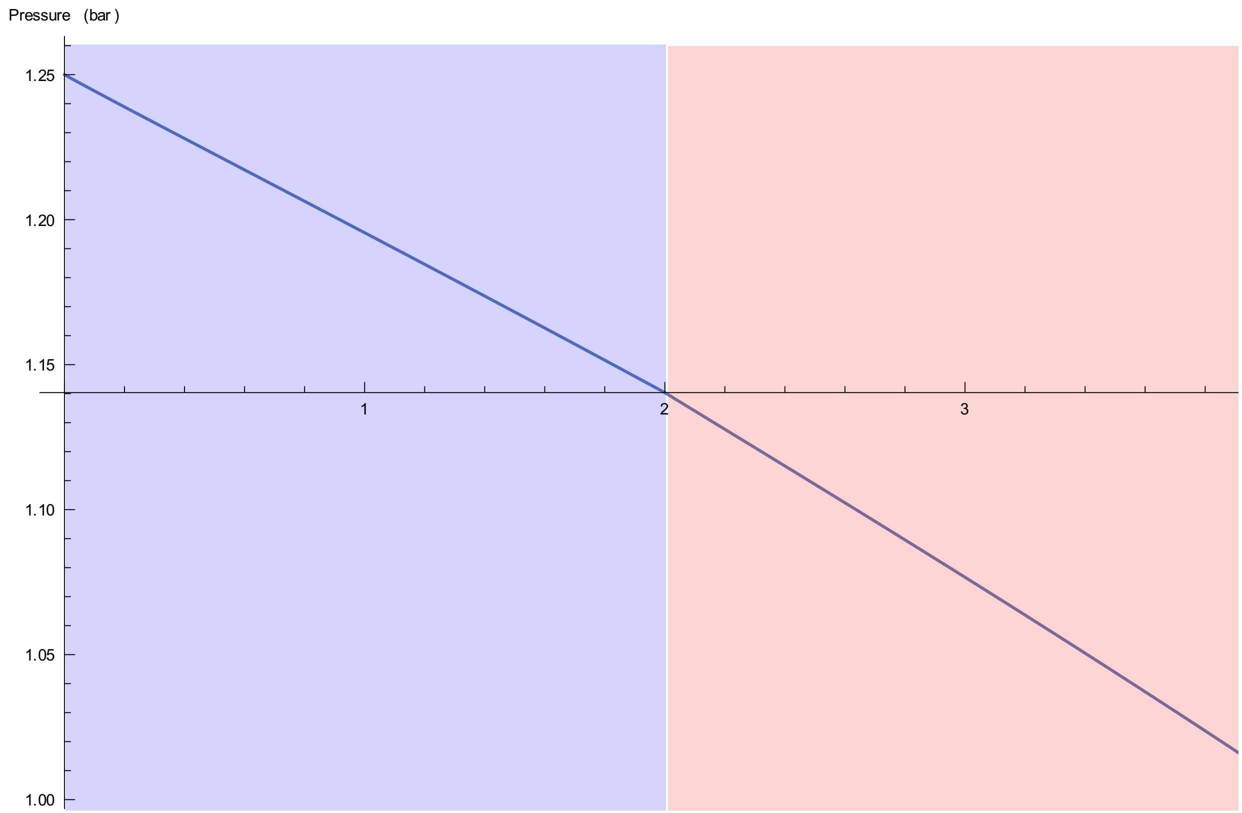
P'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458 * (1 - ϵ))/((ρg * dp * u)/μ)) * 7.7160 * 10^-8 * (u * G * FEB0)/(ρb * dp * Ac) * 10^-5 * (Ac * ρb)/FEB0,

T'[z] == (Ac * ρb)/FEB0 * (1 / (106.168 * FEB0 * (1 - X2EB[z]) * Cp1 +
      104.15 * (FST0 + FEB0 * (X2EB[z] - X2BZ[z] - X2TO[z])) * Cp2 +
      78.114 * (FBZ0 + FEB0 * X2BZ[z]) * Cp3 + 92.141 * (FTO0 + FEB0 * X2TO[z]) * Cp4 +
      2.010 * (FH20 + FEB0 * X2H2[z]) * Cp5 + 18.020 * FH2O0 * Cp6)) *
   (FEB0 * (-ΔH1 * (rc1 + rt1 * ϵ/ρb) - ΔH2 * (rc2 + rt2 * ϵ/ρb) - ΔH3 * (rc3 + rt3 * ϵ/ρb) - ΔH4 * rc4)),
  X2EB[2] == X1EB[2] /. r104, X2BZ[2] == X1BZ[2] /. r104, X2TO[2] == X1TO[2] /. r104,
  X2H2[2] == X1H2[2] /. r104, P[2] == PT[2] /. r104, T[2] == 870},
 {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
  C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];
Figure8 = Plot[{P[z] /. r204}, {z, 2, 4}, PlotRange → All,
   AxesLabel → {"Reactor height (m)", "Pressure (bar)"}], Column[{
  Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
 }, Left]]
```



Pressure profiles for these two reactors:

```
Legended [Show[Figure7 , Figure8 ],
 SwatchLegend [{Blue , Red}, {"1st reactor ", "2nd reactor "}]]
```



Conversion Profiles

For the first reactor (r101):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO,
   S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

  (*Construct the models for the thermal reactions*)
  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
```

$$kt1 = At1 * Exp\left[\frac{-Et1 * 10^3}{R * T[z]}\right];$$ (**kmol/m3hbar**)

$$kt2 = At2 * Exp\left[\frac{-Et2 * 10^3}{R * T[z]}\right];$$

$$kt3 = At3 * Exp\left[\frac{-Et3 * 10^3}{R * T[z]}\right];$$

(*Thermal reaction rates of three reactions*)

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right);$$ (**kmol/m3h**)

rt2 = kt2 * PEB;

rt3 = kt3 * PEB;

(*Construct the models for the catalytic reactions*)

$A1 = 4.594 * 10^9;$ (**kmol/kg−cath**)

$A2 = 1.060 * 10^{15};$

$A3 = 1.246 * 10^{26};$

$A4 = 8.024 * 10^{10};$

E1 = 175.38; (**kJ/mol**)

E2 = 296.29;

E3 = 474.76;

E4 = 213.78;

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right];$$ (**kmol/kg−cath**)

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

(*Catalytic reaction rates of four reactions*)

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$ (**kmol/kg−cath**)

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

(*Construct the models for the thermodynamic equilibriums*)

$AEB = 1.014 * 10^{-5};$ (**1/bar**)

$AST = 2.678 * 10^{-5};$

$AH2 = 4.519 * 10^{-7};$

$\Delta HaEB = -102.22;$ (**kJ/mol**)

$\Delta HaST = -104.56;$

$\Delta HaH2 = -117.95;$

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right];$$ (**1/bar**)

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right];$$ (**1/bar**)

(*(**The initial molar flowrates of components**)*)

FEB0 = 49.7976 * 3600/1000; (*Unit:kmol/h*)

FST0 = 0.00332919 * 3.6;

FBZ0 = 1.464 * 3.6;

FTO0 = 0.0482245 * 3.6;

FH20 = 0;

FCH40 = 0;

FC2H40 = 0;

FH2O0 = 1080 * 3.6;

FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

(*Partial pressure of components*)

$$PEB = PT[z] * \frac{\frac{FEB0}{FT0}(1 - (X1EB[z] - X1BZ[z] - X1TO[z]) - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(**1/bar**)

$$PST = PT[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (X1EB[z] - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PBZ = PT[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2 = PT[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X1H2[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PETH = PT[z] * \frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PTO = PT[z] * \frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0} * X1TO[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2O = PT[z] * \frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PMTH = PT[z] * \frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0} * X1EB[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C1ST = \frac{PST * 10^5}{R * T[z]};$$

$$C1BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C1H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C1ETH = \frac{PETH * 10^5}{R * T[z]};$$

$$C1TO = \frac{PTO * 10^5}{R * T[z]};$$

$$C1H2O = \frac{PH2O * 10^5}{R * T[z]};$$

$$C1MTH = \frac{PMTH * 10^5}{R * T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

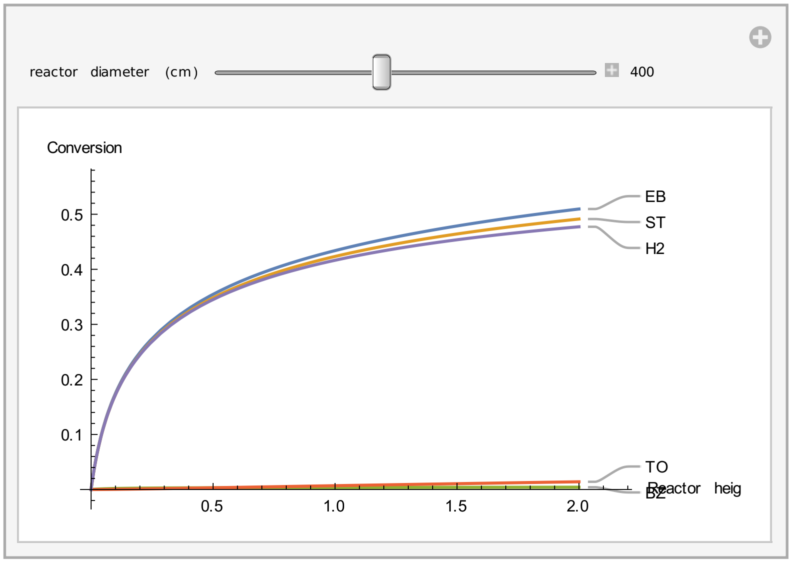
$\rho b = 1422;$

```
ϵ = 0.4312;


(*Dimensions of the reactor*)
L = 10;
Di = Dr/100;
Ac = π/4 * (Di)^2;


(*The important properties of the gas mixture*)
μ = (-10.035 + 0.25191 * T[z] - 0.000037932 * T[z] * T[z]) * 3.6 * 10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;


ρg = (10^5 * 10^-3)/(R * T[z]) * (PEB * 106.168 + PST * 104.15 + PBZ * 78.114 +
    PTO * 92.141 + PH2O * 18.020 + PH2 * 2.010 + PMTH * 16.043 + PETH * 28.054);
r105 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3) * ϵ/ρb) * (Ac * ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2 * ϵ/ρb) * (Ac * ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3 * ϵ/ρb) * (Ac * ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * ϵ/ρb) * (Ac * ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458 * (1 - ϵ))/((ρg * dp * u)/μ)) * 7.7160 * 10^-8 * (u * G * FEB0)/(ρb * dp * Ac) * 10^-5 * (Ac * ρb)/FEB0,
    T'[z] == (Ac * ρb)/FEB0 * (1/(106.168 * FEB0 * (1 - X1EB[z]) * Cp1 +
            104.15 * (FST0 + FEB0 * (X1EB[z] - X1BZ[z] - X1TO[z])) * Cp2 +
            78.114 * (FBZ0 + FEB0 * X1BZ[z]) * Cp3 + 92.141 * (FTO0 + FEB0 * X1TO[z]) * Cp4 +
            2.010 * (FH20 + FEB0 * X1H2[z]) * Cp5 + 18.020 * FH2O0 * Cp6)) *
       (FEB0 * (-ΔH1 * (rc1 + rt1 * ϵ/ρb) - ΔH2 * (rc2 + rt2 * ϵ/ρb) - ΔH3 * (rc3 + rt3 * ϵ/ρb) - ΔH4 * rc4)),
    X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 870},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
    C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];
Figure9 = Plot[{X1EB[z] /. r105, (X1EB[z] - X1BZ[z] - X1TO[z]) /. r105, X1BZ[z] /. r105,
    X1TO[z] /. r105, X1H2[z] /. r105}, {z, 0, 2}, PlotLabels → {"EB", "ST", "BZ", "TO", "H2"},
   PlotRange → All, AxesLabel → {"Reactor height (m)", "Conversion"}]], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
```



For the second reactor (r202):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
    AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
    FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
    PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
    S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},

  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
  kt3 = At3*Exp[(-Et3*10^3)/(R*T[z])];

  A1 = 4.594*10^9; (**kmol/kg-cath**)
  A2 = 1.060*10^15;
  A3 = 1.246*10^26;
  A4 = 8.024*10^10;
  E1 = 175.38; (**kJ/mol**)
```

$$E2 = 296.29;$$
$$E3 = 474.76;$$
$$E4 = 213.78;$$
$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right]; \; (** kmol/kg-cath **)$$
$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$
$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$
$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$
$$AEB = 1.014 * 10^{-5}; \; (** 1/bar **)$$
$$AST = 2.678 * 10^{-5};$$
$$AH2 = 4.519 * 10^{-7};$$
$$\Delta HaEB = -102.22; \; (** kJ/mol **)$$
$$\Delta HaST = -104.56;$$
$$\Delta HaH2 = -117.95;$$
$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; \; (** 1/bar **)$$
$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$
$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$
$$Keq = Exp\left[\frac{1}{R * T[z]} (-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z]))\right]; \; (** 1/bar **)$$

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \; (** kmol/m3h **)$$
$$rt2 = kt2 * PEB;$$
$$rt3 = kt3 * PEB;$$

$$C2EB = \frac{PEB * 10^5}{R * T[z]};$$
$$C2ST = \frac{PST * 10^5}{R * T[z]};$$
$$C2BZ = \frac{PBZ * 10^5}{R * T[z]};$$
$$C2H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$\mathrm{C2ETH} = \frac{\mathrm{PETH} * 10^5}{\mathrm{R} * \mathrm{T[z]}};$$

$$\mathrm{C2TO} = \frac{\mathrm{PTO} * 10^5}{\mathrm{R} * \mathrm{T[z]}};$$

$$\mathrm{C2H2O} = \frac{\mathrm{PH2O} * 10^5}{\mathrm{R} * \mathrm{T[z]}};$$

$$\mathrm{C2MTH} = \frac{\mathrm{PMTH} * 10^5}{\mathrm{R} * \mathrm{T[z]}};$$

$$\mathrm{S2ST} = \frac{\mathrm{X2EB[z]} - \mathrm{X2BZ[z]} - \mathrm{X2TO[z]}}{\mathrm{X2EB[z]}};$$

$$\mathrm{S2BZ} = \frac{\mathrm{X2BZ[z]}}{\mathrm{X2EB[z]}};$$

$$\mathrm{S2TO} = \frac{\mathrm{X2TO[z]}}{\mathrm{X2EB[z]}};$$

$$\mathrm{S2H2} = \frac{\mathrm{X2H2[z]}}{\mathrm{X2EB[z]}};$$

```
FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 3954.696;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;
```

$$\mathrm{PEB} = \mathrm{P[z]} * \left(\left(\frac{\mathrm{FEB0}}{\mathrm{FT0}}\,(1 - (\mathrm{X2EB[z]} - \mathrm{X2BZ[z]} - \mathrm{X2TO[z]}) - \mathrm{X2BZ[z]} - \mathrm{X2TO[z]})\right) \Big/ \left(1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X2TO[z]} + \mathrm{X2BZ[z]} + \mathrm{X2H2[z]})\right)\right);$$

(**1/bar**)

PST =

$$\mathrm{P[z]} * \left(\left(\frac{\mathrm{FST0}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X2EB[z]} - \mathrm{X2BZ[z]} - \mathrm{X2TO[z]})\right) \Big/ \left(1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X2TO[z]} + \mathrm{X2BZ[z]} + \mathrm{X2H2[z]})\right)\right);$$

$$\mathrm{PBZ} = \mathrm{P[z]} * \left(\left(\frac{\mathrm{FBZ0}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X2BZ[z]}\right) \Big/ \left(1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X2TO[z]} + \mathrm{X2BZ[z]} + \mathrm{X2H2[z]})\right)\right);$$

$$\mathrm{PH2} = \mathrm{P[z]} * \left(\left(\frac{\mathrm{FH20}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X2H2[z]}\right) \Big/ \left(1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X2TO[z]} + \mathrm{X2BZ[z]} + \mathrm{X2H2[z]})\right)\right);$$

$$\mathrm{PETH} = \mathrm{P[z]} * \left(\left(\frac{\mathrm{FC2H40}}{\mathrm{FT0}} + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * \mathrm{X2BZ[z]}\right) \Big/ \left(1 + \frac{\mathrm{FEB0}}{\mathrm{FT0}} * (\mathrm{X2TO[z]} + \mathrm{X2BZ[z]} + \mathrm{X2H2[z]})\right)\right);$$

$$PTO = P[z]*\left(\left(\frac{FTO0}{FT0} + \frac{FEB0}{FT0}*X2TO[z]\right)\Big/\left(1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])\right)\right);$$

$$PH2O = P[z]*\left(\frac{FH2O0}{FT0}\Big/\left(1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])\right)\right);$$

$$PMTH = P[z]*\left(\left(\frac{FCH40}{FT0} + \frac{FEB0}{FT0}*X2EB[z]\right)\Big/\left(1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])\right)\right);$$

$$rc1 = \left(k1*KEB*\left(PEB - \frac{PST*PH2}{Keq}\right)\right)\Big/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

(**kmol/kg−cath**)

$$rc2 = (k2*KEB*PEB)/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

$$rc3 = (k3*KEB*PEB*KH2*PH2)/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

$$rc4 = (k4*KST*PST*KH2*PH2)/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

$$\Delta H1 = 117\,690 + 41.99*(T[z] - 298.15) + \frac{-8.2026*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{6.499*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986*(T[z] - 298.15) + \frac{-7.67*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{9.592*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86*(T[z] - 298.15) + \frac{-15.1844*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{23.04*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13)*(T[z] - 298.15) + \frac{-6.9818*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{16.54*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$Cp1 = -0.43426 + 6.0671*10^{-3}*T[z] - 3.8625*10^{-6}*T[z]*T[z] + 9.1282*10^{-10}*(T[z])^3;$$ (**kJ/kgK**)

$$Cp2 = -0.26436 + 5.564*10^{-3}*T[z] - 3.0018*10^{-6}*T[z]*T[z] + 5.3317*10^{-10}*(T[z])^3;$$

$$Cp3 = -0.40599 + 6.6616*10^{-3}*T[z] - 4.5318*10^{-6}*T[z]*T[z] + 12.255*10^{-10}*(T[z])^3;$$

$$Cp4 = -0.27127 + 5.9142*10^{-3}*T[z] - 3.8631*10^{-6}*T[z]*T[z] + 9.54*10^{-10}*(T[z])^3;$$

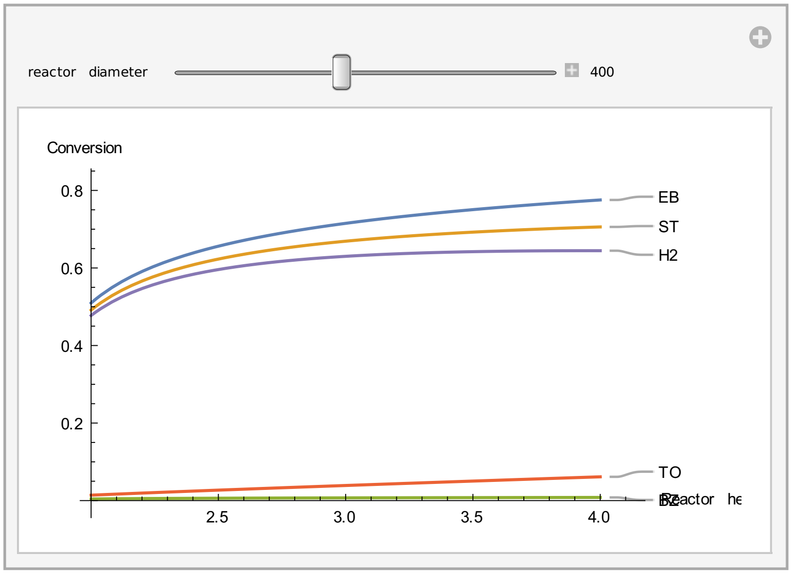
$$Cp5 = 13.57 + 4.637*10^{-3}*T[z] - 6.905*10^{-6}*T[z]*T[z] + 38.23*10^{-10}*(T[z])^3;$$

$$Cp6 = 1.7911 + 0.1069*10^{-3}*T[z] + 0.58611*10^{-6}*T[z]*T[z] - 1.998*10^{-10}*(T[z])^3;$$

$$L = 10;$$

$$Di = \frac{Dr}{100};$$

```
Ac = π/4 * (Di)^2;
dp = 5.5/1000; (**m**)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;
ρb = 1422;
ϵ = 0.4312;  (**void fraction of bed**)
ρg = (10^5*10^-3)/(R*T[z]) * (PEB*106.168 + PST*104.15 + PBZ*78.114 +
     PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r205 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
     X2BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
     X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
     P'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5 * (Ac*ρb)/FEB0,
     T'[z] ==  (Ac*ρb)/FEB0 * (1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
       (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
     X2EB[2] == X1EB[2] /. r105, X2BZ[2] == X1BZ[2] /. r105, X2TO[2] == X1TO[2] /. r105,
     X2H2[2] == X1H2[2] /. r105, P[2] == PT[2] /. r105, T[2] == 870},
    {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB,  C2ST,  C2BZ,  C2TO,
     C2H2,  C2ETH,  C2H2O, C2MTH}, {z, 2, 4}];
Figure10 = Plot[{{X2EB[z] /. r205, (X2EB[z] - X2BZ[z] - X2TO[z]) /. r205,  X2BZ[z] /. r205,
     X2TO[z] /. r205,  X2H2[z] /. r205}}, {z, 2, 4}, PlotLabels→ {"EB", "ST", "BZ", "TO", "H2"},
   PlotRange→ All, AxesLabel → {"Reactor height (m)", "Conversion"}]], Column[{
  Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



Conversion profiles for these two reactors:

Selectivity profiles

For the first reactor (r101):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO,
   S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

  (*Construct the models for the thermal reactions*)
  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
```

$$kt3 = At3 * Exp\left[\frac{-Et3 * 10^3}{R * T[z]}\right];$$

(*Thermal reaction rates of three reactions*)

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right);\ (**kmol/m3h**)$$

$$rt2 = kt2 * PEB;$$

$$rt3 = kt3 * PEB;$$

(*Construct the models for the catalytic reactions*)

$$A1 = 4.594 * 10^9;\ (**kmol/kg-cath**)$$

$$A2 = 1.060 * 10^{15};$$

$$A3 = 1.246 * 10^{26};$$

$$A4 = 8.024 * 10^{10};$$

$$E1 = 175.38;\ (**kJ/mol**)$$

$$E2 = 296.29;$$

$$E3 = 474.76;$$

$$E4 = 213.78;$$

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right];\ (**kmol/kg-cath**)$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

(*Catalytic reaction rates of four reactions*)

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};\ (**kmol/kg-cath**)$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

(*Construct the models for the thermodynamic equilibriums*)

$AEB = 1.014*10^{-5};$ (**1/bar**)

$AST = 2.678*10^{-5};$

$AH2 = 4.519*10^{-7};$

$\Delta HaEB = -102.22;$ (**kJ/mol**)

$\Delta HaST = -104.56;$

$\Delta HaH2 = -117.95;$

$$KEB = AEB*Exp\left[\frac{-\Delta HaEB*10^{3}}{R*T[z]}\right];$$ (**1/bar**)

$$KST = AST*Exp\left[\frac{-\Delta HaST*10^{3}}{R*T[z]}\right];$$

$$KH2 = AH2*Exp\left[\frac{-\Delta HaH2*10^{3}}{R*T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157-126.267*T[z]-0.002194*T[z]*T[z])}{R*T[z]}\right];$$ (**1/bar**)

(*(**The initial molar flowrates of components**)*)

FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)

FST0 = 0.00332919*3.6;

FBZ0 = 1.464*3.6;

FTO0 = 0.0482245*3.6;

FH20 = 0;

FCH40 = 0;

FC2H40 = 0;

FH2O0 = 1080*3.6;

FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

(*Partial pressure of components*)

$$PEB = PT[z]*\frac{\frac{FEB0}{FT0}(1-(X1EB[z]-X1BZ[z]-X1TO[z])-X1BZ[z]-X1TO[z])}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

(**1/bar**)

$$PST = PT[z]*\frac{\frac{FST0}{FT0}+\frac{FEB0}{FT0}*(X1EB[z]-X1BZ[z]-X1TO[z])}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PBZ = PT[z]*\frac{\frac{FBZ0}{FT0}+\frac{FEB0}{FT0}*X1BZ[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PH2 = PT[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X1H2[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PETH = PT[z] * \frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PTO = PT[z] * \frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0} * X1TO[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2O = PT[z] * \frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PMTH = PT[z] * \frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0} * X1EB[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C1ST = \frac{PST * 10^5}{R * T[z]};$$

$$C1BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C1H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C1ETH = \frac{PETH * 10^5}{R * T[z]};$$

$$C1TO = \frac{PTO * 10^5}{R * T[z]};$$

$$C1H2O = \frac{PH2O * 10^5}{R * T[z]};$$

$$C1MTH = \frac{PMTH * 10^5}{R * T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

$\rho b = 1422;$

$\epsilon = 0.4312;$

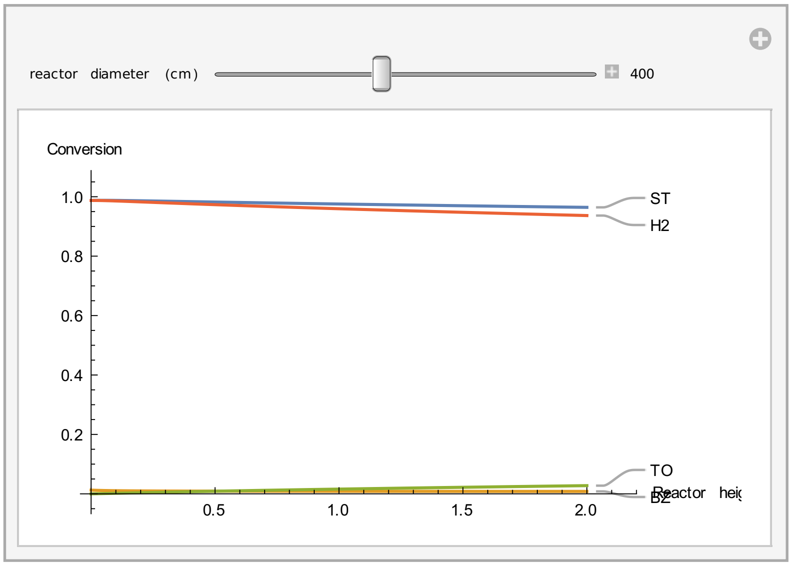
(*Dimensions of the reactor*)

L = 10;

```
Di = Dr/100;
Ac = π/4 * (Di)^2;

(*The important properties of the gas mixture*)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;

ρg = (10^5*10^-3)/(R*T[z]) * (PEB*106.168 + PST*104.15 + PBZ*78.114 +
      PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r106 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
      X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
      X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
      PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
      T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
            104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
            78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
            2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
         (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
      X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 870},
    {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
      C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO, S1H2}, {z, 0, 2}];
Figure11 = Plot[{S1ST /. r106, S1BZ /. r106, S1TO /. r106, S1H2 /. r106}, {z, 0, 2},
   PlotLabels → {"ST", "BZ", "TO", "H2"}, PlotRange → All,
   AxesLabel → {"Reactor height (m)", "Conversion"}], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



For the second reactor (r202):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
   S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},

  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
  kt3 = At3*Exp[(-Et3*10^3)/(R*T[z])];

  A1 = 4.594*10^9; (**kmol/kg-cath**)
  A2 = 1.060*10^15;
  A3 = 1.246*10^26;
  A4 = 8.024*10^10;
  E1 = 175.38; (**kJ/mol**)
```

E2 = 296.29;
E3 = 474.76;
E4 = 213.78;

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right]; (**kmol/kg-cath**)$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

$AEB = 1.014 * 10^{-5}$; (**1/bar**)
$AST = 2.678 * 10^{-5}$;
$AH2 = 4.519 * 10^{-7}$;
ΔHaEB = −102.22; (**kJ/mol**)
ΔHaST = −104.56;
ΔHaH2 = −117.95;

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; (**1/bar**)$$

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; (**1/bar**)$$

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); (**kmol/m3h**)$$

rt2 = kt2 * PEB;
rt3 = kt3 * PEB;

$$C2EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C2ST = \frac{PST * 10^5}{R * T[z]};$$

$$C2BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C2H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C2ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C2TO = \frac{PTO*10^5}{R*T[z]};$$

$$C2H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C2MTH = \frac{PMTH*10^5}{R*T[z]};$$

$$S2ST = \frac{X2EB[z] - X2BZ[z] - X2TO[z]}{X2EB[z]};$$

$$S2BZ = \frac{X2BZ[z]}{X2EB[z]};$$

$$S2TO = \frac{X2TO[z]}{X2EB[z]};$$

$$S2H2 = \frac{X2H2[z]}{X2EB[z]};$$

FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 3954.696;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

$$PEB = P[z]*\frac{\frac{FEB0}{FT0}(1 - (X2EB[z] - X2BZ[z] - X2TO[z]) - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

(**1/bar**)

$$PST = P[z]*\frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0}*(X2EB[z] - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PBZ = P[z]*\frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0}*X2BZ[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2 = P[z]*\frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0}*X2H2[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PETH = P[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X2BZ[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PTO = P[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X2TO[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PH2O = P[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PMTH = P[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X2EB[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$rc1 = \frac{k1*KEB*\left(PEB-\frac{PST*PH2}{Keq}\right)}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};\ (**kmol/kg-cath**)$$

$$rc2 = \frac{k2*KEB*PEB}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$rc3 = \frac{k3*KEB*PEB*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$rc4 = \frac{k4*KST*PST*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$\Delta H1 = 117\,690+41.99*(T[z]-298.15)+\frac{-8.2026*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{6.499*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-2.311*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510+12.986*(T[z]-298.15)+\frac{-7.67*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{9.592*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-4.125*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H3 = -54\,680+10.86*(T[z]-298.15)+\frac{-15.1844*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{23.04*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-9.9955*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

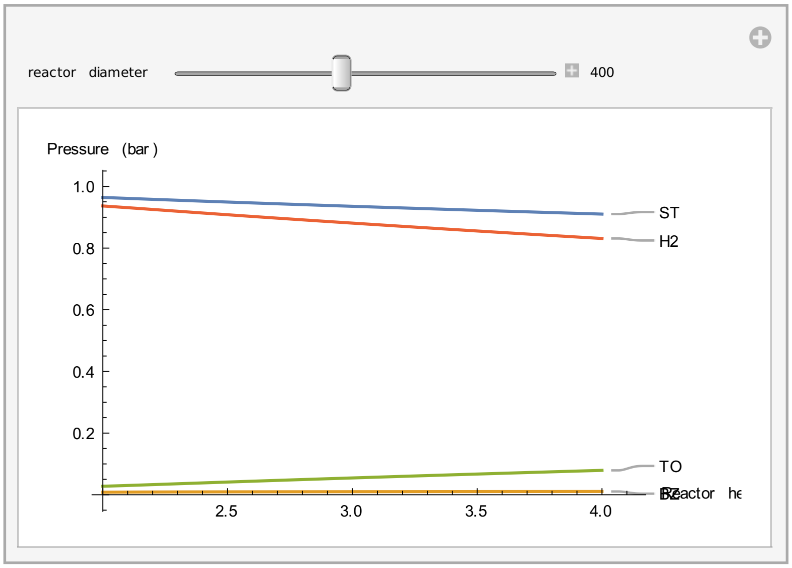
$$\Delta H4 = -172\,370+(-31.13)*(T[z]-298.15)+\frac{-6.9818*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{16.54*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-7.685*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$Cp1 = -0.43426+6.0671*10^{-3}*T[z]-3.8625*10^{-6}*T[z]*T[z]+9.1282*10^{-10}*(T[z])^3;\ (**kJ/kgK**)$$

```
Cp2 = -0.26436 + 5.564*10^-3 *T[z] - 3.0018*10^-6 *T[z]*T[z] + 5.3317*10^-10 *(T[z])^3;
Cp3 = -0.40599 + 6.6616*10^-3 *T[z] - 4.5318*10^-6 *T[z]*T[z] + 12.255*10^-10 *(T[z])^3;
Cp4 = -0.27127 + 5.9142*10^-3 *T[z] - 3.8631*10^-6 *T[z]*T[z] + 9.54*10^-10 *(T[z])^3;
Cp5 = 13.57 + 4.637*10^-3 *T[z] - 6.905*10^-6 *T[z]*T[z] + 38.23*10^-10 *(T[z])^3;
Cp6 = 1.7911 + 0.1069*10^-3 *T[z] + 0.58611*10^-6 *T[z]*T[z] - 1.998*10^-10 *(T[z])^3;

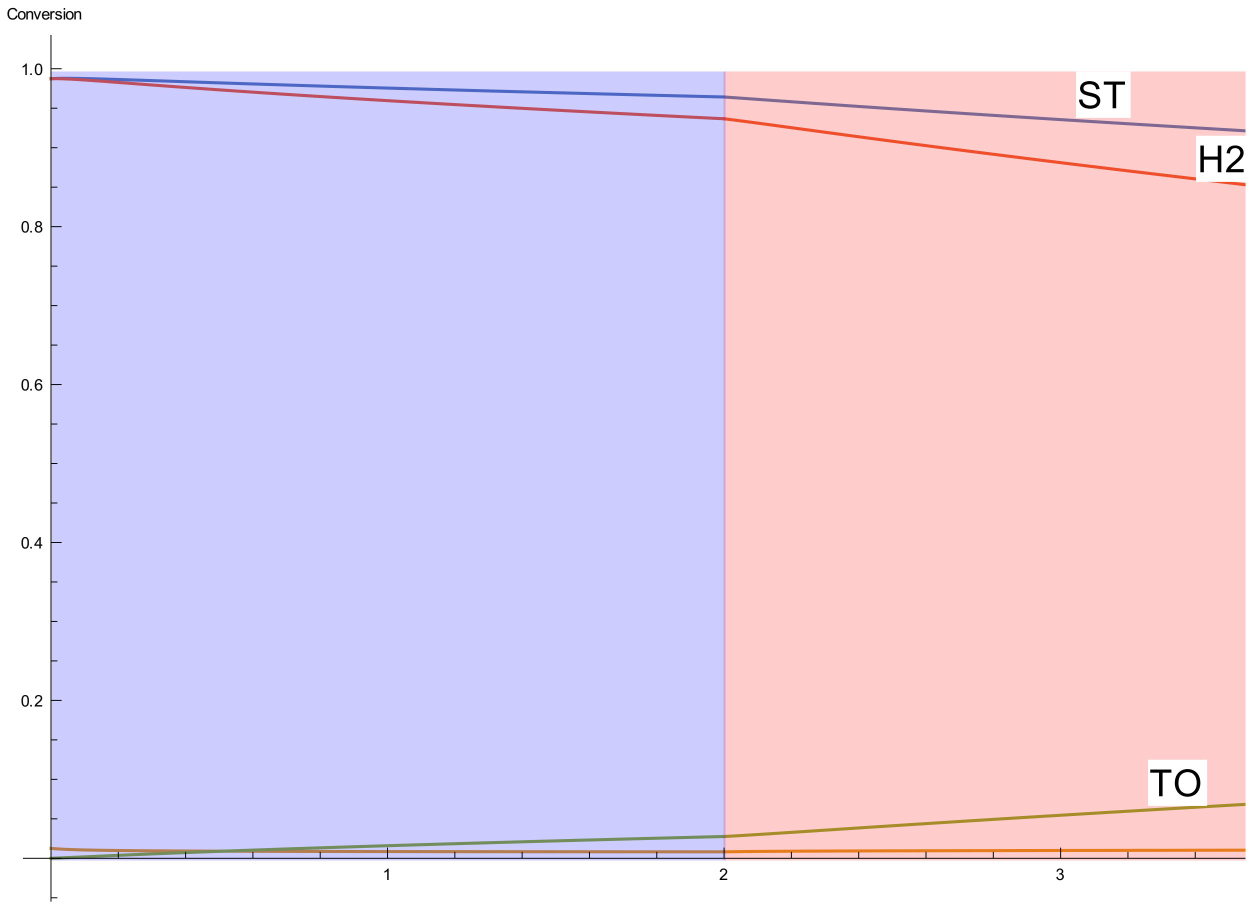
L = 10;
Di = Dr/100;
Ac = π/4 *(Di)^2;
dp = 5.5/1000; (**m**)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;
ρb = 1422;
ϵ = 0.4312; (**void fraction of bed**)
ρg = (10^5*10^-3)/(R*T[z]) *(PEB*106.168 + PST*104.15 + PBZ*78.114 +
     PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r206 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
     X2BZ'[z] == (rc2 + rt2* ϵ/ρb)* (Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3* ϵ/ρb)* (Ac*ρb)/FEB0,
     X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
     P'[z] == -(1 - ϵ)/ϵ^3 *(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) *10^-5 * (Ac*ρb)/FEB0,
     T'[z] == (Ac*ρb)/FEB0 *(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
        (FEB0*(-ΔH1*(rc1 + rt1* ϵ/ρb) - ΔH2*(rc2 + rt2* ϵ/ρb) - ΔH3*(rc3 + rt3* ϵ/ρb) - ΔH4*rc4)),
     X2EB[2] == X1EB[2] /. r106, X2BZ[2] == X1BZ[2] /. r106, X2TO[2] == X1TO[2] /. r106,
     X2H2[2] == X1H2[2] /. r106, P[2] == PT[2] /. r106, T[2] == 870},
    {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB,  C2ST,  C2BZ,  C2TO,  C2H2,
     C2ETH,  C2H2O, C2MTH, S2ST, S2BZ, S2TO,  S2H2}, {z, 2, 4}];
Figure12 = Plot[{{S2ST /. r206, S2BZ /. r206,  S2TO /. r206, S2H2 /. r206}}, {z, 2, 4},
   PlotLabels→ {"ST", "BZ", "TO", "H2"}, PlotRange→ All,
   AxesLabel→ {"Reactor height (m)", "Pressure (bar)"}], Column[{
```

```
  Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]
```



Selectivity profiles for these two reactors:

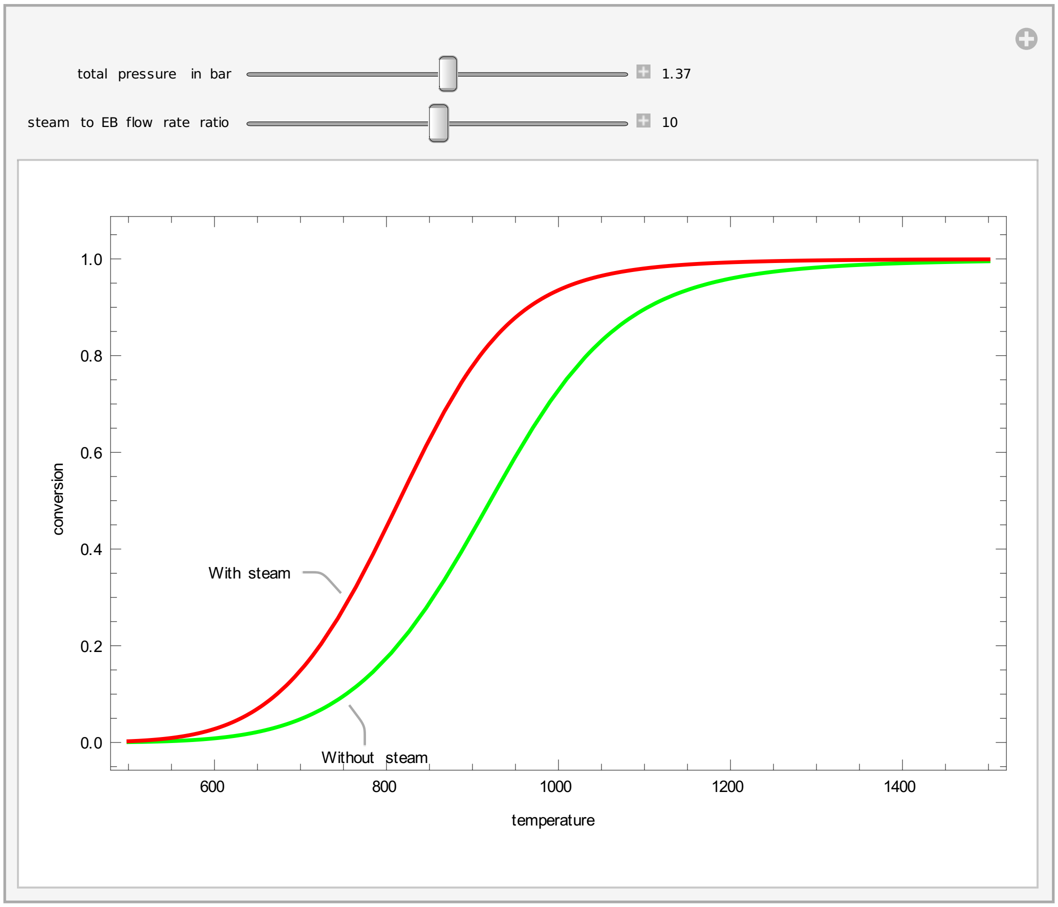
```
Legended [Show[Figure11 , Figure12 ],
  SwatchLegend [{Blue , Red}, {"1st reactor ", "2nd reactor "}]]
```


Conversion
1.0
0.8
0.6
0.4
0.2
1
2
3
ST
H2
TO

Optimization of operating conditions

Overview of effect of pressure, temperature, steam to ethylbenzene ratio on the ethylbenzene conversion

```
Manipulate[
  K[T_] := Exp[A1 + B1 / T + C1 Log[T] + D1 T];
  A1 = -13.2117277;
  B1 = -13 122.4699;
  C1 = 4.353627619;
  D1 = -0.00329709;
  F0 = 152.2;
  Fsteam = ratio F0;
  Conv[T_] := 1/(2 F0 (P + K[T])) (-K[T] Fsteam + Sqrt[(K[T] Fsteam) ^ 2 + 4 F0 (P + K[T]) K[T] (F0 + Fsteam)]);
  Conv1[T_] := 1/(2 F0 (P + K[T])) (Sqrt[4 F0 (P + K[T]) K[T] (F0)]);
  Show[Plot[Conv1[T], {T, 500, 1500}, Frame → True, FrameLabel → {"temperature", "conversion"},
     AxesOrigin → {500, 0}, PlotLabels → {Callout["Without steam", {Scaled[0.25], Right}]},
     PlotStyle → {Thick, Green}], Plot[Conv[T], {T, 500, 1500}, Frame → True,
     FrameLabel → {"temperature", "conversion"}, PlotLabels → {Callout["With steam", {Scaled[0.25], Left}]},
     AxesOrigin → {500, 0}, PlotStyle → {Thick, Red}], ImageSize → {500, 350}],
  {{P, 1.37, "total pressure in bar"}, 1, 1.7, 0.01, Appearance → "Labeled"},
  {{ratio, 10, "steam to EB flow rate ratio"}, 0, 20, 0.5, Appearance → "Labeled"}, TrackedSymbols :→ {ratio, P}]
```



Optimization of operating conditions

The effect of the ratio of steam to ethylbenzene on ethylbenzene conversion:

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Dr, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO,
   S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

  (*Construct the models for the thermal reactions*)
  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
```

Et3 = 313.06;

R = 8.314;

$$kt1 = At1 * Exp\left[\frac{-Et1 * 10^{3}}{R * T[z]}\right];\ (**kmol/m3hbar**)$$

$$kt2 = At2 * Exp\left[\frac{-Et2 * 10^{3}}{R * T[z]}\right];$$

$$kt3 = At3 * Exp\left[\frac{-Et3 * 10^{3}}{R * T[z]}\right];$$

(*Thermal reaction rates of three reactions*)

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right);\ (**kmol/m3h**)$$

rt2 = kt2 * PEB;

rt3 = kt3 * PEB;

(*Construct the models for the catalytic reactions*)

$A1 = 4.594 * 10^{9};$ (**kmol/kg−cath**)

$A2 = 1.060 * 10^{15};$

$A3 = 1.246 * 10^{26};$

$A4 = 8.024 * 10^{10};$

E1 = 175.38; (**kJ/mol**)

E2 = 296.29;

E3 = 474.76;

E4 = 213.78;

$$k1 = A1 * Exp\left[\frac{-E1 * 10^{3}}{R * T[z]}\right];\ (**kmol/kg-cath**)$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^{3}}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^{3}}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^{3}}{R * T[z]}\right];$$

(*Catalytic reaction rates of four reactions*)

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^{2}};\ (**kmol/kg-cath**)$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

(*Construct the models for the thermodynamic equilibriums*)

$AEB = 1.014 * 10^{-5}$; (**1/bar**)

$AST = 2.678 * 10^{-5}$;

$AH2 = 4.519 * 10^{-7}$;

$\Delta HaEB = -102.22$; (**kJ/mol**)

$\Delta HaST = -104.56$;

$\Delta HaH2 = -117.95$;

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; \text{ (**1/bar**)}$$

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \text{ (**1/bar**)}$$

(*(**The initial molar flowrates of components**)*)

FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)

FST0 = 0.00332919*3.6;

FBZ0 = 1.464*3.6;

FTO0 = 0.0482245*3.6;

FH20 = 0;

FCH40 = 0;

FC2H40 = 0;

FH2O0 = 49.7976*3600/1000*ratio;

FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

(*Partial pressure of components*)

$$PEB = PT[z] * \frac{\frac{FEB0}{FT0}(1 - (X1EB[z] - X1BZ[z] - X1TO[z]) - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(**1/bar**)

$$PST = PT[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (X1EB[z] - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PBZ = PT[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2 = PT[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X1H2[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PETH = PT[z] * \frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PTO = PT[z] * \frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0} * X1TO[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2O = PT[z] * \frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PMTH = PT[z] * \frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0} * X1EB[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C1ST = \frac{PST * 10^5}{R * T[z]};$$

$$C1BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C1H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C1ETH = \frac{PETH * 10^5}{R * T[z]};$$

$$C1TO = \frac{PTO * 10^5}{R * T[z]};$$

$$C1H2O = \frac{PH2O * 10^5}{R * T[z]};$$

$$C1MTH = \frac{PMTH * 10^5}{R * T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

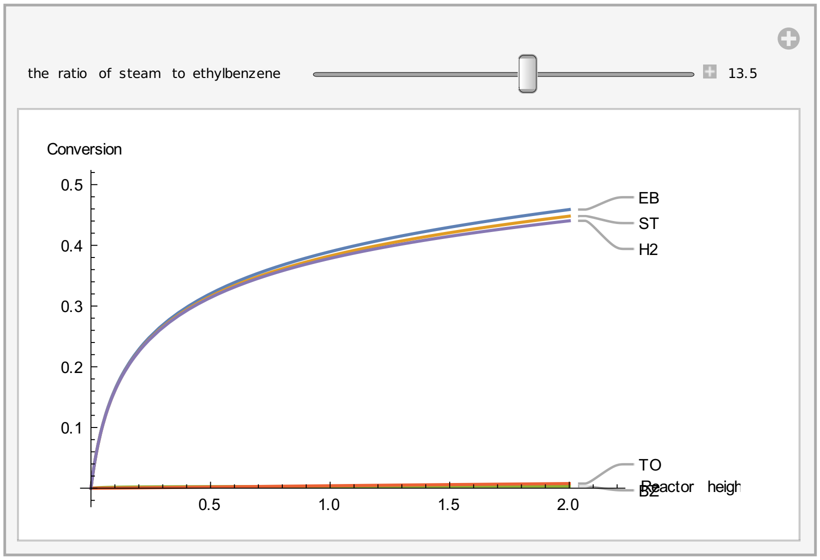
```
ρb = 1422;
ϵ = 0.4312;


(*Dimensions of the reactor*)
L = 10;
Dr = 400;
Di = Dr/100;
Ac = π/4 * (Di)^2;

(*The important properties of the gas mixture*)
μ = (-10.035 + 0.25191 * T[z] - 0.000037932 * T[z] * T[z]) * 3.6 * 10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;

ρg = (10^5 * 10^-3)/(R * T[z]) * (PEB * 106.168 + PST * 104.15 + PBZ * 78.114 +
    PTO * 92.141 + PH2O * 18.020 + PH2 * 2.010 + PMTH * 16.043 + PETH * 28.054);
r107 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3) * ϵ/ρb) * (Ac * ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2 * ϵ/ρb) * (Ac * ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3 * ϵ/ρb) * (Ac * ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * ϵ/ρb) * (Ac * ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458 * (1 - ϵ))/((ρg * dp * u)/μ)) * 7.7160 * 10^-8 * (u * G * FEB0)/(ρb * dp * Ac) * 10^-5 * (Ac * ρb)/FEB0,
    T'[z] == (Ac * ρb)/FEB0 * (1/(106.168 * FEB0 * (1 - X1EB[z]) * Cp1 +
          104.15 * (FST0 + FEB0 * (X1EB[z] - X1BZ[z] - X1TO[z])) * Cp2 +
          78.114 * (FBZ0 + FEB0 * X1BZ[z]) * Cp3 + 92.141 * (FTO0 + FEB0 * X1TO[z]) * Cp4 +
          2.010 * (FH20 + FEB0 * X1H2[z]) * Cp5 + 18.020 * FH2O0 * Cp6)) *
      (FEB0 * (-ΔH1 * (rc1 + rt1 * ϵ/ρb) - ΔH2 * (rc2 + rt2 * ϵ/ρb) - ΔH3 * (rc3 + rt3 * ϵ/ρb) - ΔH4 * rc4)),
    X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 0.65, T[0] == 870},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
    C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];
Figure13 = Plot[{X1EB[z] /. r107, (X1EB[z] - X1BZ[z] - X1TO[z]) /. r107, X1BZ[z] /. r107,
   X1TO[z] /. r107, X1H2[z] /. r107}, {z, 0, 2}, PlotLabels → {"EB", "ST", "BZ", "TO", "H2"},
```

```
    PlotRange→ All, AxesLabel → {"Reactor height (m)", "Conversion"}]], Column[{
  Control[{{ratio, 10, "the ratio of steam to ethylbenzene "}, 5, 20, 0.1, Appearance → "Labeled"}]
}, Left]]
```



Ethylbenzene conversion at 6.5, 13.5, 20.5 steam to ethylbenzene flowrate ratio

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO, S1H2,
   ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg, ratio},

  (*Construct the models for the thermal reactions*)
  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
```

$$kt3 = At3 * Exp\left[\frac{-Et3 * 10^3}{R * T[z]}\right];$$

(*Thermal reaction rates of three reactions*)

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \text{ (**kmol/m3h**)}$$

$$rt2 = kt2 * PEB;$$

$$rt3 = kt3 * PEB;$$

(*Construct the models for the catalytic reactions*)

$A1 = 4.594 * 10^9;$ (**kmol/kg−cath**)

$A2 = 1.060 * 10^{15};$

$A3 = 1.246 * 10^{26};$

$A4 = 8.024 * 10^{10};$

$E1 = 175.38;$ (**kJ/mol**)

$E2 = 296.29;$

$E3 = 474.76;$

$E4 = 213.78;$

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right]; \text{ (**kmol/kg−cath**)}$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

(*Catalytic reaction rates of four reactions*)

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2}; \text{ (**kmol/kg−cath**)}$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

```
(*Construct the models for the thermodynamic equilibriums*)
```

$$AEB = 1.014 * 10^{-5};\ (**1/bar**)$$

$$AST = 2.678 * 10^{-5};$$

$$AH2 = 4.519 * 10^{-7};$$

$$\Delta HaEB = -102.22;\ (**kJ/mol**)$$

$$\Delta HaST = -104.56;$$

$$\Delta HaH2 = -117.95;$$

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right];\ (**1/bar**)$$

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right];\ (**1/bar**)$$

```
(*(**The initial molar flowrates of components**)*)
FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 49.7976*3600/1000*ratio;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;
```

```
(*Partial pressure of components*)
```

$$PEB = PT[z] * \frac{\frac{FEB0}{FT0}\,(1 - (X1EB[z] - X1BZ[z] - X1TO[z]) - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(**1/bar**)

$$PST = PT[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (X1EB[z] - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PBZ = PT[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2 = PT[z]*\frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0}*X1H2[z]}{1 + \frac{FEB0}{FT0}*(X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PETH = PT[z]*\frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0}*X1BZ[z]}{1 + \frac{FEB0}{FT0}*(X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PTO = PT[z]*\frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0}*X1TO[z]}{1 + \frac{FEB0}{FT0}*(X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2O = PT[z]*\frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0}*(X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PMTH = PT[z]*\frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0}*X1EB[z]}{1 + \frac{FEB0}{FT0}*(X1TO[z] + X1BZ[z] + X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB*10^5}{R*T[z]};$$

$$C1ST = \frac{PST*10^5}{R*T[z]};$$

$$C1BZ = \frac{PBZ*10^5}{R*T[z]};$$

$$C1H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C1ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C1TO = \frac{PTO*10^5}{R*T[z]};$$

$$C1H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C1MTH = \frac{PMTH*10^5}{R*T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

$\rho b = 1422;$

$\epsilon = 0.4312;$

(*Dimensions of the reactor*)

L = 10;

```
Di = Dr/100;
Ac = π/4 * (Di)^2;

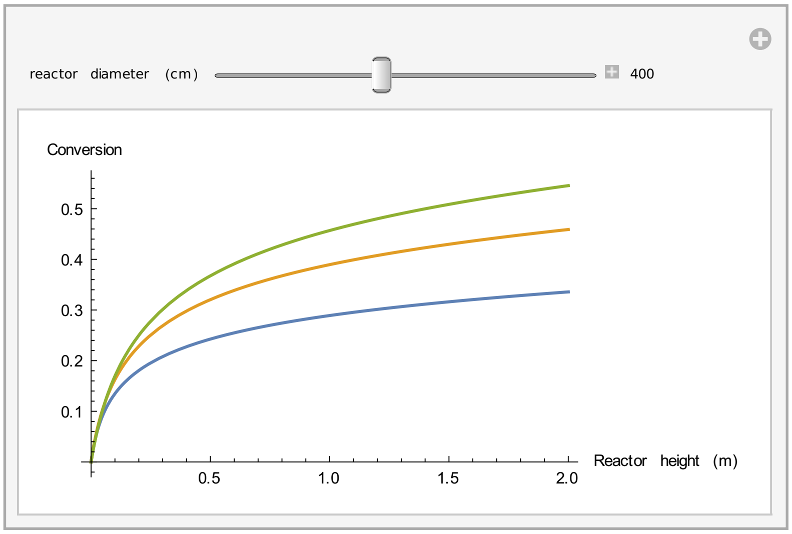
(*The important properties of the gas mixture*)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;

ρg = (10^5*10^-3)/(R*T[z]) * (PEB*106.168 + PST*104.15 + PBZ*78.114 +
    PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
ratio = 6.5;
r108 = Quiet@NDSolve[
  {X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0, X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0,
   X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0, X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
   PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
   T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
      (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
   X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 0.65, T[0] == 870},
  {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
   C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];

ratio = 13.5;
r109 = Quiet@NDSolve[
  {X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0, X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0,
   X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0, X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
```

```
PT'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5 * (Ac*ρb)/FEB0,
T'[z] == (Ac*ρb)/FEB0 * (1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
     104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
     78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
     2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
   (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
  X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 0.65, T[0] == 870},
 {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
  C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];

ratio = 20.5;
r110 = Quiet@NDSolve[
 {X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb) * (Ac*ρb)/FEB0, X1BZ'[z] == (rc2 + rt2*ϵ/ρb) * (Ac*ρb)/FEB0,
  X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb) * (Ac*ρb)/FEB0, X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb) * (Ac*ρb)/FEB0,
  PT'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5 * (Ac*ρb)/FEB0,
  T'[z] == (Ac*ρb)/FEB0 * (1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
     104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
     78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
     2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
   (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
  X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 0.65, T[0] == 870},
 {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO,
  C1H2, C1ETH, C1H2O, C1MTH}, {z, 0, 2}];
Figure14 = Plot[{X1EB[z] /. r108, X1EB[z] /. r109, X1EB[z] /. r110}, {z, 0, 2},
   PlotRange→ All, AxesLabel → {"Reactor height (m)", "Conversion"}], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



The effect of inlet temperature on the ethylbenzene conversion and selectivity of styrene:

Manipulate[

Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST, AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0, FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4, PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO, S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

(*Construct the models for the thermal reactions*)

At1 = $2.2215*10^{16}$; (kmol/m3hbar**)**

At2 = $2.4217*10^{20}$;

At3 = $3.8224*10^{17}$;

Et1 = 272.23; (kJ/mol**)**

Et2 = 352.79;

Et3 = 313.06;

R = 8.314;

$$kt1 = At1*Exp\left[\frac{-Et1*10^{3}}{R*T[z]}\right];$$ **(**kmol/m3hbar**)**

$$kt2 = At2*Exp\left[\frac{-Et2*10^{3}}{R*T[z]}\right];$$

$$kt3 = At3*Exp\left[\frac{-Et3*10^{3}}{R*T[z]}\right];$$

```
(*Thermal reaction rates of three reactions*)
```

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \text{ (**kmol/m3h**)}$$

$$rt2 = kt2 * PEB;$$

$$rt3 = kt3 * PEB;$$

```
(*Construct the models for the catalytic reactions*)
```

$$A1 = 4.594 * 10^{9}; \text{ (**kmol/kg-cath**)}$$

$$A2 = 1.060 * 10^{15};$$

$$A3 = 1.246 * 10^{26};$$

$$A4 = 8.024 * 10^{10};$$

$$E1 = 175.38; \text{ (**kJ/mol**)}$$

$$E2 = 296.29;$$

$$E3 = 474.76;$$

$$E4 = 213.78;$$

$$k1 = A1 * Exp\left[\frac{-E1 * 10^{3}}{R * T[z]}\right]; \text{ (**kmol/kg-cath**)}$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^{3}}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^{3}}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^{3}}{R * T[z]}\right];$$

```
(*Catalytic reaction rates of four reactions*)
```

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^{2}}; \text{ (**kmol/kg-cath**)}$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^{2}};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^{2}};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^{2}};$$

```
(*Construct the models for the thermodynamic equilibriums*)
```

$$AEB = 1.014 * 10^{-5}; \text{ (**1/bar**)}$$

$$AST = 2.678 * 10^{-5};$$

$AH2 = 4.519 * 10^{-7};$

$\Delta HaEB = -102.22;$ (**kJ/mol**)

$\Delta HaST = -104.56;$

$\Delta HaH2 = -117.95;$

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right];$$ (**1/bar**)

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right];$$ (**1/bar**)

(*(**The initial molar flowrates of components**)*)

FEB0 = 49.7976 * 3600/1000; (*Unit:kmol/h*)

FST0 = 0.00332919 * 3.6;

FBZ0 = 1.464 * 3.6;

FTO0 = 0.0482245 * 3.6;

FH20 = 0;

FCH40 = 0;

FC2H40 = 0;

FH2O0 = 1080 * 3.6;

FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

(*Partial pressure of components*)

$$PEB = PT[z] * \frac{\frac{FEB0}{FT0}\,(1 - (X1EB[z] - X1BZ[z] - X1TO[z]) - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(**1/bar**)

$$PST = PT[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (X1EB[z] - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PBZ = PT[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2 = PT[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X1H2[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PETH = PT[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X1BZ[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PTO = PT[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X1TO[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PH2O = PT[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PMTH = PT[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X1EB[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB*10^5}{R*T[z]};$$

$$C1ST = \frac{PST*10^5}{R*T[z]};$$

$$C1BZ = \frac{PBZ*10^5}{R*T[z]};$$

$$C1H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C1ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C1TO = \frac{PTO*10^5}{R*T[z]};$$

$$C1H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C1MTH = \frac{PMTH*10^5}{R*T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z]-X1BZ[z]-X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99*(T[z] - 298.15) + \frac{-8.2026*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{6.499*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986*(T[z] - 298.15) + \frac{-7.67*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{9.592*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86*(T[z] - 298.15) + \frac{-15.1844*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{23.04*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13)*(T[z] - 298.15) + \frac{-6.9818*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{16.54*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$Cp1 = -0.43426 + 6.0671*10^{-3}*T[z] - 3.8625*10^{-6}*T[z]*T[z] + 9.1282*10^{-10}*(T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564*10^{-3}*T[z] - 3.0018*10^{-6}*T[z]*T[z] + 5.3317*10^{-10}*(T[z])^3;$

$Cp3 = -0.40599 + 6.6616*10^{-3}*T[z] - 4.5318*10^{-6}*T[z]*T[z] + 12.255*10^{-10}*(T[z])^3;$

$Cp4 = -0.27127 + 5.9142*10^{-3}*T[z] - 3.8631*10^{-6}*T[z]*T[z] + 9.54*10^{-10}*(T[z])^3;$

$Cp5 = 13.57 + 4.637*10^{-3}*T[z] - 6.905*10^{-6}*T[z]*T[z] + 38.23*10^{-10}*(T[z])^3;$

$Cp6 = 1.7911 + 0.1069*10^{-3}*T[z] + 0.58611*10^{-6}*T[z]*T[z] - 1.998*10^{-10}*(T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

$\rho b = 1422;$

$\epsilon = 0.4312;$

(*Dimensions of the reactor*)

L = 10;

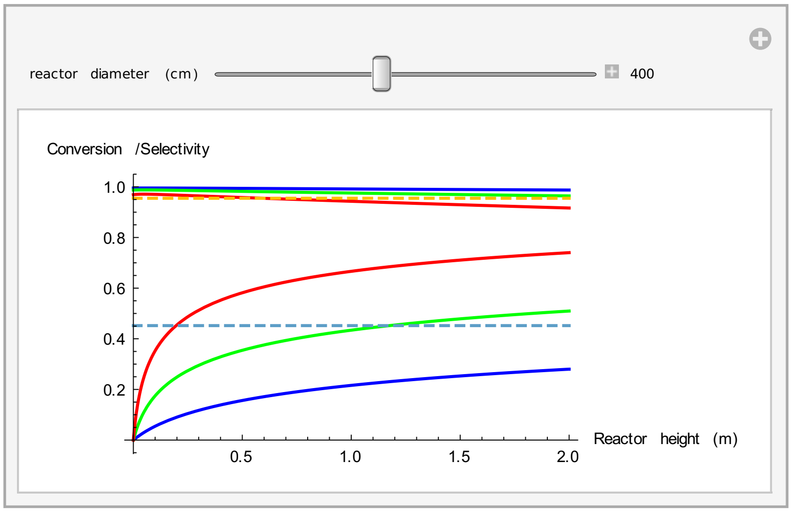
$$Di = \frac{Dr}{100};$$

$$Ac = \frac{\pi}{4}*(Di)^2;$$

```
(*The important properties of the gas mixture*)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;

ρg = (10^5*10^-3)/(R*T[z])*(PEB*106.168 + PST*104.15 + PBZ*78.114 +
    PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r111 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
        104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
        78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
        2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
      (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
    X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 820},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
    C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}, {z, 0, 2}];
r112 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
        104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
```

```
            78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
            2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
         (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
     X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 870},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
     C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}, {z, 0, 2}];
r113 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
     X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
     X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
     PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
     T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
            104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
            78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
            2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
         (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
     X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 920},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
     C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}, {z, 0, 2}];
Figure15 = Plot[{X1EB[z] /. r111, X1EB[z] /. r112, X1EB[z] /. r113, S1ST /. r111,
     S1ST /. r112, S1ST /. r113, 0.452, 0.955}, {z, 0, 2},
    PlotStyle → {Blue , Green , Red , Blue , Green , Red , Dashed , Dashed }, PlotRange → All,
    AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



The effect of inlet feed temperature on the conversion and selectivity for the second reactor:

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
   S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},

  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[-Et1*10^3/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[-Et2*10^3/(R*T[z])];
  kt3 = At3*Exp[-Et3*10^3/(R*T[z])];

  A1 = 4.594*10^9; (**kmol/kg-cath**)
  A2 = 1.060*10^15;
  A3 = 1.246*10^26;
  A4 = 8.024*10^10;
  E1 = 175.38; (**kJ/mol**)
```

```
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;
k1 = A1*Exp[(-E1*10^3)/(R*T[z])]; (**kmol/kg-cath**)
k2 = A2*Exp[(-E2*10^3)/(R*T[z])];
k3 = A3*Exp[(-E3*10^3)/(R*T[z])];
k4 = A4*Exp[(-E4*10^3)/(R*T[z])];
AEB = 1.014*10^-5; (**1/bar**)
AST = 2.678*10^-5;
AH2 = 4.519*10^-7;
ΔHaEB = -102.22; (**kJ/mol**)
ΔHaST = -104.56;
ΔHaH2 = -117.95;
KEB = AEB*Exp[(-ΔHaEB*10^3)/(R*T[z])]; (**1/bar**)
KST = AST*Exp[(-ΔHaST*10^3)/(R*T[z])];
KH2 = AH2*Exp[(-ΔHaH2*10^3)/(R*T[z])];
Keq = Exp[(-(122 725.157 - 126.267*T[z] - 0.002194*T[z]*T[z]))/(R*T[z])]; (**1/bar**)

rt1 = kt1*(PEB - (PST*PH2)/Keq); (**kmol/m3h**)
rt2 = kt2*PEB;
rt3 = kt3*PEB;

C2EB = (PEB*10^5)/(R*T[z]);
C2ST = (PST*10^5)/(R*T[z]);
C2BZ = (PBZ*10^5)/(R*T[z]);
C2H2 = (PH2*10^5)/(R*T[z]);
```

$$C2ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C2TO = \frac{PTO*10^5}{R*T[z]};$$

$$C2H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C2MTH = \frac{PMTH*10^5}{R*T[z]};$$

$$S2ST = \frac{X2EB[z] - X2BZ[z] - X2TO[z]}{X2EB[z]};$$

$$S2BZ = \frac{X2BZ[z]}{X2EB[z]};$$

$$S2TO = \frac{X2TO[z]}{X2EB[z]};$$

$$S2H2 = \frac{X2H2[z]}{X2EB[z]};$$

FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 3954.696;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

$$PEB = P[z]*\frac{\frac{FEB0}{FT0}(1 - (X2EB[z] - X2BZ[z] - X2TO[z]) - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

(**1/bar**)

$$PST = P[z]*\frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0}*(X2EB[z] - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PBZ = P[z]*\frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0}*X2BZ[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2 = P[z]*\frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0}*X2H2[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PETH = P[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X2BZ[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PTO = P[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X2TO[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PH2O = P[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$PMTH = P[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X2EB[z]}{1+\frac{FEB0}{FT0}*(X2TO[z]+X2BZ[z]+X2H2[z])};$$

$$rc1 = \frac{k1*KEB*\left(PEB-\frac{PST*PH2}{Keq}\right)}{(1+KEB*PEB+KH2*PH2+KST*PST)^2}; \text{ (**kmol/kg−cath**)}$$

$$rc2 = \frac{k2*KEB*PEB}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$rc3 = \frac{k3*KEB*PEB*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$rc4 = \frac{k4*KST*PST*KH2*PH2}{(1+KEB*PEB+KH2*PH2+KST*PST)^2};$$

$$\Delta H1 = 117\,690+41.99*(T[z]-298.15)+\frac{-8.2026*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{6.499*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-2.311*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510+12.986*(T[z]-298.15)+\frac{-7.67*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{9.592*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-4.125*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H3 = -54\,680+10.86*(T[z]-298.15)+\frac{-15.1844*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{23.04*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-9.9955*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H4 = -172\,370+(-31.13)*(T[z]-298.15)+\frac{-6.9818*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{16.54*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-7.685*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$Cp1 = -0.43426+6.0671*10^{-3}*T[z]-3.8625*10^{-6}*T[z]*T[z]+9.1282*10^{-10}*(T[z])^3; \text{ (**kJ/kgK**)}$$

$$Cp2 = -0.26436 + 5.564*10^{-3}*T[z] - 3.0018*10^{-6}*T[z]*T[z] + 5.3317*10^{-10}*(T[z])^3;$$
$$Cp3 = -0.40599 + 6.6616*10^{-3}*T[z] - 4.5318*10^{-6}*T[z]*T[z] + 12.255*10^{-10}*(T[z])^3;$$
$$Cp4 = -0.27127 + 5.9142*10^{-3}*T[z] - 3.8631*10^{-6}*T[z]*T[z] + 9.54*10^{-10}*(T[z])^3;$$
$$Cp5 = 13.57 + 4.637*10^{-3}*T[z] - 6.905*10^{-6}*T[z]*T[z] + 38.23*10^{-10}*(T[z])^3;$$
$$Cp6 = 1.7911 + 0.1069*10^{-3}*T[z] + 0.58611*10^{-6}*T[z]*T[z] - 1.998*10^{-10}*(T[z])^3;$$

$$L = 10;$$
$$Di = \frac{Dr}{100};$$
$$Ac = \frac{\pi}{4}*(Di)^2;$$
$$dp = 5.5/1000; \text{ (**m**)}$$
$$\mu = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^{-4}; \text{ (**kg/ms**)}$$
$$u = 22.003/Ac;$$
$$G = 89\,520.109/Ac;$$
$$\rho b = 1422;$$
$$\epsilon = 0.4312; \text{ (**void fraction of bed**)}$$
$$\rho g = \frac{10^5*10^{-3}}{R*T[z]}*(PEB*106.168 + PST*104.15 + PBZ*78.114 + PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);$$

$$r211 = Quiet@NDSolve\Big[\Big\{X2EB'[z] == \left(rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$
$$X2BZ'[z] == \left(rc2 + rt2*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},\ X2TO'[z] == \left(rc3 + rc4 + rt3*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$
$$X2H2'[z] == \left(rc1 - rc3 - 2\,rc4 + (rt1 - rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$
$$P'[z] == -\frac{1-\epsilon}{\epsilon^3}*\left(1.28 + \frac{458*(1-\epsilon)}{\frac{\rho g*dp*u}{\mu}}\right)*7.7160*10^{-8}*\frac{u*G*FEB0}{\rho b*dp*Ac}*10^{-5}*\frac{Ac*\rho b}{FEB0},$$
$$T'[z] == \frac{Ac*\rho b}{FEB0}*(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 + 104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 + 78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 + 2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*$$
$$\left(FEB0*\left(-\Delta H1*\left(rc1 + rt1*\frac{\epsilon}{\rho b}\right) - \Delta H2*\left(rc2 + rt2*\frac{\epsilon}{\rho b}\right) - \Delta H3*\left(rc3 + rt3*\frac{\epsilon}{\rho b}\right) - \Delta H4*rc4\right)\right),$$
$$X2EB[2] == X1EB[2] /. r111,\ X2BZ[2] == X1BZ[2] /. r111,\ X2TO[2] == X1TO[2] /. r111,$$
$$X2H2[2] == X1H2[2] /. r111,\ P[2] == PT[2] /. r111,\ T[2] == 820\Big\},$$
$$\{P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO, C2H2, C2ETH, C2H2O, C2MTH\}, \{z, 2, 4\}\Big];$$

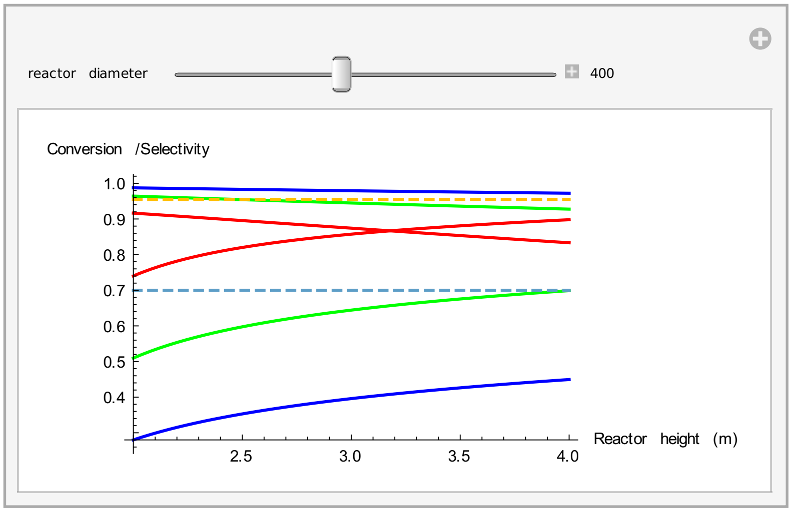
$$r212 = Quiet@NDSolve\Big[\Big\{X2EB'[z] == \left(rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$

```
    X2BZ'[z] == (rc2 + rt2 * ϵ/ρb) * (Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3 * ϵ/ρb) * (Ac*ρb)/FEB0,
    X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * ϵ/ρb) * (Ac*ρb)/FEB0,
    P'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5 * (Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0 * (1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6)) *
      (FEB0*(-ΔH1*(rc1 + rt1 * ϵ/ρb) - ΔH2*(rc2 + rt2 * ϵ/ρb) - ΔH3*(rc3 + rt3 * ϵ/ρb) - ΔH4*rc4)),
    X2EB[2] == X1EB[2] /. r112, X2BZ[2] == X1BZ[2] /. r112, X2TO[2] == X1TO[2] /. r112,
    X2H2[2] == X1H2[2] /. r112, P[2] == PT[2] /. r112, T[2] == 850},
  {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
    C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];

r213 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3) * ϵ/ρb) * (Ac*ρb)/FEB0,
    X2BZ'[z] == (rc2 + rt2 * ϵ/ρb) * (Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3 * ϵ/ρb) * (Ac*ρb)/FEB0,
    X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * ϵ/ρb) * (Ac*ρb)/FEB0,
    P'[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5 * (Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0 * (1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6)) *
      (FEB0*(-ΔH1*(rc1 + rt1 * ϵ/ρb) - ΔH2*(rc2 + rt2 * ϵ/ρb) - ΔH3*(rc3 + rt3 * ϵ/ρb) - ΔH4*rc4)),
    X2EB[2] == X1EB[2] /. r113, X2BZ[2] == X1BZ[2] /. r113, X2TO[2] == X1TO[2] /. r113,
    X2H2[2] == X1H2[2] /. r113, P[2] == PT[2] /. r113, T[2] == 880},
  {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
    C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];
Figure16 = Plot[{{X2EB[z] /. r211, X2EB[z] /. r212, X2EB[z] /. r213, S2ST /. r211, S2ST /. r212, S2ST /. r213,
      0.7, 0.955}}, {z, 2, 4}, PlotStyle -> {Blue, Green, Red, Blue, Green, Red, Dashed, Dashed},
    PlotRange -> All, AxesLabel -> {"Reactor height (m)", "Conversion/Selectivity"}], Column[{
```

Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]

}, Left]



The effect of inlet pressure on the ethylbenzene conversion and selectivity of styrene for the first reactor (r101):

Manipulate[

Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST, AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0, FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4, PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO, S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

(*Construct the models for the thermal reactions*)

At1 = $2.2215*10^{16}$; (**kmol/m3hbar**)

At2 = $2.4217*10^{20}$;

At3 = $3.8224*10^{17}$;

Et1 = 272.23; (**kJ/mol**)

Et2 = 352.79;

Et3 = 313.06;

R = 8.314;

kt1 = At1 * Exp$\left[\frac{-Et1*10^{3}}{R*T[z]}\right]$; (**kmol/m3hbar**)

kt2 = At2 * Exp$\left[\frac{-Et2*10^{3}}{R*T[z]}\right]$;

kt3 = At3 * Exp$\left[\frac{-Et3*10^{3}}{R*T[z]}\right]$;

```
(*Thermal reaction rates of three reactions*)
rt1 = kt1*(PEB - PST*PH2/Keq); (**kmol/m3h**)
rt2 = kt2*PEB;
rt3 = kt3*PEB;


(*Construct the models for the catalytic reactions*)
A1 = 4.594*10^9;  (**kmol/kg-cath**)
A2 = 1.060*10^15;
A3 = 1.246*10^26;
A4 = 8.024*10^10;
E1 = 175.38; (**kJ/mol**)
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;
k1 = A1*Exp[-E1*10^3/(R*T[z])]; (**kmol/kg-cath**)
k2 = A2*Exp[-E2*10^3/(R*T[z])];
k3 = A3*Exp[-E3*10^3/(R*T[z])];
k4 = A4*Exp[-E4*10^3/(R*T[z])];


(*Catalytic reaction rates of four reactions*)
rc1 = k1*KEB*(PEB - PST*PH2/Keq)/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2; (**kmol/kg-cath**)
rc2 = k2*KEB*PEB/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;
rc3 = k3*KEB*PEB*KH2*PH2/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;
rc4 = k4*KST*PST*KH2*PH2/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;


(*Construct the models for the thermodynamic equilibriums*)
AEB = 1.014*10^-5;  (**1/bar**)
```

```
AST = 2.678*10^-5;
AH2 = 4.519*10^-7;
ΔHaEB = -102.22; (**kJ/mol**)
ΔHaST = -104.56;
ΔHaH2 = -117.95;
```

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; \text{ (**1/bar**)}$$

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \text{ (**1/bar**)}$$

```
(*(**The initial molar flowrates of components**)*)
FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 1080*3.6;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;
```

```
(*Partial pressure of components*)
```

$$PEB = PT[z] * \frac{\frac{FEB0}{FT0}(1 - (X1EB[z] - X1BZ[z] - X1TO[z]) - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

(**1/bar**)

$$PST = PT[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (X1EB[z] - X1BZ[z] - X1TO[z])}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PBZ = PT[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * X1BZ[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PH2 = PT[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X1H2[z]}{1 + \frac{FEB0}{FT0} * (X1TO[z] + X1BZ[z] + X1H2[z])};$$

$$PETH = PT[z]*\frac{\frac{FC2H40}{FT0}+\frac{FEB0}{FT0}*X1BZ[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PTO = PT[z]*\frac{\frac{FTO0}{FT0}+\frac{FEB0}{FT0}*X1TO[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PH2O = PT[z]*\frac{\frac{FH2O0}{FT0}}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

$$PMTH = PT[z]*\frac{\frac{FCH40}{FT0}+\frac{FEB0}{FT0}*X1EB[z]}{1+\frac{FEB0}{FT0}*(X1TO[z]+X1BZ[z]+X1H2[z])};$$

(* Concentration of components*)

$$C1EB = \frac{PEB*10^5}{R*T[z]};$$

$$C1ST = \frac{PST*10^5}{R*T[z]};$$

$$C1BZ = \frac{PBZ*10^5}{R*T[z]};$$

$$C1H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C1ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C1TO = \frac{PTO*10^5}{R*T[z]};$$

$$C1H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C1MTH = \frac{PMTH*10^5}{R*T[z]};$$

(*selectivity of reaction products*)

$$S1ST = \frac{X1EB[z]-X1BZ[z]-X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(*Heat of reactions*)

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(*Heat capacities of components*)

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

$\rho b = 1422;$

$\epsilon = 0.4312;$

(*Dimensions of the reactor*)

L = 10;

$$Di = \frac{Dr}{100};$$

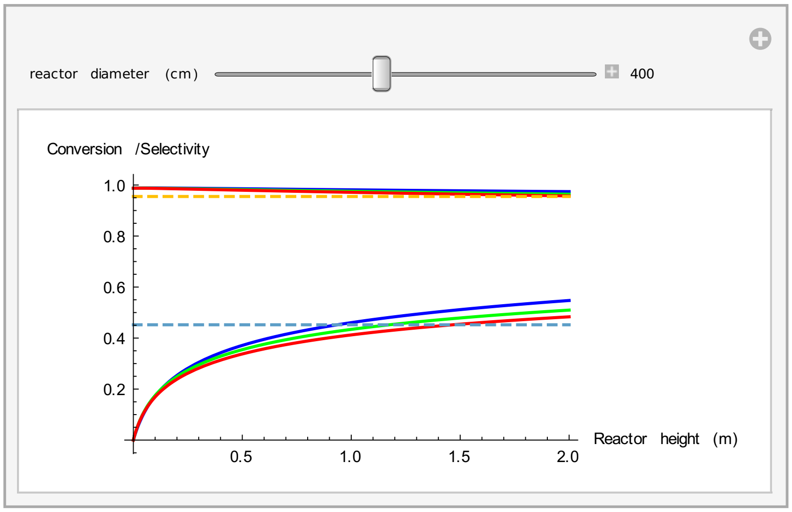
$$Ac = \frac{\pi}{4} * (Di)^2;$$

```
(*The important properties of the gas mixture*)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;

ρg = (10^5*10^-3)/(R*T[z])*(PEB*106.168 + PST*104.15 + PBZ*78.114 +
    PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r114 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
         104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
         78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
         2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
      (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
    X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 0.75, T[0] == 870},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
    C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}, {z, 0, 2}];
r115 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
    X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
         104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
```

```
78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
(FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 870},
{PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}, {z, 0, 2}];

r116 = Quiet@NDSolve[{X1EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
X1BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X1TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
X1H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
PT'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X1EB[z])*Cp1 +
104.15*(FST0 + FEB0*(X1EB[z] - X1BZ[z] - X1TO[z]))*Cp2 +
78.114*(FBZ0 + FEB0*X1BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X1TO[z])*Cp4 +
2.010*(FH20 + FEB0*X1H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
(FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.75, T[0] == 870},
{PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}, {z, 0, 2}];
Figure17 = Plot[{X1EB[z] /. r114, X1EB[z] /. r115, X1EB[z] /. r116, S1ST /. r114,
S1ST /. r115, S1ST /. r116, 0.452, 0.955}, {z, 0, 2},
PlotStyle → {Blue , Green , Red , Blue , Green , Red , Dashed , Dashed }, PlotRange → All,
AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}]], Column[{
Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



The effect of inlet pressure on the ethylbenzene conversion and selectivity of styrene for the second reactor (r202):

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
   S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},

  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
  kt3 = At3*Exp[(-Et3*10^3)/(R*T[z])];

  A1 = 4.594*10^9; (**kmol/kg-cath**)
  A2 = 1.060*10^15;
  A3 = 1.246*10^26;
  A4 = 8.024*10^10;
  E1 = 175.38; (**kJ/mol**)
```

$$E2 = 296.29;$$
$$E3 = 474.76;$$
$$E4 = 213.78;$$
$$k1 = A1 * Exp\left[\frac{-E1 * 10^{3}}{R * T[z]}\right]; \text{(**kmol/kg-cath**)}$$
$$k2 = A2 * Exp\left[\frac{-E2 * 10^{3}}{R * T[z]}\right];$$
$$k3 = A3 * Exp\left[\frac{-E3 * 10^{3}}{R * T[z]}\right];$$
$$k4 = A4 * Exp\left[\frac{-E4 * 10^{3}}{R * T[z]}\right];$$
$$AEB = 1.014 * 10^{-5}; \text{ (**1/bar**)}$$
$$AST = 2.678 * 10^{-5};$$
$$AH2 = 4.519 * 10^{-7};$$
$$\Delta HaEB = -102.22; \text{(**kJ/mol**)}$$
$$\Delta HaST = -104.56;$$
$$\Delta HaH2 = -117.95;$$
$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^{3}}{R * T[z]}\right]; \text{(**1/bar**)}$$
$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^{3}}{R * T[z]}\right];$$
$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^{3}}{R * T[z]}\right];$$
$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \text{(**1/bar**)}$$

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \text{(**kmol/m3h**)}$$
$$rt2 = kt2 * PEB;$$
$$rt3 = kt3 * PEB;$$

$$C2EB = \frac{PEB * 10^{5}}{R * T[z]};$$
$$C2ST = \frac{PST * 10^{5}}{R * T[z]};$$
$$C2BZ = \frac{PBZ * 10^{5}}{R * T[z]};$$
$$C2H2 = \frac{PH2 * 10^{5}}{R * T[z]};$$

$$C2ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C2TO = \frac{PTO*10^5}{R*T[z]};$$

$$C2H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C2MTH = \frac{PMTH*10^5}{R*T[z]};$$

$$S2ST = \frac{X2EB[z] - X2BZ[z] - X2TO[z]}{X2EB[z]};$$

$$S2BZ = \frac{X2BZ[z]}{X2EB[z]};$$

$$S2TO = \frac{X2TO[z]}{X2EB[z]};$$

$$S2H2 = \frac{X2H2[z]}{X2EB[z]};$$

FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 3954.696;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

$$PEB = P[z]*\frac{\frac{FEB0}{FT0}(1 - (X2EB[z] - X2BZ[z] - X2TO[z]) - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

(**1/bar**)

$$PST = P[z]*\frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0}*(X2EB[z] - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PBZ = P[z]*\frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0}*X2BZ[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2 = P[z]*\frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0}*X2H2[z]}{1 + \frac{FEB0}{FT0}*(X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$\text{PETH} = \text{P[z]} * \frac{\frac{\text{FC2H40}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}} * \text{X2BZ[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}} * (\text{X2TO[z]} + \text{X2BZ[z]} + \text{X2H2[z]})};$$

$$\text{PTO} = \text{P[z]} * \frac{\frac{\text{FTO0}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}} * \text{X2TO[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}} * (\text{X2TO[z]} + \text{X2BZ[z]} + \text{X2H2[z]})};$$

$$\text{PH2O} = \text{P[z]} * \frac{\frac{\text{FH2O0}}{\text{FT0}}}{1 + \frac{\text{FEB0}}{\text{FT0}} * (\text{X2TO[z]} + \text{X2BZ[z]} + \text{X2H2[z]})};$$

$$\text{PMTH} = \text{P[z]} * \frac{\frac{\text{FCH40}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}} * \text{X2EB[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}} * (\text{X2TO[z]} + \text{X2BZ[z]} + \text{X2H2[z]})};$$

$$\text{rc1} = \frac{\text{k1} * \text{KEB} * \left(\text{PEB} - \frac{\text{PST} * \text{PH2}}{\text{Keq}}\right)}{(1 + \text{KEB} * \text{PEB} + \text{KH2} * \text{PH2} + \text{KST} * \text{PST})^2}; \text{ (**kmol/kg-cath**)}$$

$$\text{rc2} = \frac{\text{k2} * \text{KEB} * \text{PEB}}{(1 + \text{KEB} * \text{PEB} + \text{KH2} * \text{PH2} + \text{KST} * \text{PST})^2};$$

$$\text{rc3} = \frac{\text{k3} * \text{KEB} * \text{PEB} * \text{KH2} * \text{PH2}}{(1 + \text{KEB} * \text{PEB} + \text{KH2} * \text{PH2} + \text{KST} * \text{PST})^2};$$

$$\text{rc4} = \frac{\text{k4} * \text{KST} * \text{PST} * \text{KH2} * \text{PH2}}{(1 + \text{KEB} * \text{PEB} + \text{KH2} * \text{PH2} + \text{KST} * \text{PST})^2};$$

$$\Delta\text{H1} = 117\,690 + 41.99 * (\text{T[z]} - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((\text{T[z]})^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3}\left((\text{T[z]})^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4}\left((\text{T[z]})^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta\text{H2} = 105\,510 + 12.986 * (\text{T[z]} - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((\text{T[z]})^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3}\left((\text{T[z]})^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4}\left((\text{T[z]})^4 - 298.15^4\right);$$

$$\Delta\text{H3} = -54\,680 + 10.86 * (\text{T[z]} - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((\text{T[z]})^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3}\left((\text{T[z]})^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4}\left((\text{T[z]})^4 - 298.15^4\right);$$

$$\Delta\text{H4} = -172\,370 + (-31.13) * (\text{T[z]} - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((\text{T[z]})^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3}\left((\text{T[z]})^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4}\left((\text{T[z]})^4 - 298.15^4\right);$$

$$\text{Cp1} = -0.43426 + 6.0671 * 10^{-3} * \text{T[z]} - 3.8625 * 10^{-6} * \text{T[z]} * \text{T[z]} + 9.1282 * 10^{-10} * (\text{T[z]})^3; \text{ (**kJ/kgK**)}$$

```
Cp2 = -0.26436 + 5.564*10^-3 *T[z] - 3.0018*10^-6 *T[z]*T[z] + 5.3317*10^-10 *(T[z])^3;
Cp3 = -0.40599 + 6.6616*10^-3 *T[z] - 4.5318*10^-6 *T[z]*T[z] + 12.255*10^-10 *(T[z])^3;
Cp4 = -0.27127 + 5.9142*10^-3 *T[z] - 3.8631*10^-6 *T[z]*T[z] + 9.54*10^-10 *(T[z])^3;
Cp5 = 13.57 + 4.637*10^-3 *T[z] - 6.905*10^-6 *T[z]*T[z] + 38.23*10^-10 *(T[z])^3;
Cp6 = 1.7911 + 0.1069*10^-3 *T[z] + 0.58611*10^-6 *T[z]*T[z] - 1.998*10^-10 *(T[z])^3;

L = 10;
Di = Dr/100;
Ac = π/4 *(Di)^2;
dp = 5.5/1000; (**m**)
μ = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^-4; (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;
ρb = 1422;
ϵ = 0.4312; (**void fraction of bed**)
ρg = (10^5 *10^-3)/(R*T[z]) *(PEB*106.168 + PST*104.15 + PBZ*78.114 +
     PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);
r214 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
     X2BZ'[z] == (rc2 + rt2 * ϵ/ρb)* (Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3 * ϵ/ρb)* (Ac*ρb)/FEB0,
     X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
     P'[z] == -(1 - ϵ)/ϵ^3 *(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) *10^-5 * (Ac*ρb)/FEB0,
     T'[z] == (Ac*ρb)/FEB0 *(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
        (FEB0*(-ΔH1*(rc1 + rt1 * ϵ/ρb) - ΔH2*(rc2 + rt2 * ϵ/ρb) - ΔH3*(rc3 + rt3 * ϵ/ρb) - ΔH4*rc4)),
     X2EB[2] == X1EB[2] /. r114, X2BZ[2] == X1BZ[2] /. r114, X2TO[2] == X1TO[2] /. r114,
     X2H2[2] == X1H2[2] /. r114, P[2] == PT[2] /. r114, T[2] == 870},
   {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
     C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];

r215 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)* ϵ/ρb)* (Ac*ρb)/FEB0,
```

$$\mathrm{X2BZ'[z]} == \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},\ \mathrm{X2TO'[z]} == \left(\mathrm{rc3} + \mathrm{rc4} + \mathrm{rt3} * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{X2H2'[z]} == \left(\mathrm{rc1} - \mathrm{rc3} - 2\ \mathrm{rc4} + (\mathrm{rt1} - \mathrm{rt3}) * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{P'[z]} == -\frac{1-\epsilon}{\epsilon^3} * \left(1.28 + \frac{458 * (1-\epsilon)}{\frac{\rho\mathrm{g} * \mathrm{dp} * \mathrm{u}}{\mu}}\right) * 7.7160 * 10^{-8} * \frac{\mathrm{u} * \mathrm{G} * \mathrm{FEB0}}{\rho\mathrm{b} * \mathrm{dp} * \mathrm{Ac}} * 10^{-5} * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{T'[z]} == \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}} * (1/(106.168 * \mathrm{FEB0} * (1 - \mathrm{X2EB[z]}) * \mathrm{Cp1} +$$
$$104.15 * (\mathrm{FST0} + \mathrm{FEB0} * (\mathrm{X2EB[z]} - \mathrm{X2BZ[z]} - \mathrm{X2TO[z]})) * \mathrm{Cp2} +$$
$$78.114 * (\mathrm{FBZ0} + \mathrm{FEB0} * \mathrm{X2BZ[z]}) * \mathrm{Cp3} + 92.141 * (\mathrm{FTO0} + \mathrm{FEB0} * \mathrm{X2TO[z]}) * \mathrm{Cp4} +$$
$$2.010 * (\mathrm{FH20} + \mathrm{FEB0} * \mathrm{X2H2[z]}) * \mathrm{Cp5} + 18.020 * \mathrm{FH2O0} * \mathrm{Cp6})) *$$
$$\left(\mathrm{FEB0} * \left(-\Delta\mathrm{H1} * \left(\mathrm{rc1} + \mathrm{rt1} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H2} * \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H3} * \left(\mathrm{rc3} + \mathrm{rt3} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H4} * \mathrm{rc4}\right)\right),$$

X2EB[2] == X1EB[2] /. r115, X2BZ[2] == X1BZ[2] /. r115, X2TO[2] == X1TO[2] /. r115,
X2H2[2] == X1H2[2] /. r115, P[2] == PT[2] /. r115, T[2] == 870},
{P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];

$$\mathrm{r216} = \mathrm{Quiet} @ \mathrm{NDSolve}\left[\left\{\mathrm{X2EB'[z]} == \left(\mathrm{rc1} + \mathrm{rc2} + \mathrm{rc3} + (\mathrm{rt1} + \mathrm{rt2} + \mathrm{rt3}) * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},\right.\right.$$

$$\mathrm{X2BZ'[z]} == \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},\ \mathrm{X2TO'[z]} == \left(\mathrm{rc3} + \mathrm{rc4} + \mathrm{rt3} * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{X2H2'[z]} == \left(\mathrm{rc1} - \mathrm{rc3} - 2\ \mathrm{rc4} + (\mathrm{rt1} - \mathrm{rt3}) * \frac{\epsilon}{\rho\mathrm{b}}\right) * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

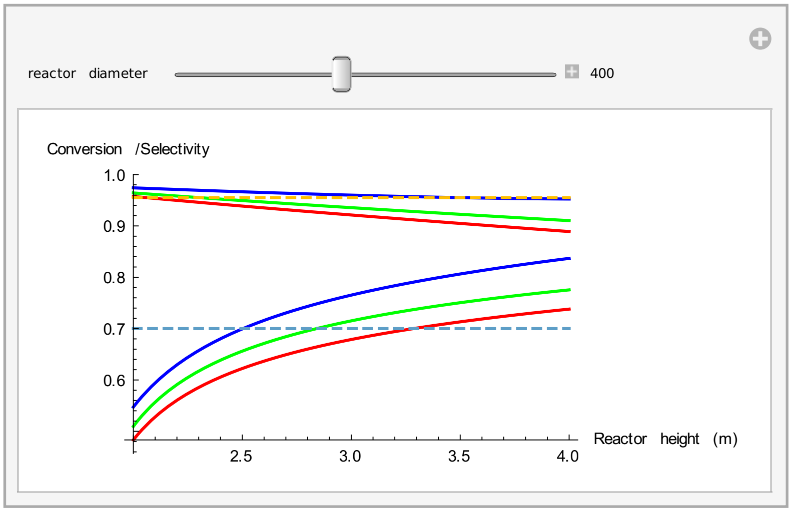
$$\mathrm{P'[z]} == -\frac{1-\epsilon}{\epsilon^3} * \left(1.28 + \frac{458 * (1-\epsilon)}{\frac{\rho\mathrm{g} * \mathrm{dp} * \mathrm{u}}{\mu}}\right) * 7.7160 * 10^{-8} * \frac{\mathrm{u} * \mathrm{G} * \mathrm{FEB0}}{\rho\mathrm{b} * \mathrm{dp} * \mathrm{Ac}} * 10^{-5} * \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}},$$

$$\mathrm{T'[z]} == \frac{\mathrm{Ac} * \rho\mathrm{b}}{\mathrm{FEB0}} * (1/(106.168 * \mathrm{FEB0} * (1 - \mathrm{X2EB[z]}) * \mathrm{Cp1} +$$
$$104.15 * (\mathrm{FST0} + \mathrm{FEB0} * (\mathrm{X2EB[z]} - \mathrm{X2BZ[z]} - \mathrm{X2TO[z]})) * \mathrm{Cp2} +$$
$$78.114 * (\mathrm{FBZ0} + \mathrm{FEB0} * \mathrm{X2BZ[z]}) * \mathrm{Cp3} + 92.141 * (\mathrm{FTO0} + \mathrm{FEB0} * \mathrm{X2TO[z]}) * \mathrm{Cp4} +$$
$$2.010 * (\mathrm{FH20} + \mathrm{FEB0} * \mathrm{X2H2[z]}) * \mathrm{Cp5} + 18.020 * \mathrm{FH2O0} * \mathrm{Cp6})) *$$
$$\left(\mathrm{FEB0} * \left(-\Delta\mathrm{H1} * \left(\mathrm{rc1} + \mathrm{rt1} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H2} * \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H3} * \left(\mathrm{rc3} + \mathrm{rt3} * \frac{\epsilon}{\rho\mathrm{b}}\right) - \Delta\mathrm{H4} * \mathrm{rc4}\right)\right),$$

X2EB[2] == X1EB[2] /. r116, X2BZ[2] == X1BZ[2] /. r116, X2TO[2] == X1TO[2] /. r116,
X2H2[2] == X1H2[2] /. r116, P[2] == PT[2] /. r116, T[2] == 870},
{P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];

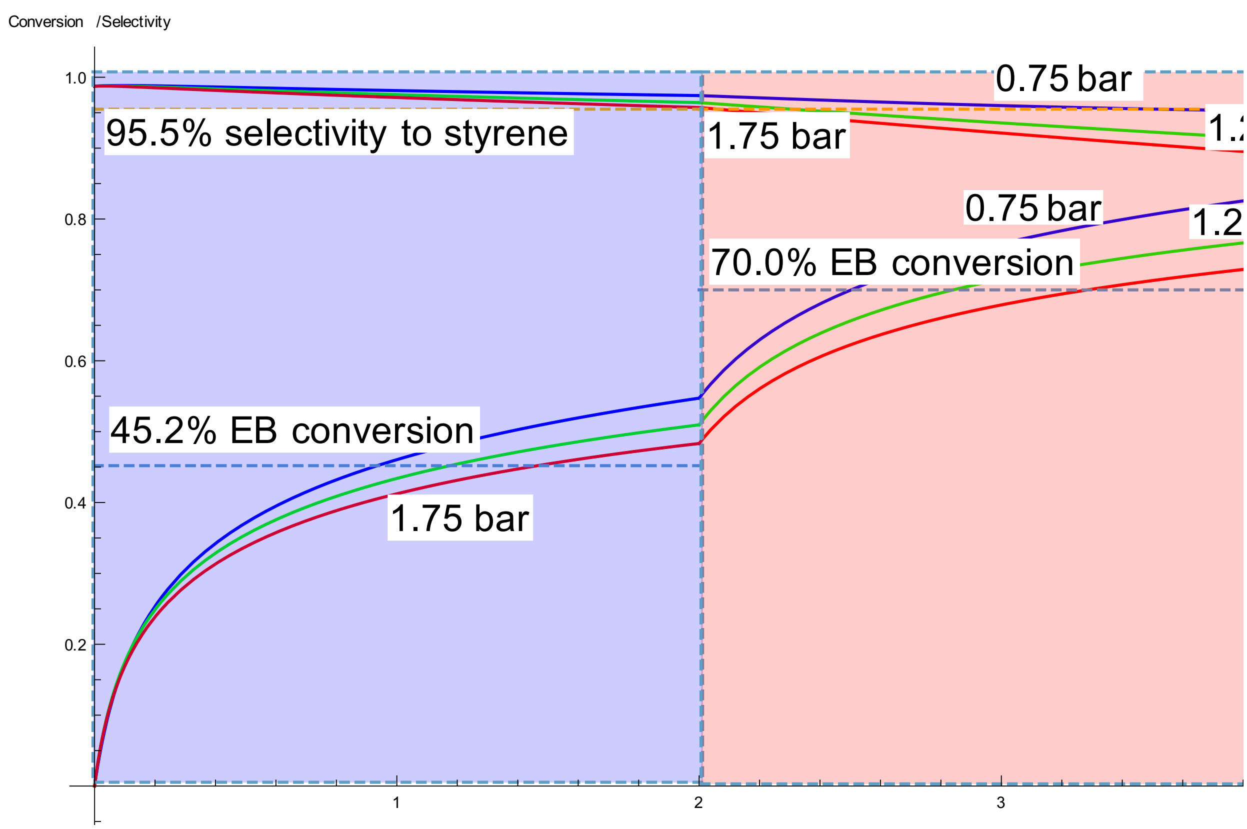
Figure18 = Plot[{{X2EB[z] /. r214, X2EB[z] /. r215, X2EB[z] /. r216, S2ST /. r214, S2ST /. r215, S2ST /. r216,
0.7, 0.955}}, {z, 2, 4}, PlotStyle → {Blue, Green, Red, Blue, Green, Red, Dashed, Dashed},
PlotRange → All, AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}], Column[{

```
    Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
  }, Left]
```



The effect of inlet pressure on EB conversion and selectivity to styrene for two reactors:

```
Legended [Show[Figure17 , Figure18 ],
  SwatchLegend [{Blue , Red}, {"1st reactor ", "2nd reactor "}]]
```



Optimization of reactor dimensions

The optimal height of the first reactor:

```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
   AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
   FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
   PH2O, PMTH, C1EB, C1ST, C1BZ, C1ETH, C1TO, C1H2, C1MTH, C1H2O, S1ST, S1BZ, S1TO,
   S1H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R, ϵ, ρg},

  (*Construct the models for the thermal reactions*)
  At1 = 2.2215*10^16; (**kmol/m3hbar**)
  At2 = 2.4217*10^20;
  At3 = 3.8224*10^17;
  Et1 = 272.23; (**kJ/mol**)
  Et2 = 352.79;
  Et3 = 313.06;
  R = 8.314;
  kt1 = At1*Exp[(-Et1*10^3)/(R*T[z])]; (**kmol/m3hbar**)
  kt2 = At2*Exp[(-Et2*10^3)/(R*T[z])];
  kt3 = At3*Exp[(-Et3*10^3)/(R*T[z])];


  (*Thermal reaction rates of three reactions*)
  rt1 = kt1*(PEB - (PST*PH2)/Keq); (**kmol/m3h**)
  rt2 = kt2*PEB;
  rt3 = kt3*PEB;


  (*Construct the models for the catalytic reactions*)
  A1 = 4.594*10^9; (**kmol/kg-cath**)
  A2 = 1.060*10^15;
  A3 = 1.246*10^26;
  A4 = 8.024*10^10;
```

$$E1 = 175.38;\ (**kJ/mol**)$$

$$E2 = 296.29;$$

$$E3 = 474.76;$$

$$E4 = 213.78;$$

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right];\ (**kmol/kg-cath**)$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

(*Catalyticreaction rates of four reactions*)

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};\ (**kmol/kg-cath**)$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

(*Construct the models for the thermodynamic equilibriums*)

$$AEB = 1.014 * 10^{-5};\ (**1/bar**)$$

$$AST = 2.678 * 10^{-5};$$

$$AH2 = 4.519 * 10^{-7};$$

$$\Delta HaEB = -102.22;\ (**kJ/mol**)$$

$$\Delta HaST = -104.56;$$

$$\Delta HaH2 = -117.95;$$

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right];\ (**1/bar**)$$

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$\text{Keq} = \text{Exp}\left[\frac{-(122\,725.157 - 126.267*\text{T[z]} - 0.002194*\text{T[z]}*\text{T[z]})}{\text{R}*\text{T[z]}}\right];\ (**1/\text{bar}**)$$

(*(**The initial molar flowrates of components**)*)

FEB0 = 49.7976*3600/1000; (*Unit:kmol/h*)

FST0 = 0.00332919*3.6;

FBZ0 = 1.464*3.6;

FTO0 = 0.0482245*3.6;

FH20 = 0;

FCH40 = 0;

FC2H40 = 0;

FH2O0 = 1080*3.6;

FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

(*Partial pressure of components*)

$$\text{PEB} = \text{PT[z]}*\frac{\frac{\text{FEB0}}{\text{FT0}}(1 - (\text{X1EB[z]} - \text{X1BZ[z]} - \text{X1TO[z]}) - \text{X1BZ[z]} - \text{X1TO[z]})}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

(**1/bar**)

$$\text{PST} = \text{PT[z]}*\frac{\frac{\text{FST0}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1EB[z]} - \text{X1BZ[z]} - \text{X1TO[z]})}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

$$\text{PBZ} = \text{PT[z]}*\frac{\frac{\text{FBZ0}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}}*\text{X1BZ[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

$$\text{PH2} = \text{PT[z]}*\frac{\frac{\text{FH20}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}}*\text{X1H2[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

$$\text{PETH} = \text{PT[z]}*\frac{\frac{\text{FC2H40}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}}*\text{X1BZ[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

$$\text{PTO} = \text{PT[z]}*\frac{\frac{\text{FTO0}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}}*\text{X1TO[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

$$\text{PH2O} = \text{PT[z]}*\frac{\frac{\text{FH2O0}}{\text{FT0}}}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

$$\text{PMTH} = \text{PT[z]}*\frac{\frac{\text{FCH40}}{\text{FT0}} + \frac{\text{FEB0}}{\text{FT0}}*\text{X1EB[z]}}{1 + \frac{\text{FEB0}}{\text{FT0}}*(\text{X1TO[z]} + \text{X1BZ[z]} + \text{X1H2[z]})};$$

(∗ Concentration of components∗)

$$C1EB = \frac{PEB*10^5}{R*T[z]};$$

$$C1ST = \frac{PST*10^5}{R*T[z]};$$

$$C1BZ = \frac{PBZ*10^5}{R*T[z]};$$

$$C1H2 = \frac{PH2*10^5}{R*T[z]};$$

$$C1ETH = \frac{PETH*10^5}{R*T[z]};$$

$$C1TO = \frac{PTO*10^5}{R*T[z]};$$

$$C1H2O = \frac{PH2O*10^5}{R*T[z]};$$

$$C1MTH = \frac{PMTH*10^5}{R*T[z]};$$

(∗selectivity of reaction products∗)

$$S1ST = \frac{X1EB[z] - X1BZ[z] - X1TO[z]}{X1EB[z]};$$

$$S1BZ = \frac{X1BZ[z]}{X1EB[z]};$$

$$S1TO = \frac{X1TO[z]}{X1EB[z]};$$

$$S1H2 = \frac{X1H2[z]}{X1EB[z]};$$

(∗Heat of reactions∗)

$$\Delta H1 = 117\,690 + 41.99*(T[z] - 298.15) + \frac{-8.2026*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{6.499*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(∗∗kJ/kmol∗∗)

$$\Delta H2 = 105\,510 + 12.986*(T[z] - 298.15) + \frac{-7.67*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) +$$

$$\frac{9.592*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-4.125*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H3=-54\,680+10.86*(T[z]-298.15)+\frac{-15.1844*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{23.04*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-9.9955*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

$$\Delta H4=-172\,370+(-31.13)*(T[z]-298.15)+\frac{-6.9818*10^{-2}}{2}*\left((T[z])^2-298.15^2\right)+$$
$$\frac{16.54*10^{-5}}{3}\left((T[z])^3-298.15^3\right)+\frac{-7.685*10^{-8}}{4}\left((T[z])^4-298.15^4\right);$$

(*Heat capacities of components*)

$Cp1=-0.43426+6.0671*10^{-3}*T[z]-3.8625*10^{-6}*T[z]*T[z]+9.1282*10^{-10}*(T[z])^3;$ (**kJ/kgK**)

$Cp2=-0.26436+5.564*10^{-3}*T[z]-3.0018*10^{-6}*T[z]*T[z]+5.3317*10^{-10}*(T[z])^3;$

$Cp3=-0.40599+6.6616*10^{-3}*T[z]-4.5318*10^{-6}*T[z]*T[z]+12.255*10^{-10}*(T[z])^3;$

$Cp4=-0.27127+5.9142*10^{-3}*T[z]-3.8631*10^{-6}*T[z]*T[z]+9.54*10^{-10}*(T[z])^3;$

$Cp5=13.57+4.637*10^{-3}*T[z]-6.905*10^{-6}*T[z]*T[z]+38.23*10^{-10}*(T[z])^3;$

$Cp6=1.7911+0.1069*10^{-3}*T[z]+0.58611*10^{-6}*T[z]*T[z]-1.998*10^{-10}*(T[z])^3;$

(*Physical properties of the catalyst*)

dp = 5.5/1000; (*m*)

$\rho b = 1422;$

$\epsilon = 0.4312;$

(*Dimensions of the reactor*)

L = 10;

$$Di=\frac{Dr}{100};$$

$$Ac=\frac{\pi}{4}*(Di)^2;$$

(*The important properties of the gas mixture*)

$\mu=(-10.035+0.25191*T[z]-0.000037932*T[z]*T[z])*3.6*10^{-4};$ (**kg/ms**)

u = 22.003/Ac;

G = 89 520.109/Ac;

$$\rho g=\frac{10^5*10^{-3}}{R*T[z]}*(PEB*106.168+PST*104.15+PBZ*78.114+$$
$$PTO*92.141+PH2O*18.020+PH2*2.010+PMTH*16.043+PETH*28.054);$$

$$
\begin{aligned}
&\text{r117} = \text{Quiet}@\text{NDSolve}\Big[\Big\{\text{X1EB}'[z] == \left(\text{rc1} + \text{rc2} + \text{rc3} + (\text{rt1} + \text{rt2} + \text{rt3}) * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{X1BZ}'[z] == \left(\text{rc2} + \text{rt2} * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\ \text{X1TO}'[z] == \left(\text{rc3} + \text{rc4} + \text{rt3} * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{X1H2}'[z] == \left(\text{rc1} - \text{rc3} - 2\,\text{rc4} + (\text{rt1} - \text{rt3}) * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{PT}'[z] == -\frac{1-\epsilon}{\epsilon^3} * \left(1.28 + \frac{458 * (1-\epsilon)}{\frac{\rho g * dp * u}{\mu}}\right) * 7.7160 * 10^{-8} * \frac{u * G * \text{FEB0}}{\rho b * dp * \text{Ac}} * 10^{-5} * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{T}'[z] == \frac{\text{Ac} * \rho b}{\text{FEB0}} * (1/(106.168 * \text{FEB0} * (1 - \text{X1EB}[z]) * \text{Cp1} +\\
&\qquad 104.15 * (\text{FST0} + \text{FEB0} * (\text{X1EB}[z] - \text{X1BZ}[z] - \text{X1TO}[z])) * \text{Cp2} +\\
&\qquad 78.114 * (\text{FBZ0} + \text{FEB0} * \text{X1BZ}[z]) * \text{Cp3} + 92.141 * (\text{FTO0} + \text{FEB0} * \text{X1TO}[z]) * \text{Cp4} +\\
&\qquad 2.010 * (\text{FH20} + \text{FEB0} * \text{X1H2}[z]) * \text{Cp5} + 18.020 * \text{FH2O0} * \text{Cp6})) *\\
&\quad\ \left(\text{FEB0} * \left(-\Delta\text{H1} * \left(\text{rc1} + \text{rt1} * \frac{\epsilon}{\rho b}\right) - \Delta\text{H2} * \left(\text{rc2} + \text{rt2} * \frac{\epsilon}{\rho b}\right) - \Delta\text{H3} * \left(\text{rc3} + \text{rt3} * \frac{\epsilon}{\rho b}\right) - \Delta\text{H4} * \text{rc4}\right)\right),\\
&\quad \text{X1EB}[0] == 0,\ \text{X1BZ}[0] == 0,\ \text{X1TO}[0] == 0,\ \text{X1H2}[0] == 0,\ \text{PT}[0] == 1.25,\ \text{T}[0] == 870\Big\},\\
&\ \{\text{PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,}\\
&\quad \text{C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}\},\ \{z, 0, 2\}\Big];
\end{aligned}
$$

$$
\begin{aligned}
&\text{r118} = \text{Quiet}@\text{NDSolve}\Big[\Big\{\text{X1EB}'[z] == \left(\text{rc1} + \text{rc2} + \text{rc3} + (\text{rt1} + \text{rt2} + \text{rt3}) * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{X1BZ}'[z] == \left(\text{rc2} + \text{rt2} * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\ \text{X1TO}'[z] == \left(\text{rc3} + \text{rc4} + \text{rt3} * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{X1H2}'[z] == \left(\text{rc1} - \text{rc3} - 2\,\text{rc4} + (\text{rt1} - \text{rt3}) * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{PT}'[z] == -\frac{1-\epsilon}{\epsilon^3} * \left(1.28 + \frac{458 * (1-\epsilon)}{\frac{\rho g * dp * u}{\mu}}\right) * 7.7160 * 10^{-8} * \frac{u * G * \text{FEB0}}{\rho b * dp * \text{Ac}} * 10^{-5} * \frac{\text{Ac} * \rho b}{\text{FEB0}},\\
&\quad \text{T}'[z] == \frac{\text{Ac} * \rho b}{\text{FEB0}} * (1/(106.168 * \text{FEB0} * (1 - \text{X1EB}[z]) * \text{Cp1} +\\
&\qquad 104.15 * (\text{FST0} + \text{FEB0} * (\text{X1EB}[z] - \text{X1BZ}[z] - \text{X1TO}[z])) * \text{Cp2} +\\
&\qquad 78.114 * (\text{FBZ0} + \text{FEB0} * \text{X1BZ}[z]) * \text{Cp3} + 92.141 * (\text{FTO0} + \text{FEB0} * \text{X1TO}[z]) * \text{Cp4} +\\
&\qquad 2.010 * (\text{FH20} + \text{FEB0} * \text{X1H2}[z]) * \text{Cp5} + 18.020 * \text{FH2O0} * \text{Cp6})) *\\
&\quad\ \left(\text{FEB0} * \left(-\Delta\text{H1} * \left(\text{rc1} + \text{rt1} * \frac{\epsilon}{\rho b}\right) - \Delta\text{H2} * \left(\text{rc2} + \text{rt2} * \frac{\epsilon}{\rho b}\right) - \Delta\text{H3} * \left(\text{rc3} + \text{rt3} * \frac{\epsilon}{\rho b}\right) - \Delta\text{H4} * \text{rc4}\right)\right),\\
&\quad \text{X1EB}[0] == 0,\ \text{X1BZ}[0] == 0,\ \text{X1TO}[0] == 0,\ \text{X1H2}[0] == 0,\ \text{PT}[0] == 1.25,\ \text{T}[0] == 870\Big\},\\
&\ \{\text{PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,}\\
&\quad \text{C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}\},\ \{z, 0, 6\}\Big];
\end{aligned}
$$

$$
\text{r119} = \text{Quiet}@\text{NDSolve}\Big[\Big\{\text{X1EB}'[z] == \left(\text{rc1} + \text{rc2} + \text{rc3} + (\text{rt1} + \text{rt2} + \text{rt3}) * \frac{\epsilon}{\rho b}\right) * \frac{\text{Ac} * \rho b}{\text{FEB0}},
$$

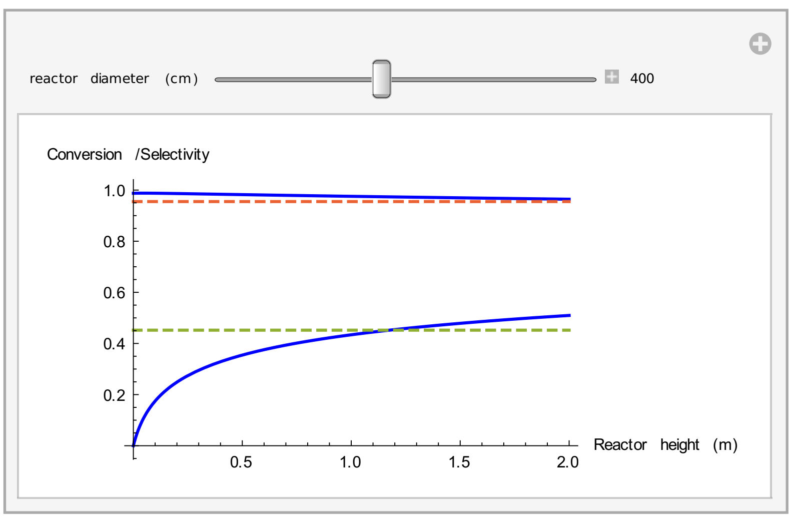
$$\mathrm{X1BZ}'[z] == \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho b}\right) * \frac{Ac * \rho b}{\mathrm{FEB0}},\ \mathrm{X1TO}'[z] == \left(\mathrm{rc3} + \mathrm{rc4} + \mathrm{rt3} * \frac{\epsilon}{\rho b}\right) * \frac{Ac * \rho b}{\mathrm{FEB0}},$$

$$\mathrm{X1H2}'[z] == \left(\mathrm{rc1} - \mathrm{rc3} - 2\,\mathrm{rc4} + (\mathrm{rt1} - \mathrm{rt3}) * \frac{\epsilon}{\rho b}\right) * \frac{Ac * \rho b}{\mathrm{FEB0}},$$

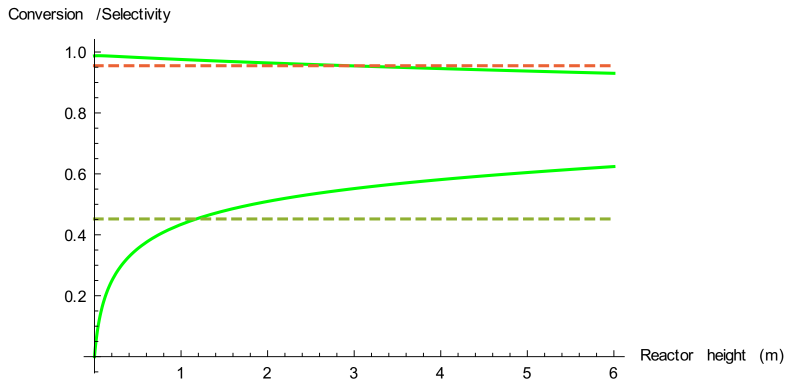
$$\mathrm{PT}'[z] == -\frac{1-\epsilon}{\epsilon^3} * \left(1.28 + \frac{458 * (1-\epsilon)}{\frac{\rho g * dp * u}{\mu}}\right) * 7.7160 * 10^{-8} * \frac{u * G * \mathrm{FEB0}}{\rho b * dp * Ac} * 10^{-5} * \frac{Ac * \rho b}{\mathrm{FEB0}},$$

$$T'[z] == \frac{Ac * \rho b}{\mathrm{FEB0}} * (1/(106.168 * \mathrm{FEB0} * (1 - \mathrm{X1EB}[z]) * \mathrm{Cp1} +$$
$$104.15 * (\mathrm{FST0} + \mathrm{FEB0} * (\mathrm{X1EB}[z] - \mathrm{X1BZ}[z] - \mathrm{X1TO}[z])) * \mathrm{Cp2} +$$
$$78.114 * (\mathrm{FBZ0} + \mathrm{FEB0} * \mathrm{X1BZ}[z]) * \mathrm{Cp3} + 92.141 * (\mathrm{FTO0} + \mathrm{FEB0} * \mathrm{X1TO}[z]) * \mathrm{Cp4} +$$
$$2.010 * (\mathrm{FH20} + \mathrm{FEB0} * \mathrm{X1H2}[z]) * \mathrm{Cp5} + 18.020 * \mathrm{FH2O0} * \mathrm{Cp6})) *$$
$$\left(\mathrm{FEB0} * \left(-\Delta H1 * \left(\mathrm{rc1} + \mathrm{rt1} * \frac{\epsilon}{\rho b}\right) - \Delta H2 * \left(\mathrm{rc2} + \mathrm{rt2} * \frac{\epsilon}{\rho b}\right) - \Delta H3 * \left(\mathrm{rc3} + \mathrm{rt3} * \frac{\epsilon}{\rho b}\right) - \Delta H4 * \mathrm{rc4}\right)\right),$$

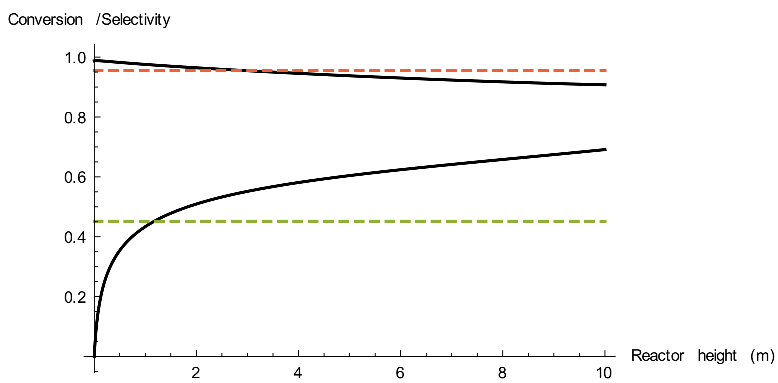
```
    X1EB[0] == 0, X1BZ[0] == 0, X1TO[0] == 0, X1H2[0] == 0, PT[0] == 1.25, T[0] == 870},
   {PT, T, X1EB, X1BZ, X1TO, X1H2, C1EB, C1ST, C1BZ, C1TO, C1H2,
    C1ETH, C1H2O, C1MTH, S1ST, S1BZ, S1TO}, {z, 0, 10}];
Figure19 = Plot[{X1EB[z] /. r117, S1ST /. r117, 0.452, 0.955}, {z, 0, 2},
   PlotStyle → {Blue , Blue , Dashed , Dashed }, PlotRange→ All,
   AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}], Column[{
  Control[{{Dr, 400, "reactor diameter (cm) "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



```
Figure20 = Plot[{X1EB[z] /. r118, {(X1EB[z] - X1BZ[z] - X1TO[z])/X1EB[z]} /. r118, 0.452, 0.955},
  {z, 0, 6}, PlotStyle → {Green , Green , Dashed , Dashed }, PlotRange→ All,
  AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}]
```




```
Figure21 = Plot[{X1EB[z] /. r119, {(X1EB[z] - X1BZ[z] - X1TO[z])/X1EB[z]} /. r119, 0.452, 0.955},
  {z, 0, 10}, PlotStyle → {Black , Black , Dashed , Dashed }, PlotRange→ All,
  AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}]
```




```
Manipulate[
 Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
    AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
    FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, FT0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
    PH2O, PMTH, C2EB, C2ST, C2BZ, C2ETH, C2TO, C2H2, C2MTH, C2H2O, S2ST, S2BZ, S2TO,
    S2H2, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, ϵ, ρg, R},

   At1 = 2.2215*10^16; (**kmol/m3hbar**)
   At2 = 2.4217*10^20;
   At3 = 3.8224*10^17;
   Et1 = 272.23; (**kJ/mol**)
   Et2 = 352.79;
   Et3 = 313.06;
   R = 8.314;
```

$$kt1 = At1 * Exp\left[\frac{-Et1 * 10^3}{R * T[z]}\right]; \text{ (**kmol/m3hbar**)}$$

$$kt2 = At2 * Exp\left[\frac{-Et2 * 10^3}{R * T[z]}\right];$$

$$kt3 = At3 * Exp\left[\frac{-Et3 * 10^3}{R * T[z]}\right];$$

$A1 = 4.594 * 10^9$; (**kmol/kg−cath**)
$A2 = 1.060 * 10^{15}$;
$A3 = 1.246 * 10^{26}$;
$A4 = 8.024 * 10^{10}$;
E1 = 175.38; (**kJ/mol**)
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;

$$k1 = A1 * Exp\left[\frac{-E1 * 10^3}{R * T[z]}\right]; \text{ (**kmol/kg−cath**)}$$

$$k2 = A2 * Exp\left[\frac{-E2 * 10^3}{R * T[z]}\right];$$

$$k3 = A3 * Exp\left[\frac{-E3 * 10^3}{R * T[z]}\right];$$

$$k4 = A4 * Exp\left[\frac{-E4 * 10^3}{R * T[z]}\right];$$

$AEB = 1.014 * 10^{-5}$; (**1/bar**)
$AST = 2.678 * 10^{-5}$;
$AH2 = 4.519 * 10^{-7}$;
ΔHaEB = −102.22; (**kJ/mol**)
ΔHaST = −104.56;
ΔHaH2 = −117.95;

$$KEB = AEB * Exp\left[\frac{-\Delta HaEB * 10^3}{R * T[z]}\right]; \text{ (**1/bar**)}$$

$$KST = AST * Exp\left[\frac{-\Delta HaST * 10^3}{R * T[z]}\right];$$

$$KH2 = AH2 * Exp\left[\frac{-\Delta HaH2 * 10^3}{R * T[z]}\right];$$

$$Keq = Exp\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right]; \text{ (**1/bar**)}$$

$$rt1 = kt1 * \left(PEB - \frac{PST * PH2}{Keq}\right); \text{ (**kmol/m3h**)}$$

rt2 = kt2 * PEB;

$$rt3 = kt3 * PEB;$$

$$C2EB = \frac{PEB * 10^5}{R * T[z]};$$

$$C2ST = \frac{PST * 10^5}{R * T[z]};$$

$$C2BZ = \frac{PBZ * 10^5}{R * T[z]};$$

$$C2H2 = \frac{PH2 * 10^5}{R * T[z]};$$

$$C2ETH = \frac{PETH * 10^5}{R * T[z]};$$

$$C2TO = \frac{PTO * 10^5}{R * T[z]};$$

$$C2H2O = \frac{PH2O * 10^5}{R * T[z]};$$

$$C2MTH = \frac{PMTH * 10^5}{R * T[z]};$$

$$S2ST = \frac{X2EB[z] - X2BZ[z] - X2TO[z]}{X2EB[z]};$$

$$S2BZ = \frac{X2BZ[z]}{X2EB[z]};$$

$$S2TO = \frac{X2TO[z]}{X2EB[z]};$$

$$S2H2 = \frac{X2H2[z]}{X2EB[z]};$$

FEB0 = 49.7976*3600/1000; (* Unit:kmol/h*)
FST0 = 0.00332919*3.6;
FBZ0 = 1.464*3.6;
FTO0 = 0.0482245*3.6;
FH20 = 0;
FCH40 = 0;
FC2H40 = 0;
FH2O0 = 3954.696;
FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0;

$$PEB = P[z] * \frac{\frac{FEB0}{FT0}(1 - (X2EB[z] - X2BZ[z] - X2TO[z]) - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

(**1/bar**)

$$PST = P[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (X2EB[z] - X2BZ[z] - X2TO[z])}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PBZ = P[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * X2BZ[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2 = P[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * X2H2[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PETH = P[z] * \frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0} * X2BZ[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PTO = P[z] * \frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0} * X2TO[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PH2O = P[z] * \frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$PMTH = P[z] * \frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0} * X2EB[z]}{1 + \frac{FEB0}{FT0} * (X2TO[z] + X2BZ[z] + X2H2[z])};$$

$$rc1 = \frac{k1 * KEB * \left(PEB - \frac{PST * PH2}{Keq}\right)}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2}; \text{ (**kmol/kg−cath**)}$$

$$rc2 = \frac{k2 * KEB * PEB}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc3 = \frac{k3 * KEB * PEB * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$rc4 = \frac{k4 * KST * PST * KH2 * PH2}{(1 + KEB * PEB + KH2 * PH2 + KST * PST)^2};$$

$$\Delta H1 = 117\,690 + 41.99 * (T[z] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[z] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86*(T[z] - 298.15) + \frac{-15.1844*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{23.04*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-9.9955*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13)*(T[z] - 298.15) + \frac{-6.9818*10^{-2}}{2}*\left((T[z])^2 - 298.15^2\right) + \frac{16.54*10^{-5}}{3}\left((T[z])^3 - 298.15^3\right) + \frac{-7.685*10^{-8}}{4}\left((T[z])^4 - 298.15^4\right);$$

$Cp1 = -0.43426 + 6.0671*10^{-3}*T[z] - 3.8625*10^{-6}*T[z]*T[z] + 9.1282*10^{-10}*(T[z])^3;$ (**kJ/kgK**)
$Cp2 = -0.26436 + 5.564*10^{-3}*T[z] - 3.0018*10^{-6}*T[z]*T[z] + 5.3317*10^{-10}*(T[z])^3;$
$Cp3 = -0.40599 + 6.6616*10^{-3}*T[z] - 4.5318*10^{-6}*T[z]*T[z] + 12.255*10^{-10}*(T[z])^3;$
$Cp4 = -0.27127 + 5.9142*10^{-3}*T[z] - 3.8631*10^{-6}*T[z]*T[z] + 9.54*10^{-10}*(T[z])^3;$
$Cp5 = 13.57 + 4.637*10^{-3}*T[z] - 6.905*10^{-6}*T[z]*T[z] + 38.23*10^{-10}*(T[z])^3;$
$Cp6 = 1.7911 + 0.1069*10^{-3}*T[z] + 0.58611*10^{-6}*T[z]*T[z] - 1.998*10^{-10}*(T[z])^3;$

L = 10;
$Di = \frac{Dr}{100};$
$Ac = \frac{\pi}{4}*(Di)^2;$
dp = 5.5/1000; (**m**)
$\mu = (-10.035 + 0.25191*T[z] - 0.000037932*T[z]*T[z])*3.6*10^{-4};$ (**kg/ms**)
u = 22.003/Ac;
G = 89 520.109/Ac;
$\rho b = 1422;$
$\epsilon = 0.4312;$ (**void fraction of bed**)

$$\rho g = \frac{10^5*10^{-3}}{R*T[z]}*(PEB*106.168 + PST*104.15 + PBZ*78.114 + PTO*92.141 + PH2O*18.020 + PH2*2.010 + PMTH*16.043 + PETH*28.054);$$

$$r217 = Quiet@NDSolve\left[\left\{X2EB'[z] == \left(rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},\right.\right.$$

$$X2BZ'[z] == \left(rc2 + rt2*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},\ X2TO'[z] == \left(rc3 + rc4 + rt3*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$

$$X2H2'[z] == \left(rc1 - rc3 - 2\,rc4 + (rt1 - rt3)*\frac{\epsilon}{\rho b}\right)*\frac{Ac*\rho b}{FEB0},$$

$$P'[z] == -\frac{1-\epsilon}{\epsilon^3}*\left(1.28 + \frac{458*(1-\epsilon)}{\frac{\rho g*dp*u}{\mu}}\right)*7.7160*10^{-8}*\frac{u*G*FEB0}{\rho b*dp*Ac}*10^{-5}*\frac{Ac*\rho b}{FEB0},$$

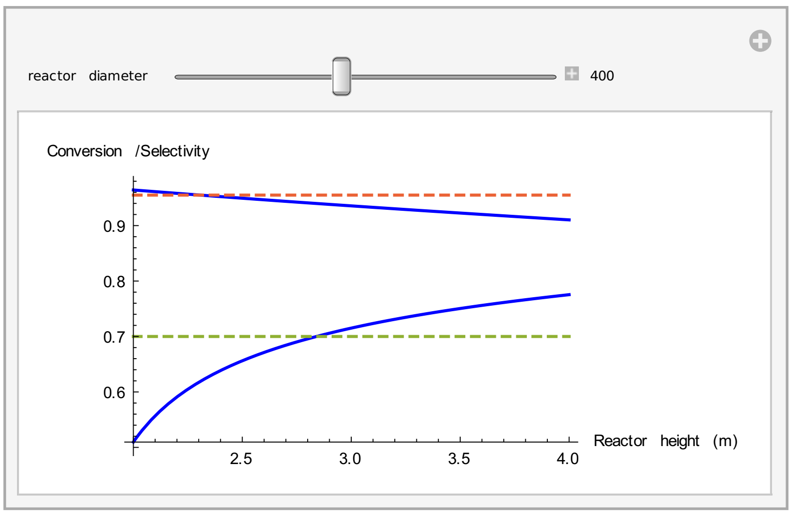
$$T'[z] == \frac{Ac*\rho b}{FEB0}*(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 + 104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 + 78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 + 2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*$$

```
      (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
    X2EB[2] == X1EB[2] /. r117, X2BZ[2] == X1BZ[2] /. r117, X2TO[2] == X1TO[2] /. r117,
    X2H2[2] == X1H2[2] /. r117, P[2] == PT[2] /. r117, T[2] == 870},
   {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
    C2H2, C2ETH, C2H2O, C2MTH}, {z, 2, 4}];

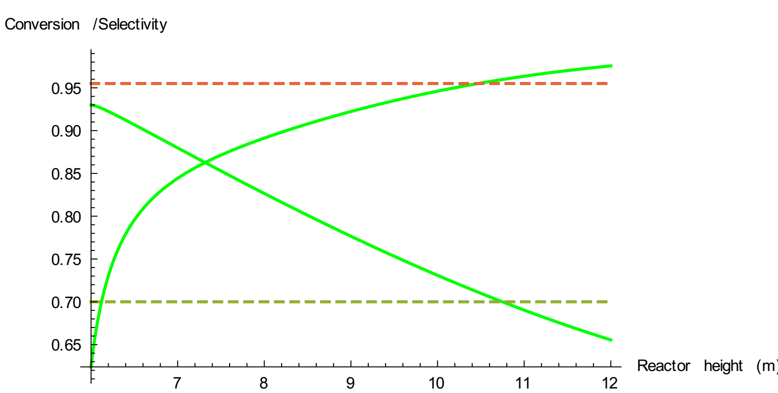
r218 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    X2BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
    X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    P'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
      (FEB0*(-ΔH1*(rc1 + rt1*ϵ/ρb) - ΔH2*(rc2 + rt2*ϵ/ρb) - ΔH3*(rc3 + rt3*ϵ/ρb) - ΔH4*rc4)),
    X2EB[6] == X1EB[6] /. r118, X2BZ[6] == X1BZ[6] /. r118, X2TO[6] == X1TO[6] /. r118,
    X2H2[6] == X1H2[6] /. r118, P[6] == PT[6] /. r118, T[6] == 870},
   {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB, C2ST, C2BZ, C2TO,
    C2H2, C2ETH, C2H2O, C2MTH}, {z, 6, 12}];

r219 = Quiet@NDSolve[{X2EB'[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    X2BZ'[z] == (rc2 + rt2*ϵ/ρb)*(Ac*ρb)/FEB0, X2TO'[z] == (rc3 + rc4 + rt3*ϵ/ρb)*(Ac*ρb)/FEB0,
    X2H2'[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*ϵ/ρb)*(Ac*ρb)/FEB0,
    P'[z] == -(1 - ϵ)/ϵ^3*(1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ))*7.7160*10^-8*(u*G*FEB0)/(ρb*dp*Ac)*10^-5*(Ac*ρb)/FEB0,
    T'[z] == (Ac*ρb)/FEB0*(1/(106.168*FEB0*(1 - X2EB[z])*Cp1 +
          104.15*(FST0 + FEB0*(X2EB[z] - X2BZ[z] - X2TO[z]))*Cp2 +
          78.114*(FBZ0 + FEB0*X2BZ[z])*Cp3 + 92.141*(FTO0 + FEB0*X2TO[z])*Cp4 +
          2.010*(FH20 + FEB0*X2H2[z])*Cp5 + 18.020*FH2O0*Cp6))*
```

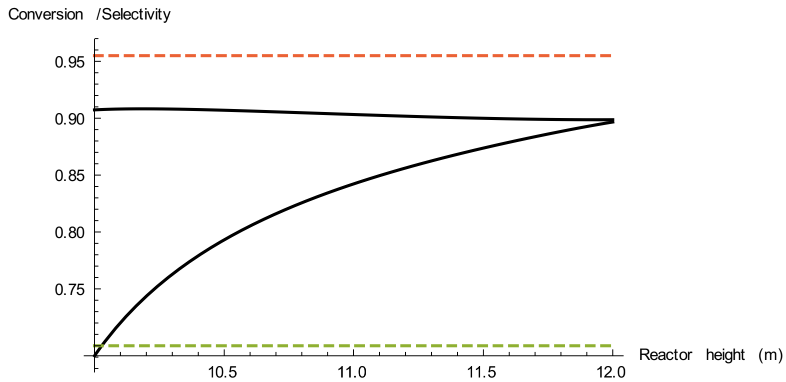
```
(FEB0 * (-ΔH1 * (rc1 + rt1 * ϵ/ρb) - ΔH2 * (rc2 + rt2 * ϵ/ρb) - ΔH3 * (rc3 + rt3 * ϵ/ρb) - ΔH4 * rc4)),
    X2EB[10] == X1EB[10] /. r119, X2BZ[10] == X1BZ[10] /. r119, X2TO[10] == X1TO[10] /. r119,
    X2H2[10] == X1H2[10] /. r119, P[10] == PT[10] /. r119, T[10] == 870},
  {P, T, X2EB, X2BZ, X2TO, X2H2, C2EB,  C2ST,  C2BZ,  C2TO,
    C2H2,  C2ETH,  C2H2O, C2MTH}, {z, 10, 20}];
Figure22 = Plot[{{X2EB[z] /. r217, S2ST /. r217, 0.7, 0.955}}, {z, 2, 4},
    PlotStyle → {Blue, Blue, Dashed, Dashed}, PlotRange → All,
    AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}], Column[{
  Control[{{Dr, 400, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]
```



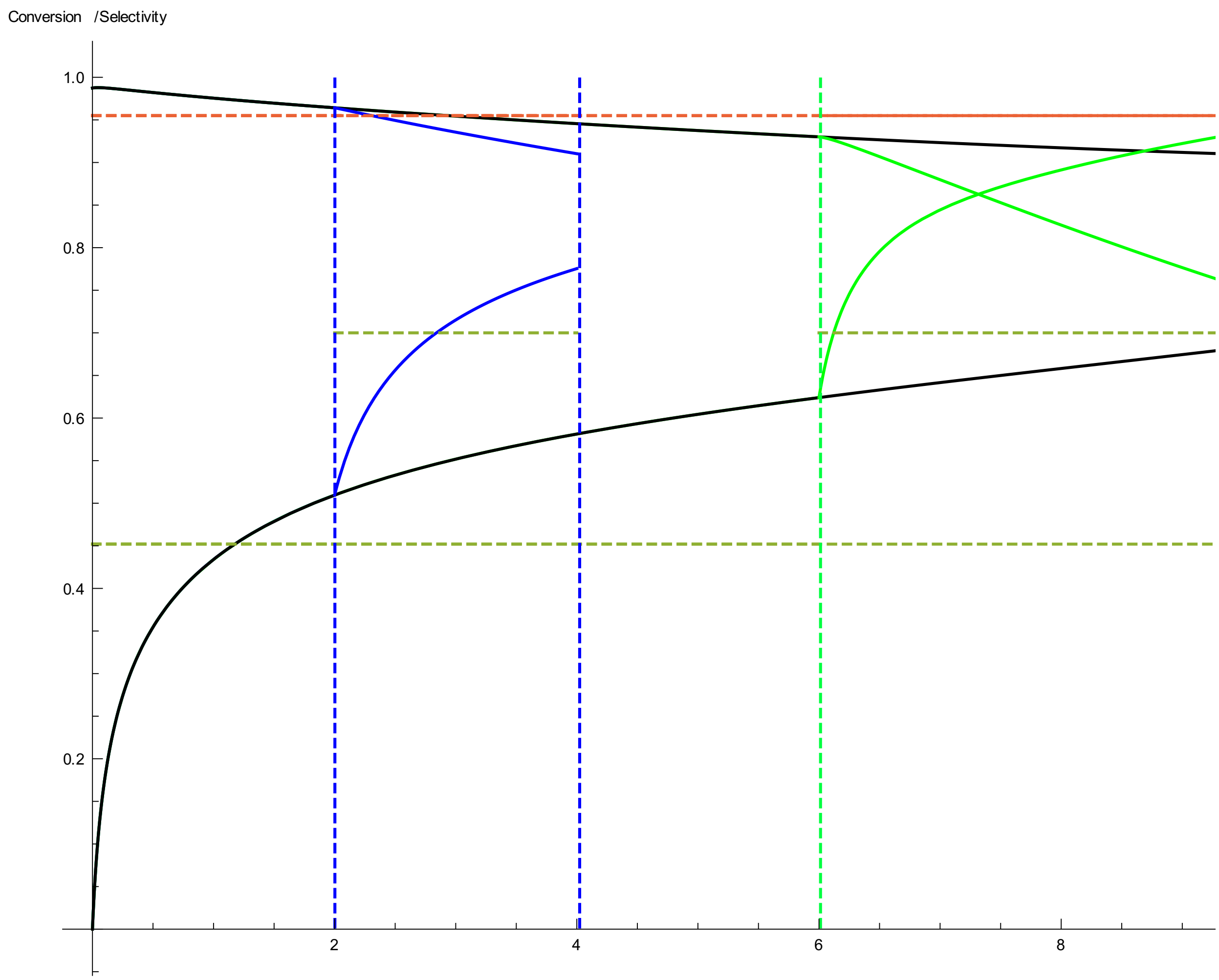

```
Figure23 = Plot[{X2EB[z] /. r218, {(X2EB[z] - X2BZ[z] - X2TO[z])/X2EB[z]} /. r218,  0.7, 0.955},
  {z, 6, 12}, PlotStyle → {Green , Green , Dashed , Dashed }, PlotRange → All,
  AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}]
```



```
Figure24 = Plot[{X2EB[z] /. r219, {(X2EB[z] - X2BZ[z] - X2TO[z])/X2EB[z]} /. r219, 0.7, 0.955},
  {z, 10, 12}, PlotStyle → {Black, Black, Dashed, Dashed}, PlotRange → All,
  AxesLabel → {"Reactor height (m)", "Conversion/Selectivity"}]
```




```
Legended[Show[Figure19, Figure20, Figure21, Figure22, Figure23, Figure24],
 SwatchLegend[{Blue, Green, Black},
  {"two 2m height reactors", "two 6m height reactors", "two 10m height reactors"}]]
```



Comparison with literature [1]

Resetting the inlet flow information and dimension of reactors according to the literature before running simulations

```
Manipulate[
  Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST,
     AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2, rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0,
```

```
FBZ0, FTO0, FH20, FCH40, FC2H40, FH2o0, PEB, PST, PBZ, PETH, PTO, PH2, PCH4, PC2H4,
PH2o, PMTH, ΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb},
At1 = 2.2215*10^16; (**kmol/m3hbar**)
At2 = 2.4217*10^20;
At3 = 3.8224*10^17;
Et1 = 272.23; (**kJ/mol**)
Et2 = 352.79;
Et3 = 313.06;
kt1 = At1*Exp[(-Et1*10^3)/(8.314*T[W])]; (**kmol/m3hbar**)
kt2 = At2*Exp[(-Et2*10^3)/(8.314*T[W])];
kt3 = At3*Exp[(-Et3*10^3)/(8.314*T[W])];
A1 = 4.594*10^9; (**kmol/kg-cath**)
A2 = 1.060*10^15;
A3 = 1.246*10^26;
A4 = 8.024*10^10;
E1 = 175.38; (**kJ/mol**)
E2 = 296.29;
E3 = 474.76;
E4 = 213.78;
k1 = A1*Exp[(-E1*10^3)/(8.314*T[W])]; (**kmol/kg-cath**)
k2 = A2*Exp[(-E2*10^3)/(8.314*T[W])];
k3 = A3*Exp[(-E3*10^3)/(8.314*T[W])];
k4 = A4*Exp[(-E4*10^3)/(8.314*T[W])];
AEB = 1.014*10^-5; (**1/bar**)
AST = 2.678*10^-5;
AH2 = 4.519*10^-7;
ΔHaEB = -102.22; (**kJ/mol**)
ΔHaST = -104.56;
ΔHaH2 = -117.95;
KEB = AEB*Exp[(-ΔHaEB*10^3)/(8.314*T[W])]; (**1/bar**)
KST = AST*Exp[(-ΔHaST*10^3)/(8.314*T[W])];
KH2 = AH2*Exp[(-ΔHaH2*10^3)/(8.314*T[W])];
```

$$Keq = Exp[(-(122\,725.157 - 126.267*T[W] - 0.002194*T[W]*T[W]))/(8.314*T[W])];$$

(**1/bar**)

$$rt1 = kt1*\left(PEB - \frac{PST*PH2}{Keq}\right); \text{(**kmol/m3h**)}$$

$$rt2 = kt2*PEB;$$

$$rt3 = kt3*PEB;$$

$$FEB0 = 707; \text{(**kmol/h**)}$$

$$FST0 = 7.104;$$

$$FBZ0 = 0.293;$$

$$FTO0 = 4.968;$$

$$FH20 = 0;$$

$$FCH40 = 0;$$

$$FC2H40 = 0;$$

$$FH2o0 = 7777;$$

$$FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2o0;$$

$$PEB = PT[W]*\left(\left(\frac{FEB0}{FT0}(1 - (XEB[W] - XBZ[W] - XTO[W]) - XBZ[W] - XTO[W])\right)\Big/ \left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

(**1/bar**)

$$PST = PT[W]*\left(\left(\frac{FST0}{FT0} + \frac{FEB0}{FT0}*(XEB[W] - XBZ[W] - XTO[W])\right)\Big/\left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

$$PBZ = PT[W]*\left(\left(\frac{FBZ0}{FT0} + \frac{FEB0}{FT0}*XBZ[W]\right)\Big/\left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

$$PH2 = PT[W]*\left(\left(\frac{FH20}{FT0} + \frac{FEB0}{FT0}*XH2[W]\right)\Big/\left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

$$PETH = PT[W]*\left(\left(\frac{FC2H40}{FT0} + \frac{FEB0}{FT0}*XBZ[W]\right)\Big/\left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

$$PTO = PT[W]*\left(\left(\frac{FTO0}{FT0} + \frac{FEB0}{FT0}*XTO[W]\right)\Big/\left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

$$PH2o = PT[W]*\left(\frac{FH2o0}{FT0}\Big/\left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

$$PMTH = PT[W]*\left(\left(\frac{FCH40}{FT0} + \frac{FEB0}{FT0}*XEB[W]\right)\Big/\left(1 + \frac{FEB0}{FT0}*(XTO[W] + XBZ[W] + XH2[W])\right)\right);$$

$$rc1 = \left(k1*KEB*\left(PEB - \frac{PST*PH2}{Keq}\right)\right)\Big/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

(**kmol/kg−cath**)

$$rc2 = (k2*KEB*PEB)/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

$$rc3 = (k3*KEB*PEB*KH2*PH2)/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

$$rc4 = (k4*KST*PST*KH2*PH2)/(1 + KEB*PEB + KH2*PH2 + KST*PST)^2;$$

$$(**\frac{\epsilon_B}{\rho_B}=0.000303**)$$

$$\Delta H1 = 117\,690 + 41.99 * (T[W] - 298.15) + \frac{-8.2026 * 10^{-2}}{2} * \left((T[W])^2 - 298.15^2\right) + \frac{6.499 * 10^{-5}}{3}\left((T[W])^3 - 298.15^3\right) + \frac{-2.311 * 10^{-8}}{4}\left((T[W])^4 - 298.15^4\right);$$

(**kJ/kmol**)

$$\Delta H2 = 105\,510 + 12.986 * (T[W] - 298.15) + \frac{-7.67 * 10^{-2}}{2} * \left((T[W])^2 - 298.15^2\right) + \frac{9.592 * 10^{-5}}{3}\left((T[W])^3 - 298.15^3\right) + \frac{-4.125 * 10^{-8}}{4}\left((T[W])^4 - 298.15^4\right);$$

$$\Delta H3 = -54\,680 + 10.86 * (T[W] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[W])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3}\left((T[W])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4}\left((T[W])^4 - 298.15^4\right);$$

$$\Delta H4 = -172\,370 + (-31.13) * (T[W] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[W])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3}\left((T[W])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4}\left((T[W])^4 - 298.15^4\right);$$

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[W] - 3.8625 * 10^{-6} * T[W] * T[W] + 9.1282 * 10^{-10} * (T[W])^3;$ (**kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[W] - 3.0018 * 10^{-6} * T[W] * T[W] + 5.3317 * 10^{-10} * (T[W])^3;$

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[W] - 4.5318 * 10^{-6} * T[W] * T[W] + 12.255 * 10^{-10} * (T[W])^3;$

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[W] - 3.8631 * 10^{-6} * T[W] * T[W] + 9.54 * 10^{-10} * (T[W])^3;$

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[W] - 6.905 * 10^{-6} * T[W] * T[W] + 38.23 * 10^{-10} * (T[W])^3;$

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[W] + 0.58611 * 10^{-6} * T[W] * T[W] - 1.998 * 10^{-10} * (T[W])^3;$

$L = 219.19;$

$$Di = \frac{Dr}{100};$$

$$Ac = \frac{\pi}{4} * (Di)^2;$$

$dp = 5.5/1000;$ (**m**)

$\mu = (-10.035 + 0.25191 * T[W] - 0.000037932 * T[W] * T[W]) * 3.6 * 10^{-4};$ (**kg/ms**)

$u = 139.0877413220332/Ac;$

$G = 216\,412.01750800002/Ac;$

$\rho b = 1422;$

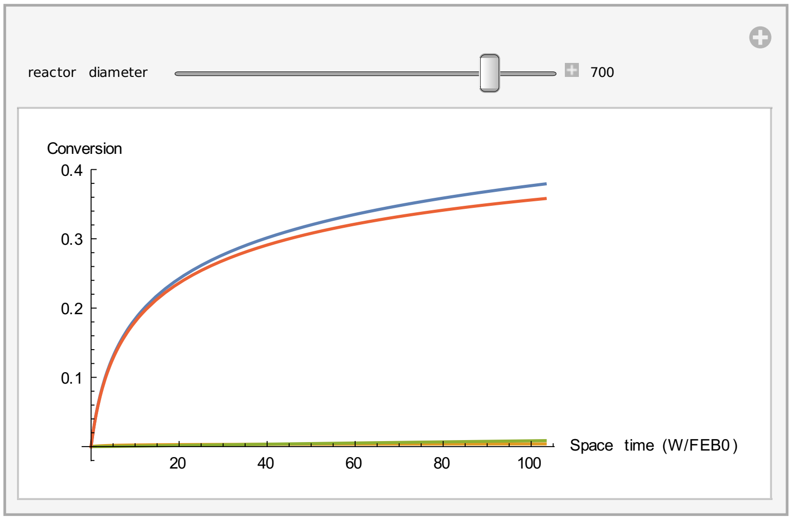
$\epsilon = 0.4312;$ (**void fraction of bed**)

$$\rho g = \frac{10^5 * 10^{-3}}{8.314 * T[W]} * (PEB * 106.168 + PST * 104.15 + PBZ * 78.114 + PTO * 92.141 + PH2o * 18.020 + PH2 * 2.010 + PMTH * 16.043 + PETH * 28.054);$$

```
s15 = Quiet@NDSolve[{XEB'[W] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3) * 0.000303),
    XBZ'[W] == (rc2 + rt2 * 0.000303), XTO'[W] == (rc3 + rc4 + rt3 * 0.000303),
    XH2'[W] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * 0.000303),
```

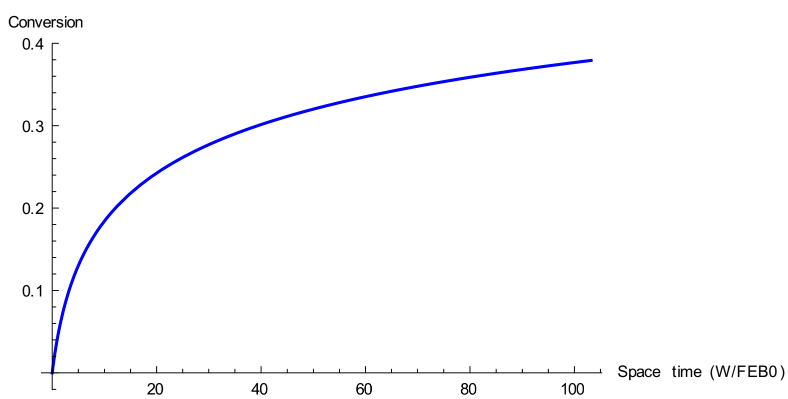
```
      PT'[W] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5,
      T'[W] == (1/(106.168*FEB0*(1 - XEB[W])*Cp1 +
                104.15*(FST0 + FEB0*(XEB[W] - XBZ[W] - XTO[W]))*Cp2 +
                78.114*(FBZ0 + FEB0*XBZ[W])*Cp3 + 92.141*(FTO0 + FEB0*XTO[W])*Cp4 +
                2.010*(FH20 + FEB0*XH2[W])*Cp5 + 18.020*FH2o0*Cp6))*
          (FEB0*(-ΔH1*(rc1 + rt1*0.000303) - ΔH2*(rc2 + rt2*0.000303) -
                ΔH3*(rc3 + rt3*0.000303) - ΔH4*rc4)),
      XEB[0] == 0, XBZ[0] == 0, XTO[0] == 0, XH2[0] == 0, PT[0] == 1.25, T[0] == 886},
    {PT, T, XEB, XBZ, XTO, XH2}, {W, 0, 103.18}];
s16 = Quiet@NDSolve[{XEB'[W] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*0.000303),
      XBZ'[W] == (rc2 + rt2*0.000303), XTO'[W] == (rc3 + rc4 + rt3*0.000303),
      XH2'[W] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*0.000303),
      PT'[W] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5,
      T'[W] == (1/(106.168*FEB0*(1 - XEB[W])*Cp1 +
                104.15*(FST0 + FEB0*(XEB[W] - XBZ[W] - XTO[W]))*Cp2 +
                78.114*(FBZ0 + FEB0*XBZ[W])*Cp3 + 92.141*(FTO0 + FEB0*XTO[W])*Cp4 +
                2.010*(FH20 + FEB0*XH2[W])*Cp5 + 18.020*FH2o0*Cp6))*
          (FEB0*(-ΔH1*(rc1 + rt1*0.000303) - ΔH2*(rc2 + rt2*0.000303) -
                ΔH3*(rc3 + rt3*0.000303) - ΔH4*rc4)),
      XEB[103.18] == 0.3874204642104947, XBZ[103.18] == 0.003908770904199895,
      XTO[103.18] == 0.008259243954145309,
      XH2[103.18] == 0.3669932053980045, PT[103.18] == 1.11, T[103.18] == 898.2},
    {PT, T, XEB, XBZ, XTO, XH2}, {W, 103.18, 219.19}];
s17 = Quiet@NDSolve[{XEB'[W] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3)*0.000303),
      XBZ'[W] == (rc2 + rt2*0.000303), XTO'[W] == (rc3 + rc4 + rt3*0.000303),
      XH2'[W] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3)*0.000303),
      PT'[W] == -(1 - ϵ)/ϵ^3 * (1.28 + (458*(1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160*10^-8 * (u*G*FEB0)/(ρb*dp*Ac) * 10^-5,
      T'[W] == (1/(106.168*FEB0*(1 - XEB[W])*Cp1 +
                104.15*(FST0 + FEB0*(XEB[W] - XBZ[W] - XTO[W]))*Cp2 +
                78.114*(FBZ0 + FEB0*XBZ[W])*Cp3 + 92.141*(FTO0 + FEB0*XTO[W])*Cp4 +
                2.010*(FH20 + FEB0*XH2[W])*Cp5 + 18.020*FH2o0*Cp6))*
          (FEB0*(-ΔH1*(rc1 + rt1*0.000303) - ΔH2*(rc2 + rt2*0.000303) -
                ΔH3*(rc3 + rt3*0.000303) - ΔH4*rc4)),
      XEB[219.19] == 0.7100790974754088, XBZ[219.19] == 0.009805048792484946,
      XTO[219.19] == 0.04996796938047778, XH2[219.19] == 0.6003381099219698,
      PT[219.19] == 0.92, T[219.19] == 897.6},
    {PT, T, XEB, XBZ, XTO, XH2}, {W, 219.19, 350}];
```

```
Figure = Plot[{XEB[W] /. s15, XBZ[W] /. s15, XTO[W] /. s15, XH2[W] /. s15}, {W, 0, 103.18},
    PlotRange → All, AxesLabel → {"Space time (W/FEB0)", "Conversion"}], Column[{
  Control[{{Dr, 700, "reactor diameter "}, 100, 800, 10, Appearance → "Labeled"}]
}, Left]]
```



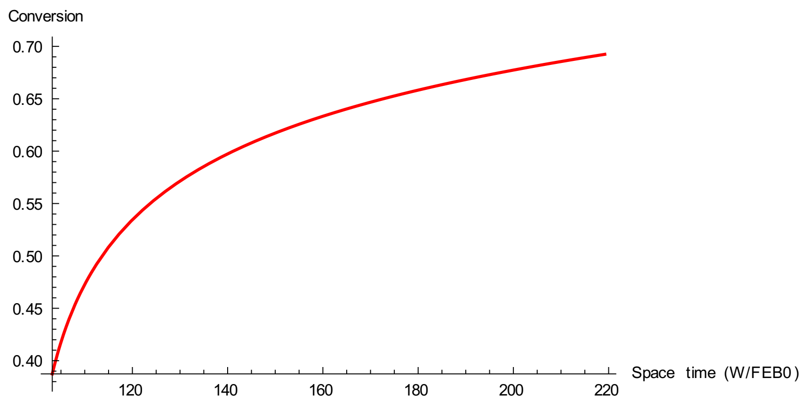
EB Conversion profile for the first reactor:

```
figure26 = Plot[{XEB[W] /. s15}, {W, 0, 103.18}, PlotRange → All,
  PlotStyle → Blue, AxesLabel → {"Space time (W/FEB0)", "Conversion "}]
```



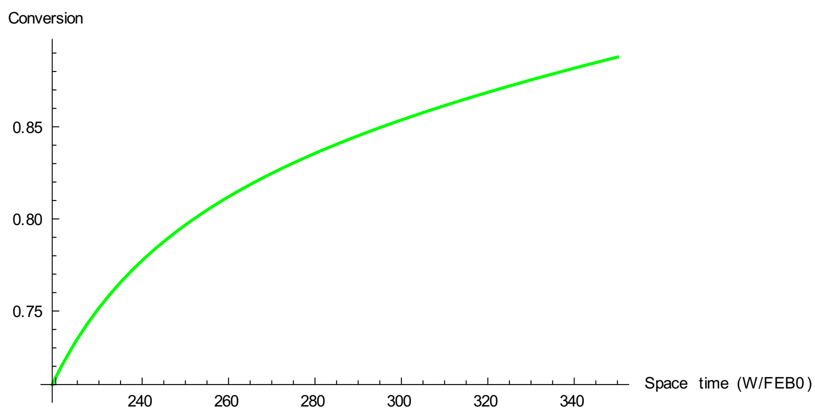
EB conversion profile for the second reactor:

```
figure27 = Plot[{XEB[W] /. s16}, {W, 103.18 , 219.19 }, PlotRange → All,
  PlotStyle → Red, AxesLabel → {"Space time (W/FEB0)", "Conversion "}]
```



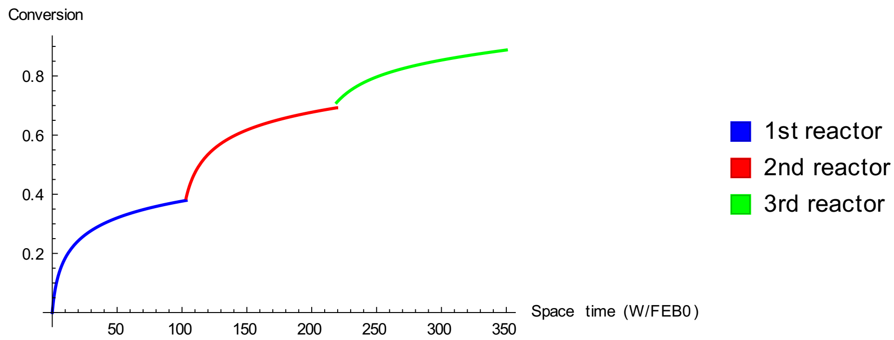
EB conversion profile for the third reactor:

```
figure28 = Plot[{XEB[W] /. s17}, {W, 219.19 , 350}, PlotRange → All,
  PlotStyle → Green, AxesLabel → {"Space time (W/FEB0)", "Conversion "}]
```

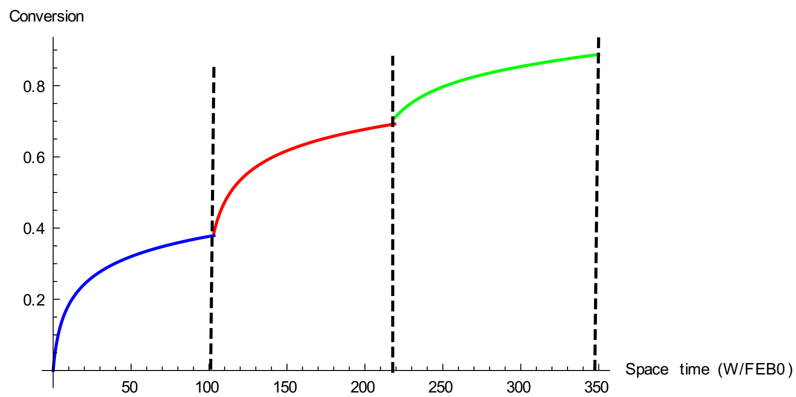


Overview of EB conversion profile for three reactors in series:

```
Legended [Show[figure26 , figure27 , figure28 ],
 SwatchLegend [{Blue , Red , Green }, {"1st reactor ", "2nd reactor ", "3rd reactor "}]]
```



Comparison with literature



[1] Lee, W.J. and G.F. Froment, Ethylbenzene dehydrogenation into styrene: Kinetic modeling and reactor simulation. Industrial and Engineering Chemistry

Research, 2008. 47(23): p. 9183-9194.

Appendix:

comments on codes

Manipulate[

```
Module[{At1, At2, At3, Et1, Et2, Et3, kt1, kt2, kt3, k1, k2, k3, k4, A1, A2, A3, A4, E1, E2, E3, E4, AEB, AST, AH2, ΔHaEB, ΔHaST, ΔHaH2, KEB, KST, KH2,
  rt1, rt2, rt3, rc1, rc2, rc3, rc4, Keq, FEB0, FST0, FBZ0, FTO0, FH20, FCH40, FC2H40, FH2O0, PEB, PST, PBZ, PETH, PTO, PH2, PH2O, PMTH,
  CEB, CST, CBZ, CETH, CTO, CH2, CMTH, CH2O, CΔH1, ΔH2, ΔH3, ΔH4, Cp1, Cp2, Cp3, Cp4, Cp5, Cp6, L, Di, Ac, dp, μ, u, G, ρb, R},


  (**Construct the models for the thermal reactions **)

  At1 = 2.2215 * 10^16; (**The preexponential factor for the first thermal reaction . Unit:kmol/m^3hbar**)
  At2 = 2.4217 * 10^20; (**The preexponential factor for the second thermal reaction . Unit:kmol/m^3hbar**)
  At3 = 3.8224 * 10^17; (**The preexponential factor for the third thermal reaction . Unit:kmol/m^3hbar**)
  Et1 = 272.23; (**The activation energy for the first thermal reaction . Unit:kJ/mol**)
  Et2 = 352.79; (**The activation energy for the second thermal reaction . Unit:kJ/mol**)
  Et3 = 313.06; (**The activation energy for the third thermal reaction . Unit:kJ/mol**)
  R = 8.314; (**gas constant**)
  kt1 = At1 * Exp[(-Et1 * 10^3)/(R * T[z])]; (**The rate coefficient of the first thermal reaction . Unit:kmol/m^3hbar**)
  kt2 = At2 * Exp[(-Et2 * 10^3)/(R * T[z])]; (**The rate coefficient of the first thermal reaction . Unit:kmol/m^3hbar**)
  kt3 = At3 * Exp[(-Et3 * 10^3)/(R * T[z])]; (**The rate coefficient of the first thermal reaction . Unit:kmol/m^3hbar**)


  (**Construct the models for the catalytic reactions **)

  A1 = 4.594 * 10^9; (**The preexponential factor for the first catalytic reaction . Unit:kmol/kg-cath**)
  A2 = 1.060 * 10^15; (**The preexponential factor for the second catalytic reaction . Unit:kmol/kg-cath**)
  A3 = 1.246 * 10^26; (**The preexponential factor for the third catalytic reaction . Unit:kmol/kg-cath**)
  A4 = 8.024 * 10^10; (**The preexponential factor for the fourth catalytic reaction . Unit:kmol/kg-cath**)
  E1 = 175.38; (**The activation energy for the first catalytic reaction . Unit:kJ/mol**)
  E2 = 296.29; (**The activation energy for the second catalytic reaction . Unit:kJ/mol**)
  E3 = 474.76; (**The activation energy for the third catalytic reaction . Unit:kJ/mol**)
  E4 = 213.78; (**The activation energy for the fourth catalytic reaction . Unit:kJ/mol**)
  k1 = A1 * Exp[(-E1 * 10^3)/(R * T[z])]; (**The rate coefficient of the first catalytic reaction . Unit:kmol/kg-cath**)
  k2 = A2 * Exp[(-E2 * 10^3)/(R * T[z])]; (**The rate coefficient of the second catalytic reaction . Unit:kmol/kg-cath**)
```

$$k3 = A3 * \mathrm{Exp}\left[\frac{-E3 * 10^{3}}{R * T[z]}\right];$$ (**The rate coefficient of the third catalytic reaction . Unit:kmol/kg−cath**)

$$k4 = A4 * \mathrm{Exp}\left[\frac{-E4 * 10^{3}}{R * T[z]}\right];$$ (**The rate coefficient of the fourth catalytic reaction . Unit:kmol/kg−cath**)

(**Construct the models for the thermodynamic equilibriums **)

$$AEB = 1.014 * 10^{-5};$$ (**Preexponential factor of ethylbenzene adsoprtion . Unit:1/bar**)

$$AST = 2.678 * 10^{-5};$$ (**Preexponential factor of styrene adsoprtion . Unit:1/bar**)

$$AH2 = 4.519 * 10^{-7};$$ (**Preexponential factor of hydrogen adsoprtion . Unit:1/bar**)

$$\Delta HaEB = -102.22;$$ (**Adsorption enthalpy of ethylbenzene . Unit:kJ/mol**)

$$\Delta HaST = -104.56;$$ (**Adsorption enthalpy of styrene . Unit:kJ/mol**)

$$\Delta HaH2 = -117.95;$$ (**Adsorption enthalpy of hydrogen . Unit:kJ/mol**)

$$KEB = AEB * \mathrm{Exp}\left[\frac{-\Delta HaEB * 10^{3}}{R * T[z]}\right];$$ (**The adsorption equilibrium constant of ethylbenzene . Unit:1/bar**)

$$KST = AST * \mathrm{Exp}\left[\frac{-\Delta HaST * 10^{3}}{R * T[z]}\right];$$ (**The adsorption equilibrium constant of styrene . Unit:1/bar**)

$$KH2 = AH2 * \mathrm{Exp}\left[\frac{-\Delta HaH2 * 10^{3}}{R * T[z]}\right];$$ (**The adsorption equilibrium constant of hydrogen . Unit:1/bar**)

$$Keq = \mathrm{Exp}\left[\frac{-(122\,725.157 - 126.267 * T[z] - 0.002194 * T[z] * T[z])}{R * T[z]}\right];$$

(**The kinetic equilibrium constant for the first reversible reaction .Unit:1/bar**)

(*(**Partial pressure of components **)*)

$$PEB = PT[z] * \frac{\frac{FEB0}{FT0}(1 - (XEB[z] - XBZ[z] - XTO[z]) - XBZ[z] - XTO[z])}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of ethylbenzene . Unit:1/bar**)

$$PST = PT[z] * \frac{\frac{FST0}{FT0} + \frac{FEB0}{FT0} * (XEB[z] - XBZ[z] - XTO[z])}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of styrene . Unit:1/bar**)

$$PBZ = PT[z] * \frac{\frac{FBZ0}{FT0} + \frac{FEB0}{FT0} * XBZ[z]}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of benzene . Unit:1/bar**)

$$PH2 = PT[z] * \frac{\frac{FH20}{FT0} + \frac{FEB0}{FT0} * XH2[z]}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of hydrogen . Unit:1/bar**)

$$PETH = PT[z] * \frac{\frac{FC2H40}{FT0} + \frac{FEB0}{FT0} * XBZ[z]}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of ethylene . Unit:1/bar**)

$$PTO = PT[z] * \frac{\frac{FTO0}{FT0} + \frac{FEB0}{FT0} * XTO[z]}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of toluene . Unit:1/bar**)

$$PH2O = PT[z] * \frac{\frac{FH2O0}{FT0}}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of water . Unit:1/bar**)

$$PMTH = PT[z] * \frac{\frac{FCH40}{FT0} + \frac{FEB0}{FT0} * XEB[z]}{1 + \frac{FEB0}{FT0} * (XTO[z] + XBZ[z] + XH2[z])};$$ (**The partial pressure of methane . Unit:1/bar**)

```
(*(** Concentration of components **)*)
CEB = PEB * 10^5 / (R * T[z]); (**The concentration of ethylbenzene . Unit:mol/m^3**)
CST = PST * 10^5 / (R * T[z]); (**The concentration of styrene . Unit:mol/m^3**)
CBZ = PBZ * 10^5 / (R * T[z]); (**The concentration of benzene . Unit:mol/m^3**)
CH2 = PH2 * 10^5 / (R * T[z]); (**The concentration of hydrogen . Unit:mol/m^3**)
CETH = PETH * 10^5 / (R * T[z]); (**The concentration of ethylene . Unit:mol/m^3**)
CTO = PTO * 10^5 / (R * T[z]); (**The concentration of toluene . Unit:mol/m^3**)
CH2O = PH2O * 10^5 / (R * T[z]); (**The concentration of water . Unit:mol/m^3**)
CMTH = PMTH * 10^5 / (R * T[z]); (**The concentration of methane . Unit:mol/m^3**)

(*(**Thermal reaction rates of three reactions **)*)
rt1 = kt1 * (PEB - PST * PH2 / Keq); (**The reaction rate of the first thermal reaction . Unit:kmol/m^3h**)
rt2 = kt2 * PEB ; (**The reaction rate of the second thermal reaction . Unit:kmol/m^3h**)
rt3 = kt3 * PEB ; (**The reaction rate of the third thermal reaction . Unit:kmol/m^3h**)

(*(**Catalytic reaction rates of four reactions **)*)
rc1 = k1 * KEB * (PEB - PST*PH2/Keq) / (1 + KEB * PEB + KH2 * PH2 + KST * PST)^2; (**The reaction rate of the first catalytic reaction . Unit: kmol/kg-cath**)
rc2 = k2 * KEB * PEB / (1 + KEB * PEB + KH2 * PH2 + KST * PST)^2; (**The reaction rate of the second catalytic reaction . Unit: kmol/kg-cath**)
rc3 = k3 * KEB * PEB * KH2 * PH2 / (1 + KEB * PEB + KH2 * PH2 + KST * PST)^2; (**The reaction rate of the third catalytic reaction . Unit: kmol/kg-cath**)
rc4 = k4 * KST * PST * KH2 * PH2 / (1 + KEB * PEB + KH2 * PH2 + KST * PST)^2; (**The reaction rate of the fourth catalytic reaction . Unit: kmol/kg-cath**)

(*(**Heat of reactions **)*)
ΔH1 = 117 690 +41.99 * (T[z] - 298.15) + (-8.2026 * 10^-2)/2 * ((T[z])^2 -298.15^2) + (6.499 * 10^-5)/3 ((T[z])^3 -298.15^3) + (-2.311 * 10^-8)/4 ((T[z])^4 -298.15^4);
(**Reaction enthalpy of the first reaction . Unit:kJ/kmol**)
ΔH2 = 105 510 +12.986 * (T[z] - 298.15) + (-7.67 * 10^-2)/2 * ((T[z])^2 -298.15^2) + (9.592 * 10^-5)/3 ((T[z])^3 -298.15^3) + (-4.125 * 10^-8)/4 ((T[z])^4 -298.15^4);
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(**Reaction enthalpy of the second reaction . Unit :kJ/kmol **)

$$\Delta H3 = -54680 + 10.86 * (T[z] - 298.15) + \frac{-15.1844 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{23.04 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-9.9955 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(**Reaction enthalpy of the third reaction . Unit :kJ/kmol **)

$$\Delta H4 = -172370 + (-31.13) * (T[z] - 298.15) + \frac{-6.9818 * 10^{-2}}{2} * \left((T[z])^2 - 298.15^2\right) + \frac{16.54 * 10^{-5}}{3} \left((T[z])^3 - 298.15^3\right) + \frac{-7.685 * 10^{-8}}{4} \left((T[z])^4 - 298.15^4\right);$$

(**Reaction enthalpy of the fourth reaction . Unit :kJ/kmol **)

(*(**Heat capacities of components **)*)

$Cp1 = -0.43426 + 6.0671 * 10^{-3} * T[z] - 3.8625 * 10^{-6} * T[z] * T[z] + 9.1282 * 10^{-10} * (T[z])^3;$ (**Heat capacity of ethylbenzene . Unit :kJ/kgK**)

$Cp2 = -0.26436 + 5.564 * 10^{-3} * T[z] - 3.0018 * 10^{-6} * T[z] * T[z] + 5.3317 * 10^{-10} * (T[z])^3;$ (**Heat capacity of styrene . Unit :kJ/kgK**)

$Cp3 = -0.40599 + 6.6616 * 10^{-3} * T[z] - 4.5318 * 10^{-6} * T[z] * T[z] + 12.255 * 10^{-10} * (T[z])^3;$ (**Heat capacity of benzene . Unit :kJ/kgK**)

$Cp4 = -0.27127 + 5.9142 * 10^{-3} * T[z] - 3.8631 * 10^{-6} * T[z] * T[z] + 9.54 * 10^{-10} * (T[z])^3;$ (**Heat capacity of toluene . Unit :kJ/kgK**)

$Cp5 = 13.57 + 4.637 * 10^{-3} * T[z] - 6.905 * 10^{-6} * T[z] * T[z] + 38.23 * 10^{-10} * (T[z])^3;$ (**Heat capacity of hydrogen . Unit :kJ/kgK**)

$Cp6 = 1.7911 + 0.1069 * 10^{-3} * T[z] + 0.58611 * 10^{-6} * T[z] * T[z] - 1.998 * 10^{-10} * (T[z])^3;$ (**Heat capacity of water . Unit :kJ/kgK**)

(*(**Physical properties of the catalyst we chose **)*)

L = 10; (**Length of the reactor . Unit :m**)

dp = 5.5 / 1000; (**Catalyst equivalent pellet diameter . Unit :m**)

$\rho b = 1422;$ (**Catalyst bulk diameter . Unit :kg−cat/m^3**)

$\epsilon = 0.4312;$ (**void fraction of bed . Unit : m^3/m^3**)

(*(**Dimensions of the reactor **)*)

$Di = \frac{Dr}{100};$ (**Diameter of the reactor . Unit : m.Dr is the diamter of the reactor in cm **)

$Ac = \frac{\pi}{4} * (Di)^2;$ (**The cross section area of the reactor . Unit : m^2**)

(**The important properties of the gas mixture **)

$\mu = (-10.035 + 0.25191 * T[z] - 0.000037932 * T[z] * T[z]) * 3.6 * 10^{-4};$ (**The viscosity of the mixture . Unit :kg/ms **)

u = 22.00279 / Ac;

(**The superficial velocity of the inlet feed stream , which is the volumetric flowrate divided by the cross section area . Unit : m^3/m^2s**)

G = 89 520.109 / Ac;

(**The superficial velocity of the inlet feed stream , which is the mass flowrate divided by the cross section area . Unit : kg/m^2h**)

$$\rho g = \frac{10^5 * 10^{-3}}{R * T[z]} * (PEB * 106.168 + PST * 104.15 + PBZ * 78.114 + PTO * 92.141 + PH2O * 18.020 + PH2 * 2.010 + PMTH * 16.043 + PETH * 28.054);$$

(*(**Density of the gas mixture . Unit : kg/m^3**)*)

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(**The initial molar flowrates of components **)

FEB0 = 49.7976 * 3600 / 1000; (**The initial molar flowrate of ethylbenzene . Unit :kmol /h**)

FST0 = 0.00332919 * 3.6; (**The initial molar flowrate of styrene . Unit :kmol /h**)

FBZ0 = 1.464 * 3.6; (**The initial molar flowrate of benzene . Unit :kmol /h**)

FTO0 = 0.0482245 * 3.6; (**The initial molar flowrate of toluene . Unit :kmol /h**)

FH20 = 0; (**The initial molar flowrate of hydrogen . Unit :kmol /h**)

FCH40 = 0; (**The initial molar flowrate of methane . Unit :kmol /h**)

FC2H40 = 0; (**The initial molar flowrate of ethylene . Unit :kmol /h**)

FH2O0 = 1080 * 3.6; (**The initial molar flowrate of water . Unit :kmol /h**)

FT0 = FEB0 + FST0 + FBZ0 + FTO0 + FH20 + FCH40 + FC2H40 + FH2O0 ; (**The total molar flowrate of the gas mixture . Unit :kmol /h**)


s1 = Quiet @NDSolve[{XEB '[z] == (rc1 + rc2 + rc3 + (rt1 + rt2 + rt3) * (ϵ / ρb)) * (Ac * ρb)/FEB0, (**Mass balance differential equation for ethylbenzene **)

    XBZ '[z] == (rc2 + rt2 * (ϵ / ρb)) * (Ac * ρb)/FEB0, (**Mass balance differential equation for benzene **)

    XTO '[z] == (rc3 + rc4 + rt3 * (ϵ / ρb)) * (Ac * ρb)/FEB0, (**Mass balance differential equation for toluene **)

    XH2 '[z] == (rc1 - rc3 - 2 rc4 + (rt1 - rt3) * (ϵ / ρb)) * (Ac * ρb)/FEB0, (**Mass balance differential equation for hydrogen **)

    PT '[z] == -(1 - ϵ)/ϵ^3 * (1.28 + (458 * (1 - ϵ))/((ρg*dp*u)/μ)) * 7.7160 * 10^-8 * (u * G * FEB0)/(ρb * dp * Ac) * 10^-5 * (Ac * ρb)/FEB0,

    (**The Ergun equation for pressure drop. Note that the pressure is in bar**)

    T '[z] == (Ac * ρb)/FEB0 * (1 / (106.168 * FEB0 * (1 - XEB [z]) * Cp1 + 104.15 * (FST0 + FEB0 * (XEB [z] - XBZ [z] - XTO [z])) * Cp2 + 78.114 *

                (FBZ0 + FEB0 * XBZ [z]) * Cp3 + 92.141 * (FTO0 + FEB0 * XTO [z]) * Cp4 + 2.010 * (FH20 + FEB0 * XH2 [z]) * Cp5 + 18.020 * FH2O0 * Cp6)) *

       (FEB0 * (-ΔH1 * (rc1 + rt1 * (ϵ / ρb)) - ΔH2 * (rc2 + rt2 * (ϵ / ρb)) - ΔH3 * (rc3 + rt3 * (ϵ / ρb)) - ΔH4 * rc4 )), (**Energy balance differential equation **)

    XEB [0] == 0, (**The initial conversion of ethylbenzene is zero **)

    XBZ [0] == 0, (**The initial conversion of benzene is zero **)

    XTO [0] == 0, (**The initial conversion of toluene is zero **)

    XH2 [0] == 0, (**The initial conversion of hydrogen is zero **)

    PT [0] == 2.7, (**The initial pressure of the mixture . Unit : bar**)

    T[0] == 893.15 (**The initial temperature of the mixture . Unit : K**)

  }, {CEB , CST, CBZ , CTO , CH2, CETH , CH2O , CMTH }, {z, 0, L}]; (**Solve the differnetial equations simultaneously with results returned to s1**)


Figure = Plot[{CEB /. s1, CST /. s1, CBZ /. s1, CTO /. s1, CH2 /. s1, CETH /. s1, CMTH /. s1}, {z, 0, L}, PlotRange → All,

    PlotLabels → {"EB ", "ST ", "BZ ", "TO ", "H2 ", "ETH ", "MTH ", "Water "}, AxesLabel → {"Reactor length (m)", "Concentration (mol/cum )"}]], Column [{

  Control[{{Dr, 400, "reactor diameter (cm ) "}, 100, 800, 10, Appearance → "Labeled "}]

}, Left ]]
```