

Wolfram LEP tutorial

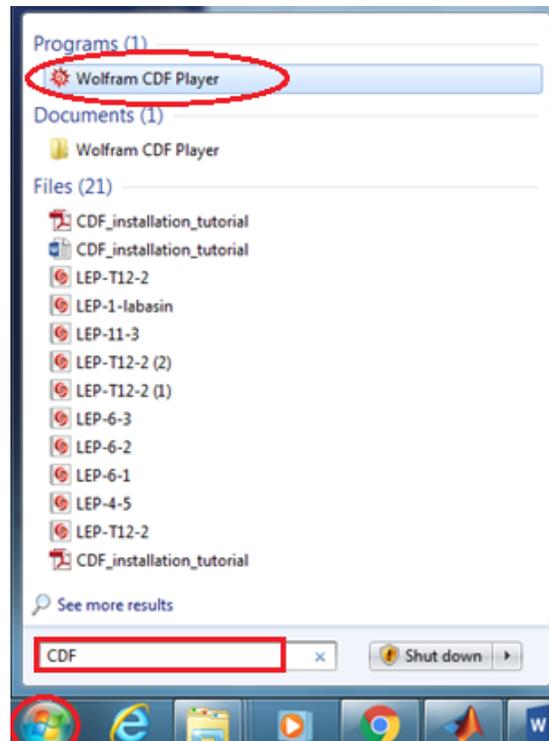
Step 1: Open chapter 12 and click on LEP-T12-2.cdf under “Wolfram CDF Code” section. After clicking, you should see that the file is downloaded in the bottom of the browser

The screenshot shows the Wolfram LEP tutorial website. At the top, there are navigation links for "Elements of Chemical Reaction Engineering 5th Edition" and "Essentials of Chemical Reaction Engineering". Below these are book covers and a "Home Problem Solving Updates and FAQs" link. A table of contents (TOC) is visible with chapters 1 through 18 and Appendices. The main content area is titled "Chapter 12: Steady-State Nonisothermal Reactor Design: Flow Reactors with Heat Exchange" and includes a section for "Living Example Problems". A table lists various example problems and their corresponding code files. The file "LEP-T12-2.cdf" is circled in red. At the bottom, a download bar shows the file "LEP-T12-2.cdf" has been downloaded, also circled in red.

Living Example Problem	Polymath™ Code	Matlab Code	Wolfram CDF Code *	AspenTech™
LEP Table 12-2 computer experiment	LEP-T12-2.pol	LEP-T12-2.zip	LEP-T12-2.cdf	--
Example 12-1 Isomerization of Normal Butane with Heat Exchanger	a) Co-current: LEP-12-1a.pol	a) Co-current: LEP-12-1a.zip	a) Co-current: LEP-12-1a.cdf	--
	b) Countercurrent: LEP-12-1b.pol	b) Countercurrent: LEP-12-1b.zip	b) Countercurrent: LEP-12-1b.cdf	
	c) Constant T_a : LEP-12-1c.pol	c) Constant T_a : LEP-12-1c.zip	c) Constant T_a : LEP-12-1c.cdf	
	d) Adiabatic: LEP-12-1d.pol	d) Adiabatic: LEP-12-1d.zip	d) Adiabatic: LEP-12-1d.cdf	

Step 2: To run the file, click on the file you just downloaded. If you are able to open it then go to Step 6. If you are not able to open it then follow the Steps 3-5

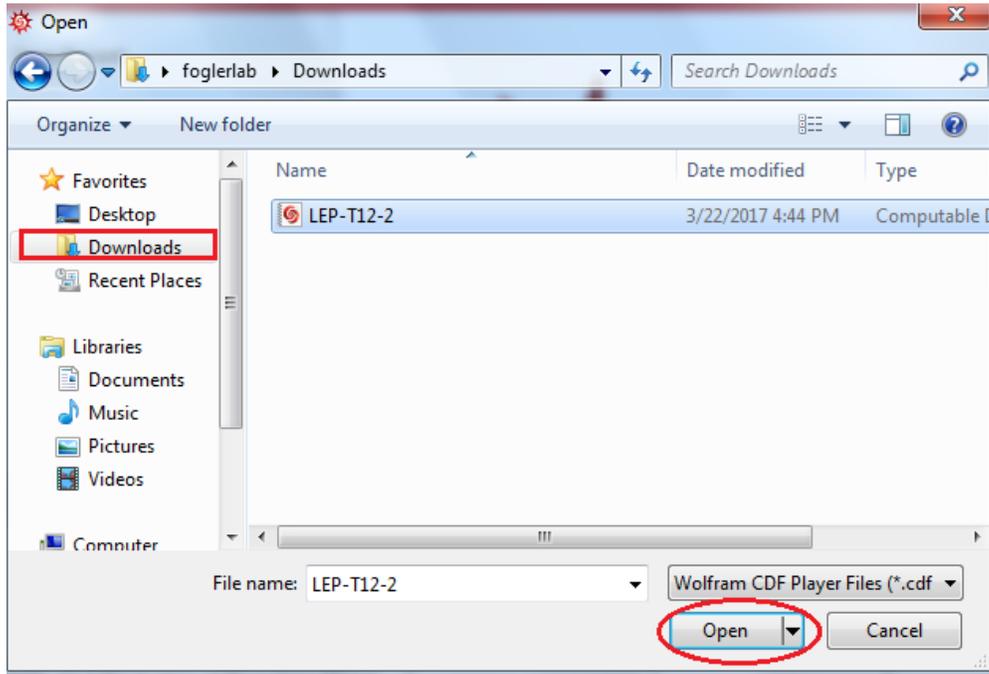
Step 3: Click on the "Start" button in the bottom left corner of the screen and type CDF. You will find that Wolfram CDF Player is present under Programs menu. Click to open the CDF player



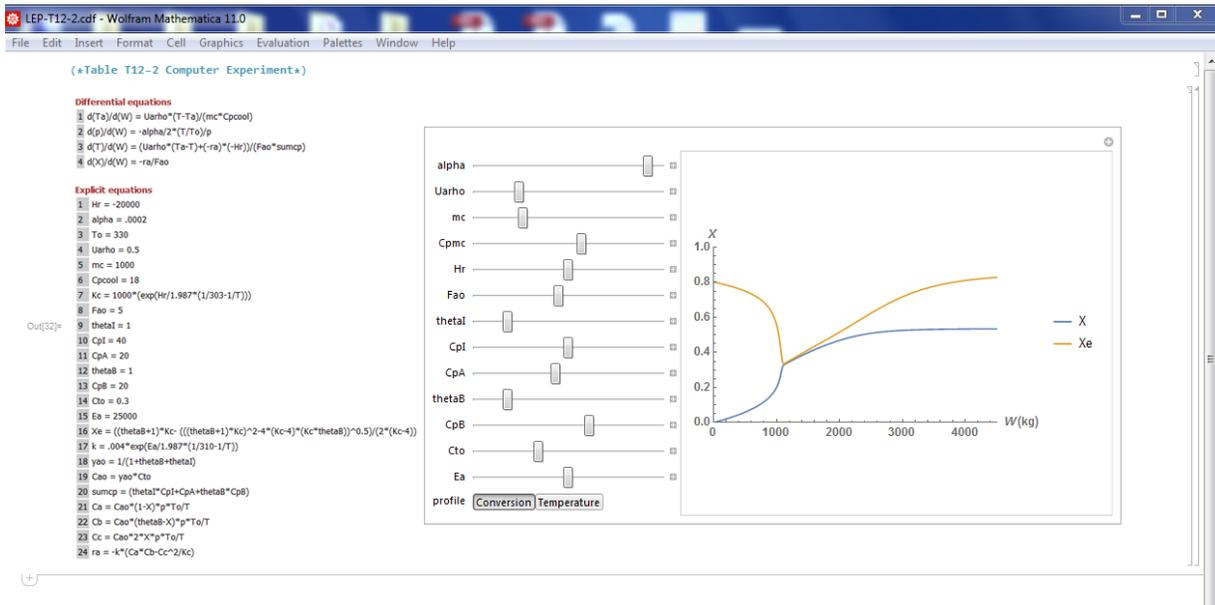
Step 4: The following window will appear. Click "Open" which is present on the left panel of CDF player



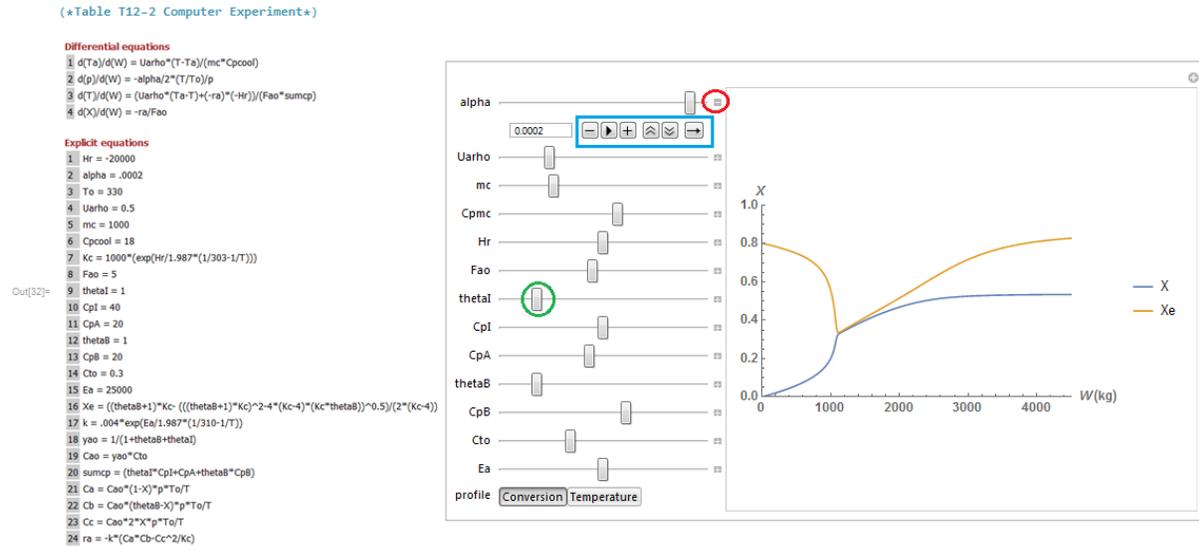
Step 5: Choose the location where your file is present using the menu present on left side. By default, it should be in Downloads. Select the file LEP-T12-2 and click Open



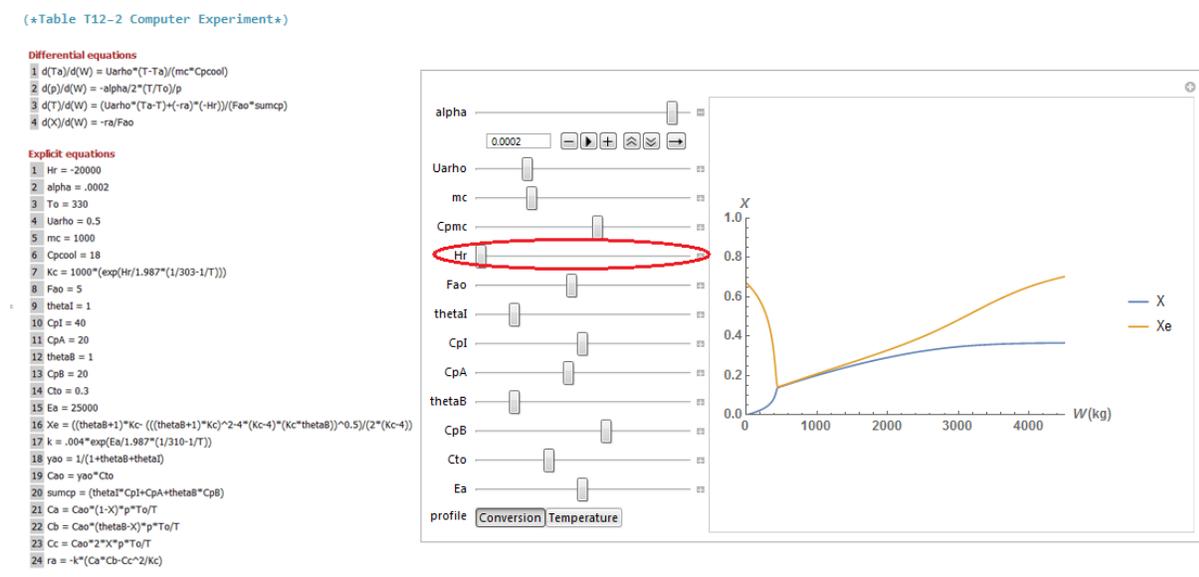
Step 6: After opening the file, you should see the following window. If the graph doesn't appear, then press Shift+Enter



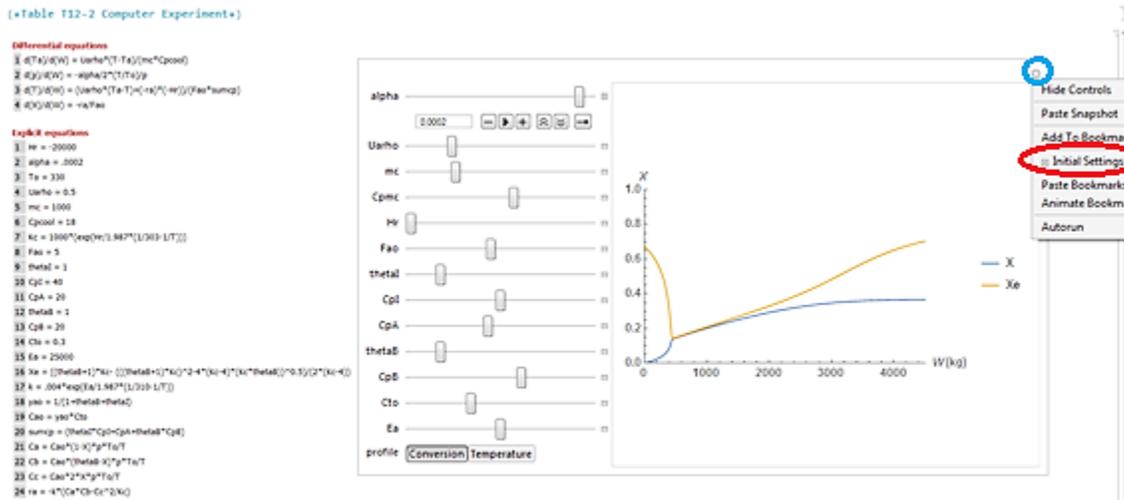
Step 7: To view the effects of changing various parameters on the graph, use slide bars (shown by green circle). You can move the slide bar from extreme left (minimum value of parameter) to extreme right (maximum value of parameter). To view and set the values of the variables, click “+” button present on the right of each slider (shown by red). You can also play animation using various buttons present (shown by blue rectangle)



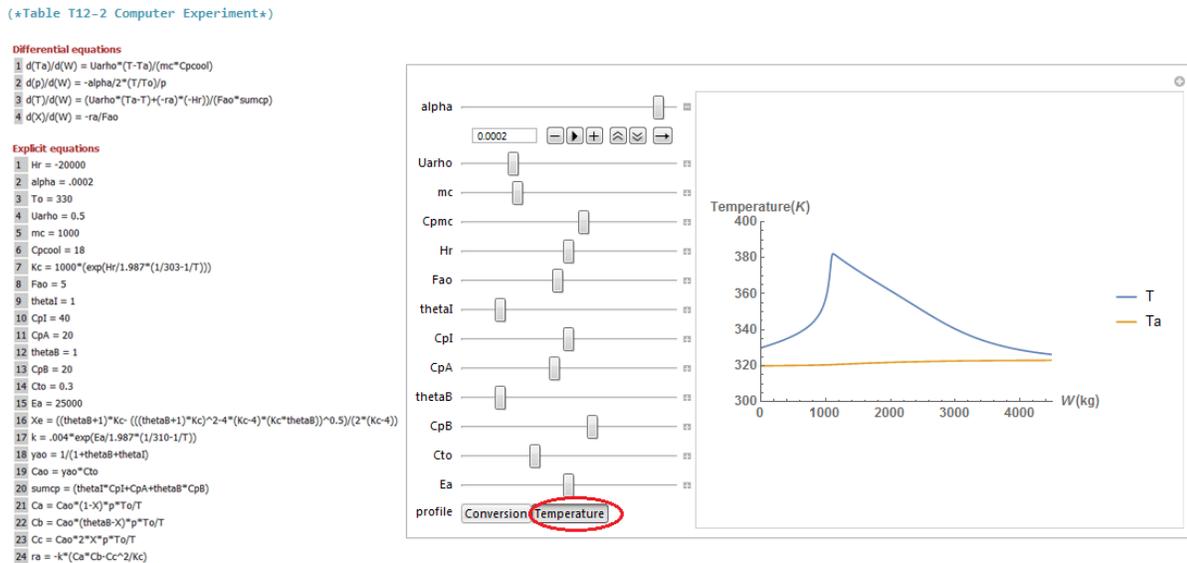
Step 8: Let’s change only Hr value from -20000 to the minimum allowed in the slide bar. Take the slide bar of Hr to the left extreme and see how the graph changes



Step 9: To go back to initial values of all the parameter, you can either close the program and re-open OR click on the “+” button on the top right corner of graph and choose “Initial settings”. If you don’t reset the values, then simulation will retain new value of the parameter. Let’s reset the parameter value



Step 10: To view temperature profile, click on Temperature tab present in the profile option. Use slide bar to see the effect of various parameters



Step 11: Currently, you can't see the codes written for this simulation as codes are hidden. If you wish to see the code or make any changes (to make changes you need MATHEMATICA), you can double click on the right most vertical bar. In the below screenshot, under red rectangle, you can see two bars. You need to double click on the bar which is shown by blue color

After you double click, you will see the complete codes as shown below

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(*Table T12-2 Computer Experiments*)

Differential equations
1 dT/dW(K) = Uairho*(T-Fa)/(mc*Cp)
2 dW/dW(K) = -alpha*(T-Ta)
3 dT/dW(K) = Uairho*(T-Ta)/(mc*Cp) + alpha*(T-Ta)/(rho*W)
4 dW/dW(K) = -alpha*Fao

Explicit equations
1 Hr = -20000
2 alpha = .0002
3 Ta = 300
4 Uairho = 0.5
5 mc = 1000
6 Cpocd = 18
7 ka = 1000*exp(91.987*(1/300-1/T))
8 Fao = 5
9 thetal = 1
10 Cpl = 40
11 CpA = 20
12 thetaB = 1
13 CpB = 20
14 Cto = 0.3
15 Eo = 25000
16 Xe = ((thetal+1)*Ka - ((thetal+1)*Ka)^2-4*(Ka-4)*(Ka*thetal)^0.5)/(2*(Ka-4))
17 k = .004*exp(Ka/1.887*(1/300-1/T))
18 yao = 1/(1+thetal+thetal)
19 Cao = yao*Chi
20 sumcp = (thetal*Cpl+CpA+thetal*CpB)
21 Ca = Cao*(1-X)^2*Ta/T
22 Cc = Cao*(thetal+1)*Ta/T
23 ca = Cao*(1-X)^2*Ta/T
24 ra = 4*(Ca*Cc-Cc^2)/Kc

Manipulate[
Module[{sol1, pl1t, pl2t, yao},
Kc[T] := 1000 * (Exp[Hr / 1.987 * (1 / 300 - 1 / T)])];
ka[T] := .004 * Exp[ka / 1.987 * (1 / 300 - 1 / T)];
yao = 1 / (1 + thetal + thetal);
To := 300;
Xe[KC] := ((thetal + 1) * Kc[T] - (((thetal + 1) * Kc[T])^2 - 4 * (Kc[T] - 4) * (Kc[T] + thetal) ^ 0.5) / (2 * (Kc[T] - 4)));
sumcp = (thetal * Cpl + CpA + thetal * CpB);
Ca[X, p, T] := Cao * (1 - X[u]) * p[u] * To / T[u];
Cb[X, p, T] := Cao * (thetal * X[u]) * p[u] * To / T[u];
Cc[X, p, T] := Cao * 2 * X[u] * p[u] * To / T[u];
ra[ka, Ca, Cb, Cc, Kc] := -ka[X, p, T] * (Ca[X, p, T] + Cb[X, p, T] - (Cc[X, p, T])^2 / Kc[T]);
sol1 = NSolve[{Ta[u] == Uairho * (T[u] - Ta[u]) / (mc * Cpmc), p'[u] == -alpha / 2 * (T[u] / To) / p[u], T'[u] == (Uairho * (Ta[u] - T[u]) + (-ra[ka, Ca, Cb, Cc, Kc]) * (-Hr)) / (Fao + sumcp), X'[u] == -ra[ka, Ca, Cb, Cc, Kc] / Fao, Ta[0] = 300, p[0] = 1, T[0] = 300, X[0] = 0}, {Ta, p, T, X}, {t, 0, 4500}];
pl1t = Plot[Evaluate[X[u] /. sol1], Evaluate[ra[KC] /. sol1], {t, 0, 4500}, AxesLabel -> {W[kg], X}, PlotLegends -> {"X"}, "ta", PlotRange -> {{0, 4500}, {0, 1}}, BaseStyle -> {FontWeight -> "Bold", FontSize -> 12}];
pl2t = Plot[Evaluate[T[u] /. sol1], Evaluate[Ta[u] /. sol1], {t, 0, 4500}, AxesLabel -> {W[kg], Temperature[K]}, PlotRange -> {{0, 4500}, {300, 400}}, PlotLegends -> {"T", "Ta"}, BaseStyle -> {FontWeight -> "Bold", FontSize -> 12}];
Switch[ctrl, 1, Show[pl1t], 2, Show[pl2t]];
{{alpha, .0002}, {Uairho, 0.5}, {mc, 1000}, {Cpocd, 18}, {{Hr, -20000}, -30000, -10000, 1000}, {{Fao, 5}, 1, 10, 1}, {{thetal, 1}, 0.2, 5, 0.2}, {{Cpl, 40}, 20, 60, 5}, {{CpA, 20}, 5, 40, 2}, {{thetalB, 1}, 0.2, 5, 0.2}, {{CpB, 20}, 4, 30, 2}, {{Cto, 0.3}, 0.05, 0.8, 0.02}, {{Eo, 25000}, 10000, 40000, 2000},
Differential equations
1 dT/dW(K) = Uairho*(T-Fa)/(mc*Cp)
2 dW/dW(K) = -alpha*(T-Ta)
3 dT/dW(K) = Uairho*(T-Ta)/(mc*Cp) + alpha*(T-Ta)/(rho*W)
4 dW/dW(K) = -alpha*Fao

Explicit equations
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13 CpB = 20
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16 Xe = ((thetal+1)*Ka - ((thetal+1)*Ka)^2-4*(Ka-4)*(Ka*thetal)^0.5)/(2*(Ka-4))
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19 Cao = yao*Chi
20 sumcp = (thetal*Cpl+CpA+thetal*CpB)
21 Ca = Cao*(1-X)^2*Ta/T
22 Cc = Cao*(thetal+1)*Ta/T
23 ca = Cao*(1-X)^2*Ta/T
24 ra = 4*(Ca*Cc-Cc^2)/Kc

Manipulate[
Module[{sol1, pl1t, pl2t, yao},
Kc[T] := 1000 * (Exp[Hr / 1.987 * (1 / 300 - 1 / T)])];
ka[T] := .004 * Exp[ka / 1.987 * (1 / 300 - 1 / T)];
yao = 1 / (1 + thetal + thetal);
To := 300;
Xe[KC] := ((thetal + 1) * Kc[T] - (((thetal + 1) * Kc[T])^2 - 4 * (Kc[T] - 4) * (Kc[T] + thetal) ^ 0.5) / (2 * (Kc[T] - 4)));
sumcp = (thetal * Cpl + CpA + thetal * CpB);
Ca[X, p, T] := Cao * (1 - X[u]) * p[u] * To / T[u];
Cb[X, p, T] := Cao * (thetal * X[u]) * p[u] * To / T[u];
Cc[X, p, T] := Cao * 2 * X[u] * p[u] * To / T[u];
ra[ka, Ca, Cb, Cc, Kc] := -ka[X, p, T] * (Ca[X, p, T] + Cb[X, p, T] - (Cc[X, p, T])^2 / Kc[T]);
sol1 = NSolve[{Ta[u] == Uairho * (T[u] - Ta[u]) / (mc * Cpmc), p'[u] == -alpha / 2 * (T[u] / To) / p[u], T'[u] == (Uairho * (Ta[u] - T[u]) + (-ra[ka, Ca, Cb, Cc, Kc]) * (-Hr)) / (Fao + sumcp), X'[u] == -ra[ka, Ca, Cb, Cc, Kc] / Fao, Ta[0] = 300, p[0] = 1, T[0] = 300, X[0] = 0}, {Ta, p, T, X}, {t, 0, 4500}];
pl1t = Plot[Evaluate[X[u] /. sol1], Evaluate[ra[KC] /. sol1], {t, 0, 4500}, AxesLabel -> {W[kg], X}, PlotLegends -> {"X"}, "ta", PlotRange -> {{0, 4500}, {0, 1}}, BaseStyle -> {FontWeight -> "Bold", FontSize -> 12}];
pl2t = Plot[Evaluate[T[u] /. sol1], Evaluate[Ta[u] /. sol1], {t, 0, 4500}, AxesLabel -> {W[kg], Temperature[K]}, PlotRange -> {{0, 4500}, {300, 400}}, PlotLegends -> {"T", "Ta"}, BaseStyle -> {FontWeight -> "Bold", FontSize -> 12}];
Switch[ctrl, 1, Show[pl1t], 2, Show[pl2t]];
{{ctrl, 1, "profile"}, {1 -> "Conversion", 2 -> "Temperature"}]

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