Example 10.3.1 from Davis and Davis
Froment, Ind Eng Chem 59 (1967)

Here are the dimensionless equations. You want to make “y1”, not “y2”

In[1]:=
```
eq1 = pe ( D[ y1[r, z], {r, 2}] + 1 / r D[ y1[r, z], r]) +
  β1 (k1 ( 1 - y1[r, z] - y2[r, z]) - k2 y1[r, z])
```

Out[1]=
$$\beta 1\ (-k2\, y1[r,z] + k1\ (1 - y1[r,z] - y2[r,z])) + pe \left(\frac{y1^{(1,0)}[r,z]}{r} + y1^{(2,0)}[r,z]\right)$$

In[2]:=
```
eq2 = pe ( D[ y2[r, z], {r, 2}] + 1 / r D[ y2[r, z], r]) +
  β1 (k2 y1[r, z] + k3 (1 - y1[r, z] - y2[r, z]))
```

Out[2]=
$$\beta 1\ (k2\, y1[r,z] + k3\ (1 - y1[r,z] - y2[r,z])) + pe \left(\frac{y2^{(1,0)}[r,z]}{r} + y2^{(2,0)}[r,z]\right)$$

In[3]:=
```
eq3 = bo ( D[ θ[r, z], {r, 2}] + 1 / r D[ θ[r, z], r]) +
  β2 (k1 ( 1 - y1[r, z] - y2[r, z]) - k2 y1[r, z]) +
  β3 (k2 y1[r, z] + k3 (1 - y1[r, z] - y2[r, z]))
```

Out[3]=
$$\beta 2\ (-k2\, y1[r,z] + k1\ (1 - y1[r,z] - y2[r,z])) + \beta 3\ (k2\, y1[r,z] + k3\ (1 - y1[r,z] - y2[r,z])) + bo \left(\frac{\theta^{(1,0)}[r,z]}{r} + \theta^{(2,0)}[r,z]\right)$$

In[4]:=
```
eqs = { D[y1[r, z], z] == eq1, D[y2[r, z], z] == eq2, D[θ[r, z], z] == eq3,
  y1[r, 0] == 0, y2[r, 0] == 0, θ[r, 0] == 1, ((D[y1[r, z], r]) /. r → eps) == 0,
  ((D[y2[r, z], r]) /. r → eps ) == 0, ((D[θ[r, z], r]) /. r → eps) == 0,
  ((D[y1[r, z], r]) /. r → 1) == 0, ((D[y2[r, z], r]) /. r → 1) == 0,
  ((D[θ[r, z], r]) /. r → 1) == hw ( θw - θ[1, z])}
```

Out[4]=
$$\Big\{y1^{(0,1)}[r,z] == \beta 1\ (-k2\, y1[r,z] + k1\ (1 - y1[r,z] - y2[r,z])) + pe \left(\frac{y1^{(1,0)}[r,z]}{r} + y1^{(2,0)}[r,z]\right),\ y2^{(0,1)}[r,z] ==$$
$$\beta 1\ (k2\, y1[r,z] + k3\ (1 - y1[r,z] - y2[r,z])) + pe \left(\frac{y2^{(1,0)}[r,z]}{r} + y2^{(2,0)}[r,z]\right),$$
$$\theta^{(0,1)}[r,z] == \beta 2\ (-k2\, y1[r,z] + k1\ (1 - y1[r,z] - y2[r,z])) + \beta 3\ (k2\, y1[r,z] + k3\ (1 - y1[r,z] - y2[r,z])) + bo \left(\frac{\theta^{(1,0)}[r,z]}{r} + \theta^{(2,0)}[r,z]\right),$$
$$y1[r,0] == 0,\ y2[r,0] == 0,\ \theta[r,0] == 1,\ y1^{(1,0)}[eps,z] == 0,\ y2^{(1,0)}[eps,z] == 0,\ \theta^{(1,0)}[eps,z] == 0,\ y1^{(1,0)}[1,z] == 0,$$
$$y2^{(1,0)}[1,z] == 0,\ \theta^{(1,0)}[1,z] == hw\ (\theta w - \theta[1,z])\Big\}$$

In[5]:=
```
eqs /.
 {k1 → Exp[-1.74 + 21.6 (1 - 1/θ[r, z])], k2 → Exp[-4.24 + 25.1 (1 - 1/θ[r, z])],
  k3 → Exp[-3.89 + 22.9 (1 - 1/θ[r, z])], pe → 5.706, bo → 10.97,
  hw → 2.5, β1 → 5.106, β2 → 3.144, β3 → 11.16, θw → 1, eps → .0001}
```

Out[5]=

$$\Big\{y1^{(0,1)}[r,z] == 5.106\left(-e^{-4.24+25.1\left(1-\frac{1}{\theta[r,z]}\right)}\,y1[r,z]+e^{-1.74+21.6\left(1-\frac{1}{\theta[r,z]}\right)}\,(1-y1[r,z]-y2[r,z])\right)+5.706\left(\frac{y1^{(1,0)}[r,z]}{r}+y1^{(2,0)}[r,z]\right),$$

$$y2^{(0,1)}[r,z] == 5.106\left(e^{-4.24+25.1\left(1-\frac{1}{\theta[r,z]}\right)}\,y1[r,z]+e^{-3.89+22.9\left(1-\frac{1}{\theta[r,z]}\right)}\,(1-y1[r,z]-y2[r,z])\right)+5.706\left(\frac{y2^{(1,0)}[r,z]}{r}+y2^{(2,0)}[r,z]\right),$$

$$\theta^{(0,1)}[r,z] == 3.144\left(-e^{-4.24+25.1\left(1-\frac{1}{\theta[r,z]}\right)}\,y1[r,z]+e^{-1.74+21.6\left(1-\frac{1}{\theta[r,z]}\right)}\,(1-y1[r,z]-y2[r,z])\right)+11.16\left(e^{-4.24+25.1\left(1-\frac{1}{\theta[r,z]}\right)}\,y1[r,z]+e^{-3.89+22.9\left(1-\frac{1}{\theta[r,z]}\right)}\,(1-y1[r,z]-y2[r,z])\right)+10.97\left(\frac{\theta^{(1,0)}[r,z]}{r}+\theta^{(2,0)}[r,z]\right),\ y1[r,0]==0,\ y2[r,0]==0,$$

$$\theta[r,0]==1,\ y1^{(1,0)}[0.0001,z]==0,\ y2^{(1,0)}[0.0001,z]==0,\ \theta^{(1,0)}[0.0001,z]==0,\ y1^{(1,0)}[1,z]==0,\ y2^{(1,0)}[1,z]==0,\ \theta^{(1,0)}[1,z]==2.5\,(1-\theta[1,z])\Big\}$$

In[6]:=
```
NDSolve[%5, {y1[r, z], y2[r, z], θ[r, z]}, {r, .001, 1},
 {z, 0, 1}, Method → {"PDEDiscretization" → {"MethodOfLines",
    "SpatialDiscretization" → {"TensorProductGrid", "MinPoints" → 1000}}}]
```

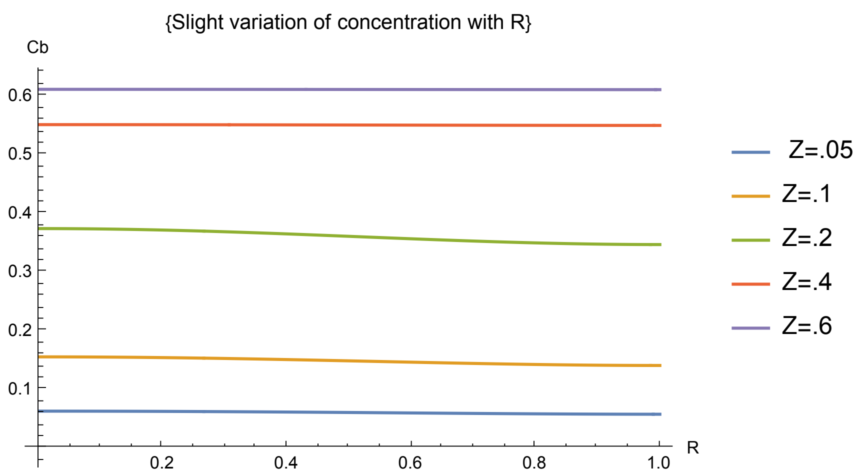
Out[6]=
```
{{y1[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}}
                                    Output: scalar
                                    Data not in notebook; Store now » ][r, z],
  y2[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}}
                                    Output: scalar
                                    Data not in notebook; Store now » ][r, z],
  θ[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}}
                                   Output: scalar
                                   Data not in notebook; Store now » ][r, z]}}
```

In[7]:=
```
ans = NDSolve[%5, {y1[r, z], y2[r, z], θ[r, z]}, {r, .0001, 1}, {z, 0, 1}]
```

Out[7]=
```
{{y1[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}} Output: scalar ][r, z],
  y2[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}} Output: scalar ][r, z],
  θ[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}} Output: scalar ][r, z]}}
```

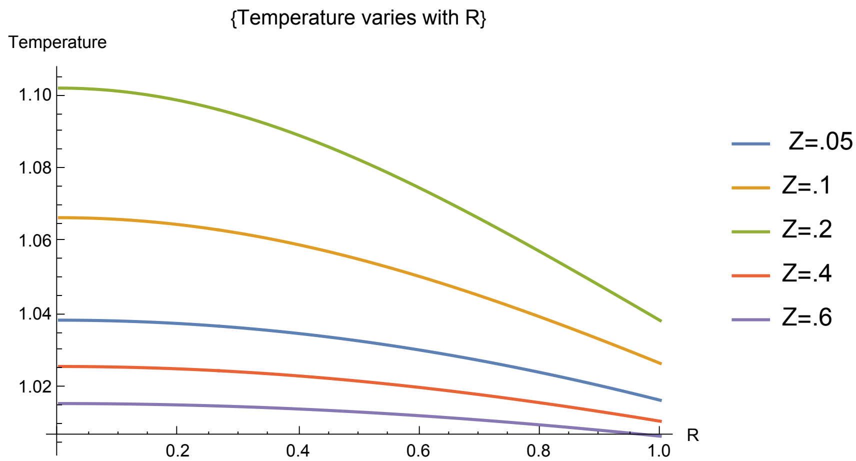
In[12]:=
```
Plot[{(y1[r, z] /. ans[[1]]) /. z → .05, (y1[r, z] /. ans[[1]]) /. z → .1,
   (y1[r, z] /. ans[[1]]) /. z → .2, (y1[r, z] /. ans[[1]]) /. z → .4,
   (y1[r, z] /. ans[[1]]) /. z → .6}, {r, .001, 1}, AxesLabel → {"R", "Cb"},
  PlotLegends → {" Z=.05", "Z=.1", "Z=.2", "Z=.4", "Z=.6"},
  PlotLabel → {"Slight variation of concentration with R"}]
```

Out[12]=



In[13]:=
```
Plot[{(θ[r, z] /. ans[[1]]) /. z → .05, (θ[r, z] /. ans[[1]]) /. z → .1,
   (θ[r, z] /. ans[[1]]) /. z → .2, (θ[r, z] /. ans[[1]]) /. z → .4,
   (θ[r, z] /. ans[[1]]) /. z → .6}, {r, .001, 1}, AxesLabel → {"R", "Temperature"},
  PlotLegends → {" Z=.05", "Z=.1", "Z=.2", "Z=.4", "Z=.6"},
  PlotLabel → {"Temperature varies with R"}]
```

Out[13]=

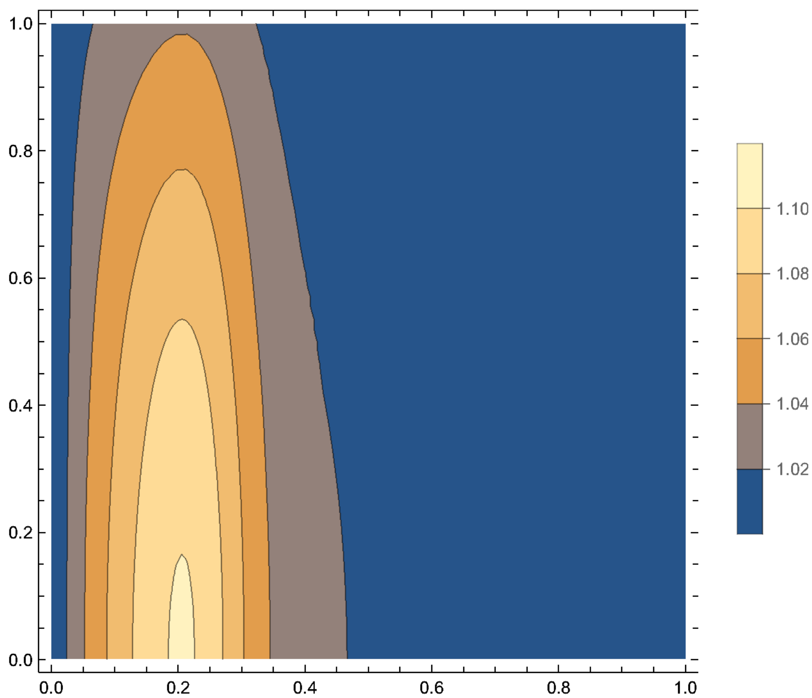


Contour plot of temperature

In[21]:=

```
ContourPlot[θ[r, z] /. ans[[1]], {z, 0, 1}, {r, .001, 1},
 AxesLabel → {"axial distance", "radial location"}, PlotLegends → Automatic]
```

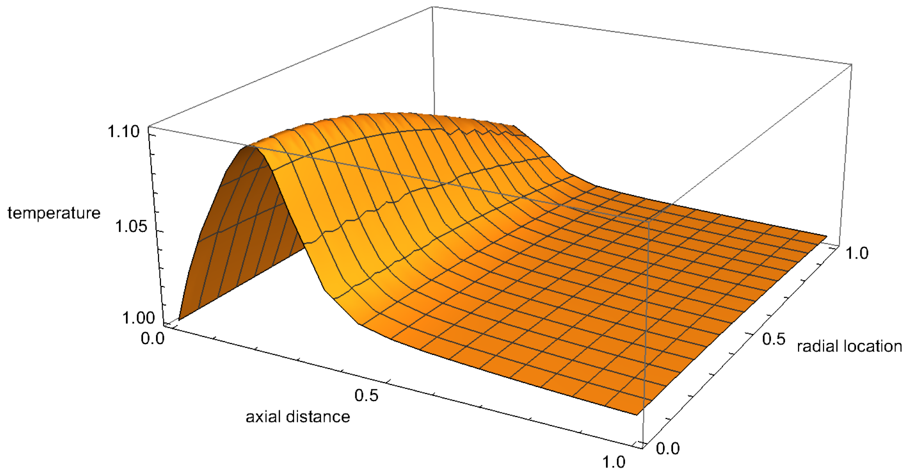
Out[21]=



3D plot of temperature

In[18]:=
```
Plot3D[θ[r, z] /. ans[[1]], {z, 0, 1}, {r, .001, 1},
 AxesLabel → {"axial distance", "radial location", "temperature"}]
```

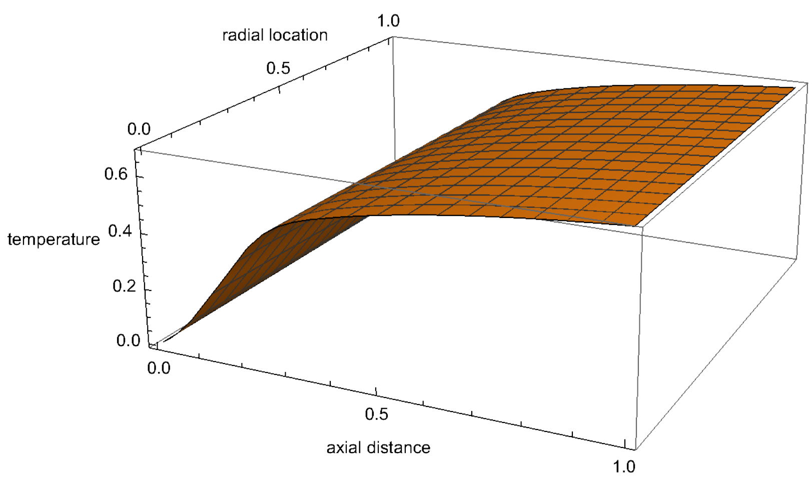
Out[18]=



3-D plot of product

In[19]:=
```
Plot3D[y1[r, z] /. ans[[1]], {z, 0, 1}, {r, .001, 1},
 AxesLabel → {"axial distance", "radial location", "temperature"}]
```

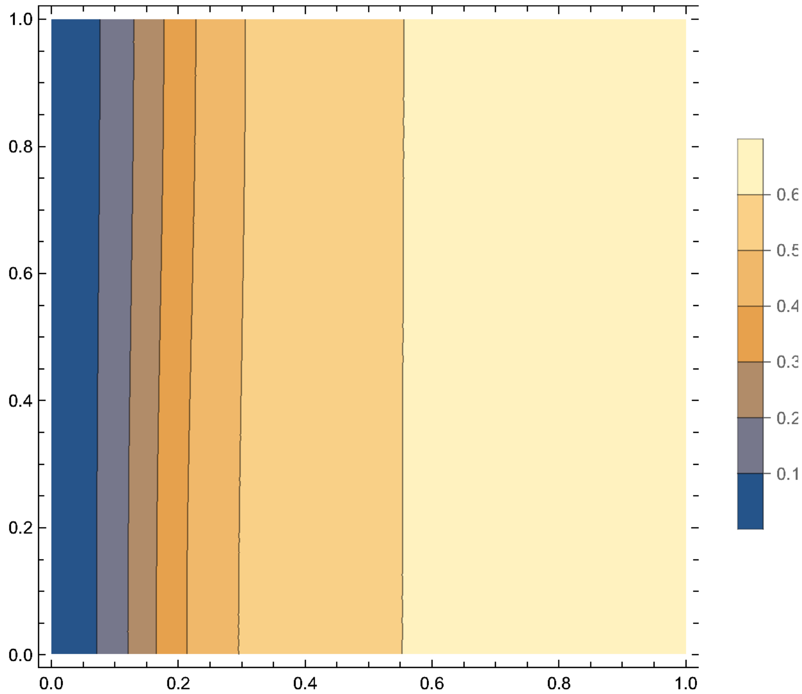
Out[19]=



Contour plot of product

In[22]:=
```
ContourPlot[y1[r, z] /. ans[[1]], {z, 0, 1}, {r, .001, 1},
 AxesLabel → {"axial distance", "radial location"}, PlotLegends → Automatic]
```

Out[22]=



Reduce cooling slightly, hw from 2.5 to 2.4

In[56]:=
```
eqs /.
 {k1 → Exp[-1.74 + 21.6 (1 - 1 / θ[r, z])], k2 → Exp[-4.24 + 25.1 (1 - 1 / θ[r, z])],
  k3 → Exp[-3.89 + 22.9 (1 - 1 / θ[r, z])], pe → 5.706, bo → 10.97,
  hw → 2.4, β1 → 5.106, β2 → 3.144, β3 → 11.16, θw → 1, eps → .0001}
```

Out[56]=
```
{y1^(0,1)[r, z] ==
  5.106 (-e^(-4.24+25.1 (1-1/θ[r,z])) y1[r, z] + e^(-1.74+21.6 (1-1/θ[r,z])) (1 - y1[r, z] - y2[r, z])) +
   5.706 (y1^(1,0)[r, z]/r + y1^(2,0)[r, z]), y2^(0,1)[r, z] ==
  5.106 (e^(-4.24+25.1 (1-1/θ[r,z])) y1[r, z] + e^(-3.89+22.9 (1-1/θ[r,z])) (1 - y1[r, z] - y2[r, z])) +
   5.706 (y2^(1,0)[r, z]/r + y2^(2,0)[r, z]), θ^(0,1)[r, z] ==
  3.144 (-e^(-4.24+25.1 (1-1/θ[r,z])) y1[r, z] + e^(-1.74+21.6 (1-1/θ[r,z])) (1 - y1[r, z] - y2[r, z])) +
   11.16 (e^(-4.24+25.1 (1-1/θ[r,z])) y1[r, z] + e^(-3.89+22.9 (1-1/θ[r,z])) (1 - y1[r, z] - y2[r, z])) +
   10.97 (θ^(1,0)[r, z]/r + θ^(2,0)[r, z]), y1[r, 0] == 0, y2[r, 0] == 0,
 θ[r, 0] == 1, y1^(1,0)[0.0001, z] == 0, y2^(1,0)[0.0001, z] == 0,
 θ^(1,0)[0.0001, z] == 0, y1^(1,0)[1, z] == 0,
 y2^(1,0)[1, z] == 0, θ^(1,0)[1, z] == 2.4 (1 - θ[1, z])}
```

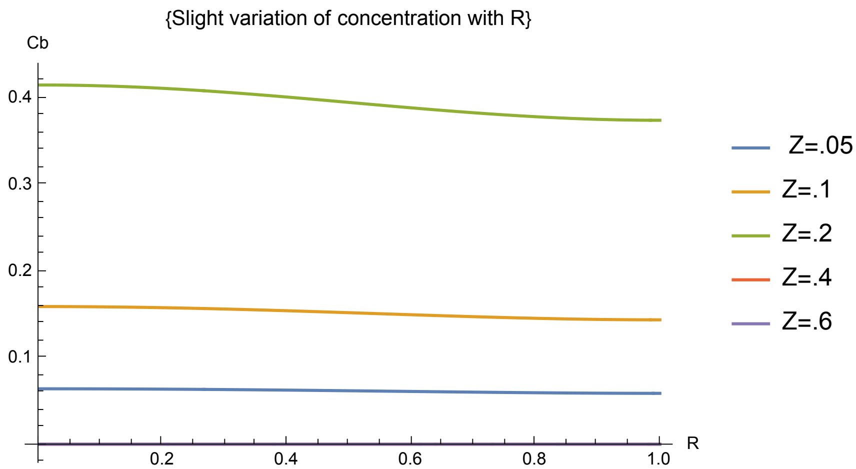
In[57]:=
```
ans2 = NDSolve[%, {y1[r, z], y2[r, z], θ[r, z]}, {r, .0001, 1}, {z, 0, 1}]
```

Out[57]=
```
{{y1[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}} Output: scalar ][r, z],
  y2[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}} Output: scalar ][r, z],
  θ[r, z] → InterpolatingFunction[ Domain: {{0.0001, 1.}, {0., 1.}} Output: scalar ][r, z]}}
```

We see that our product reacts further to CO2 and water

In[59]:=
```
Plot[{(y1[r, z] /. ans2[[1]]) /. z → .05, (y1[r, z] /. ans2[[1]]) /. z → .1,
   (y1[r, z] /. ans2[[1]]) /. z → .2, (y1[r, z] /. ans2[[1]]) /. z → .4,
   (y1[r, z] /. ans2[[1]]) /. z → .6}, {r, .001, 1}, AxesLabel → {"R", "Cb"},
 PlotLegends → {" Z=.05", "Z=.1", "Z=.2", "Z=.4", "Z=.6"},
 PlotLabel → {"Slight variation of concentration with R"}]
```

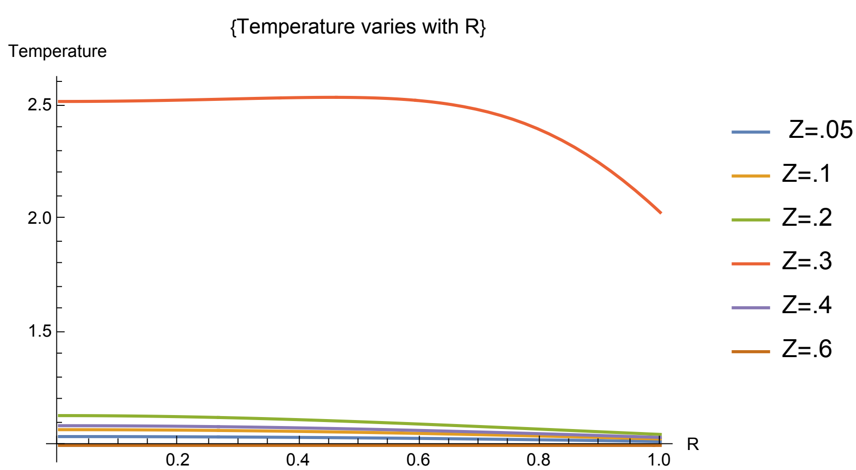
Out[59]=



Maybe not surprising the temperature gets very high!

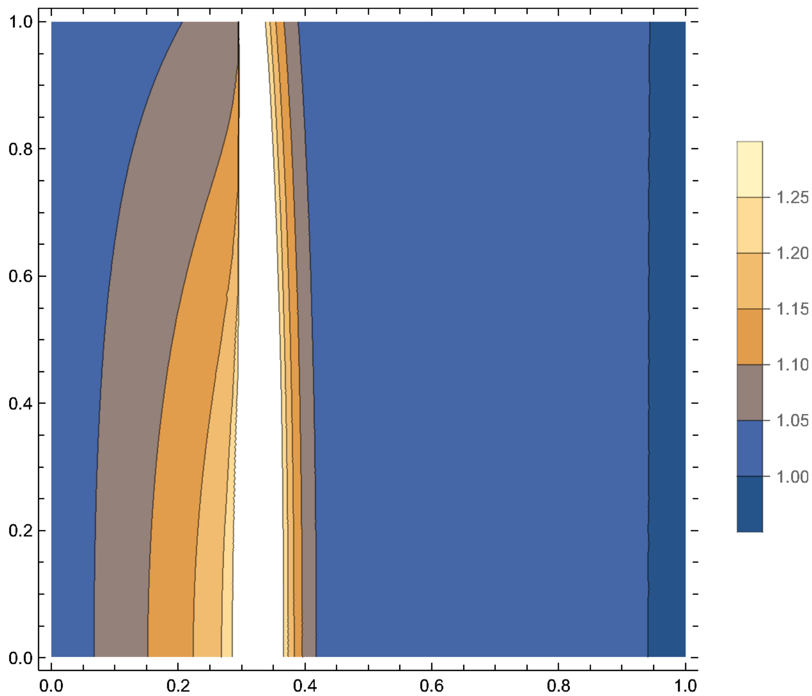
In[65]:=
```
Plot[{(θ[r, z] /. ans2[[1]]) /. z → .05, (θ[r, z] /. ans2[[1]]) /. z → .1,
   (θ[r, z] /. ans2[[1]]) /. z → .2, (θ[r, z] /. ans2[[1]]) /. z → .3,
   (θ[r, z] /. ans2[[1]]) /. z → .4, (θ[r, z] /. ans2[[1]]) /. z → .6},
 {r, .001, 1}, AxesLabel → {"R", "Temperature"},
 PlotLegends → {" Z=.05", "Z=.1", "Z=.2", "Z=.3", "Z=.4", "Z=.6"},
 PlotLabel → {"Temperature varies with R"}, PlotRange → All]
```

Out[65]=



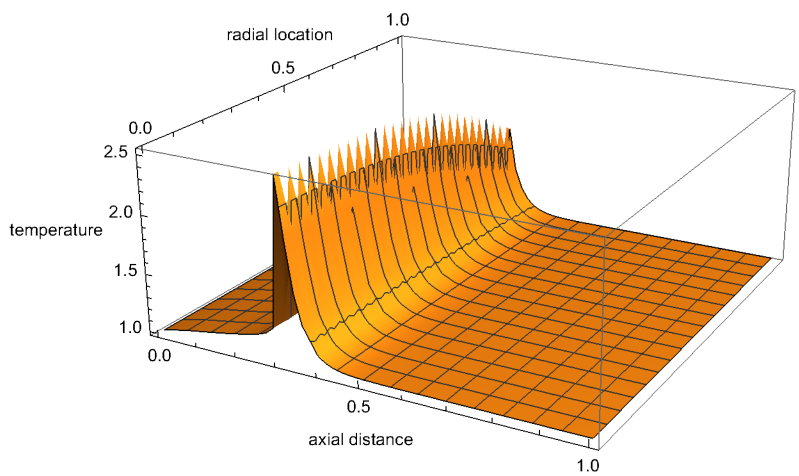
In[62]:=
```
ContourPlot[θ[r, z] /. ans2[[1]], {z, 0, 1}, {r, .001, 1},
 AxesLabel → {"axial distance", "radial location"}, PlotLegends → Automatic]
```

Out[62]=



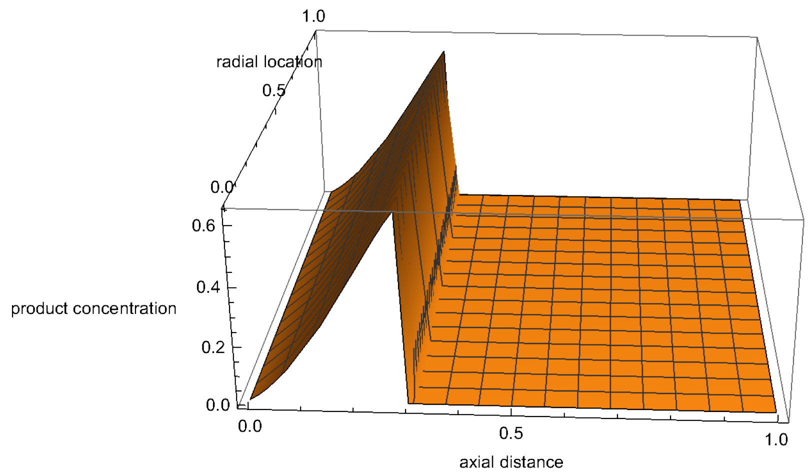

```
In[66]:= Plot3D[θ[r, z] /. ans2[[1]], {z, 0, 1}, {r, .001, 1},
          AxesLabel → {"axial distance", "radial location", "temperature"}, PlotRange → All]
```

Out[66]=



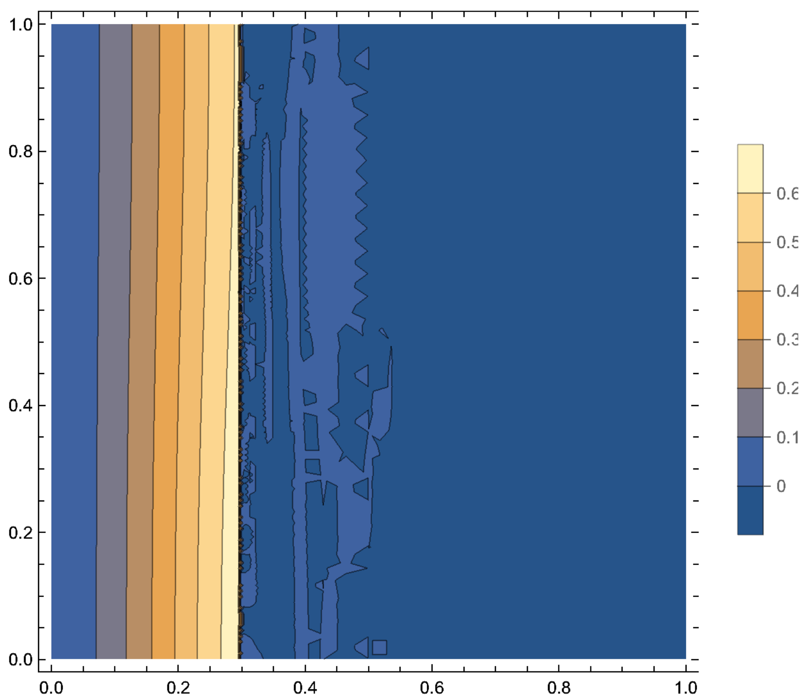

```
In[68]:= Plot3D[y1[r, z] /. ans2[[1]], {z, 0, 1}, {r, .001, 1},
          AxesLabel → {"axial distance", "radial location", "product concentration"}]
```

Out[68]=



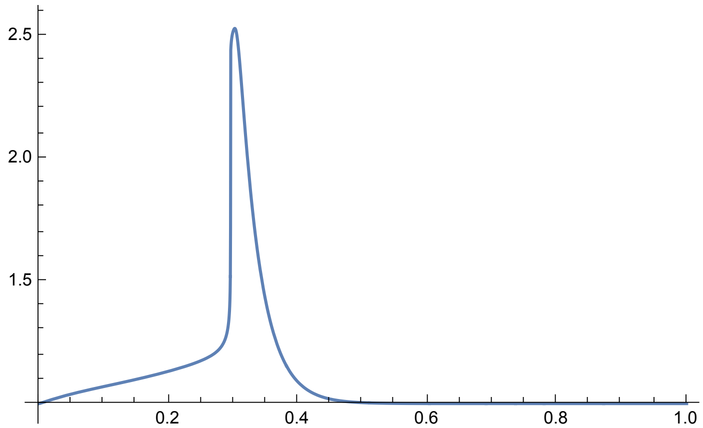

```
In[70]:= ContourPlot[y1[r, z] /. ans2[[1]], {z, 0, 1}, {r, .001, 1},
  AxesLabel → {"axial distance", "radial location"}, PlotLegends → Automatic]
```

Out[70]=



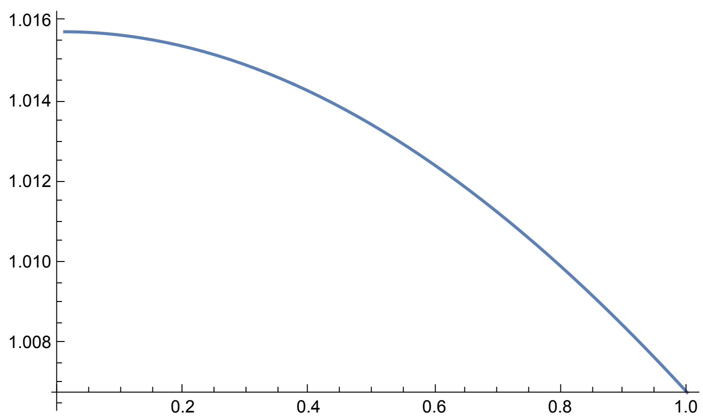
In[72]:=
```
Plot[(θ[r, z] /. ans2[[1]]) /. r → .01, {z, 0, 1}, PlotRange → All]
```

Out[72]=



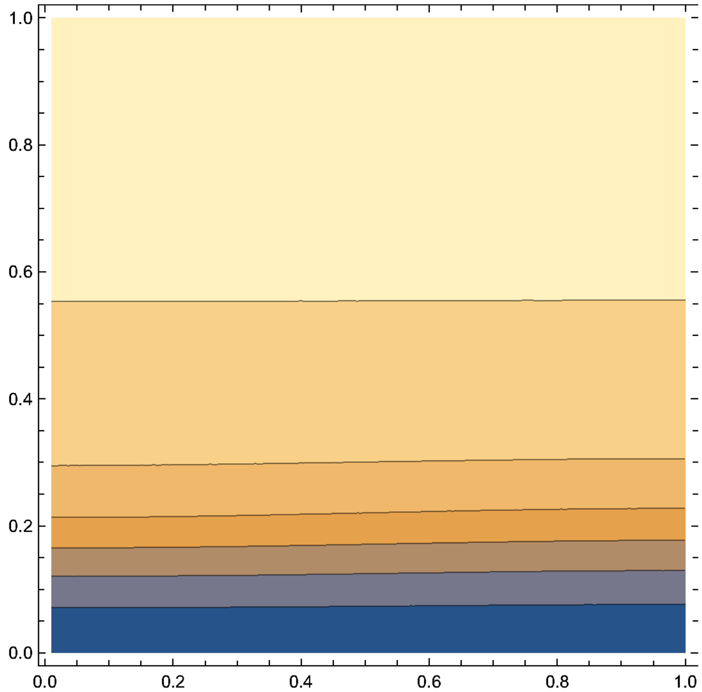
In[∘]:=
```
Plot[(θ[r, z] /. %39[[1]]) /. z → .6, {r, .01, 1}]
```

Out[∘]=



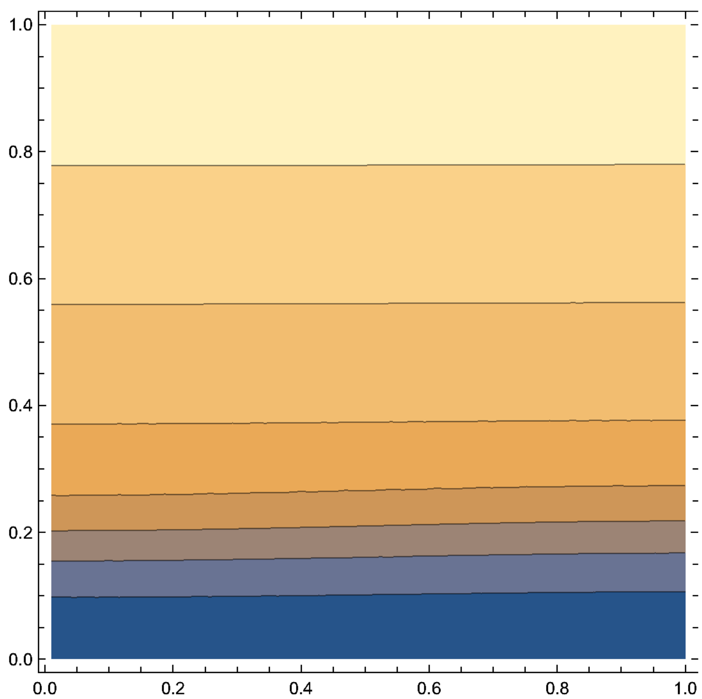
In[∘]:=
```
ContourPlot[y1[r, z] /. %119[[1]], {r, .01, 1}, {z, 0, 1}]
```

Out[∘]=



In[∘]:=
```
ContourPlot[y2[r, z] /. %119[[1]], {r, .01, 1}, {z, 0, 1}]
```

Out[∘]=



In[∘]:=
```
ContourPlot[θ[r, z] /. %119[[1]], {r, .01, 1}, {z, 0, 1}]
```

Out[∘]=