Checking the Beer Paper with *Mathematica*: Question 5

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Run this command once per experiment to clear out model solution variables stored in memory.

In[1]:=
```
Clear[solution, bubbledata]
```

Enter parameters in model.

In[2]:=
```
ρbeer = 1.010 * 10^3;
g = 9.807;
R = 8.3145;
P = 1.013 * 10^5;
mCO2 = 4.401 * 10^-2;
η = 1.3 * 10^-3;
T = 281;
k = 7.5 * 10^-3;
```

Solve the system of ordinary differential equations (ODE) with initial data numerically.

In[10]:=
```
Clear[k, d]
```

In[11]:=
```
solution[k_, d_] := NDSolve[
  {n'[t] == 4 * π * k * (3 * n[t] * R * T / (4 * π * (P - g * ρbeer * x[t])))^(2/3),
   x'[t] == y[t],
   y'[t] ==
    g * (ρbeer * R * T / (mCO2 * (P - g * ρbeer * x[t])) - 1) - (d * y[t] / (mCO2 * n[t])) * (3 * n[t] * R * T / (4 * π * (P - g * ρbeer * x[t])))^(2/3),
   x[0] == -0.156,
   y[0] == 0,
   n[0] == 9 * 10^-10},
  {x, y, n}, {t, 5}];
```

In[12]:=
```
solution[2 * 10^-3, 260]
```

Out[12]=
```
{{x → InterpolatingFunction[{{0., 5.}}, <>],
  y → InterpolatingFunction[{{0., 5.}}, <>],
  n → InterpolatingFunction[{{0., 5.}}, <>]}}
```

In[13]:=
```
solution[2 * 10^-3, 260][[1]]
```

Out[13]=
```
{x → InterpolatingFunction[{{0., 5.}}, <>],
 y → InterpolatingFunction[{{0., 5.}}, <>],
 n → InterpolatingFunction[{{0., 5.}}, <>]}
```

Use the solution to the system of ODE to find bubble radius at each time increment and display bubble data in a table.

In[14]:=
$$r[t_] := \left(\frac{3 * n[t] * R * T}{4 * \pi * (P - g * \rho_{beer} * x[t])}\right)^{1/3};$$

In[15]:=
```
bubbledata[k_, d_] := Table[
   Evaluate[{t, 100 * x[t], r[t] / r[0]} /. solution[k, d][[1]]], {t, 0, 3.78, 0.54}];
```

In[16]:=
```
bubbledata[2 * 10^-3, 260]
```

Out[16]=
```
{{0., -15.6, 1.}, {0.54, -14.0351, 1.1453}, {1.08, -12.258, 1.29098},
 {1.62, -10.2679, 1.43712}, {2.16, -8.06435, 1.58375},
 {2.7, -5.64642, 1.73093}, {3.24, -3.01333, 1.8787}, {3.78, -0.164137, 2.02714}}
```

In[17]:=
$$\texttt{TableForm}\left[\texttt{bubbledata}[2 * 10^{-3}, 260],\ \texttt{TableHeadings} \to \left\{\texttt{None}, \left\{\texttt{"time (sec)"}, \texttt{"depth (cm)"}, \texttt{"}\frac{\texttt{radius}}{\texttt{initial radius}}\texttt{"}\right\}\right\}\right]$$

Out[17]//TableForm=

time (sec)	depth (cm)	$\frac{\text{radius}}{\text{initial radius}}$
0.	-15.6	1.
0.54	-14.0351	1.1453
1.08	-12.258	1.29098
1.62	-10.2679	1.43712
2.16	-8.06435	1.58375
2.7	-5.64642	1.73093
3.24	-3.01333	1.8787
3.78	-0.164137	2.02714

Make a list of the actual data values, with {time, depth, and radius/initial radius} for each time t = 0, 0.54, ... , 3.78 seconds.

In[18]:=
```
actualdata =
  {{0, -15.6, 1}, {0.54, -14.4, 1.15}, {1.08, -12.2, 1.29}, {1.62, -10.4, 1.44},
   {2.16, -8.6, 1.58}, {2.70, -6.0, 1.73}, {3.24, -3.2, 1.88}, {3.78, 0, 2.03}};
```

Error[k,d] finds the sum of the square errors (SSE) between model's bubble depth and measured bubble depth, as a function of the parameters k and d .

In[19]:=
```
Error[k_, d_] :=
 Sum[(bubbledata[k, d][[i, 2]] - actualdata[[i, 2]])^2, {i, 1, Length[actualdata]}]
```

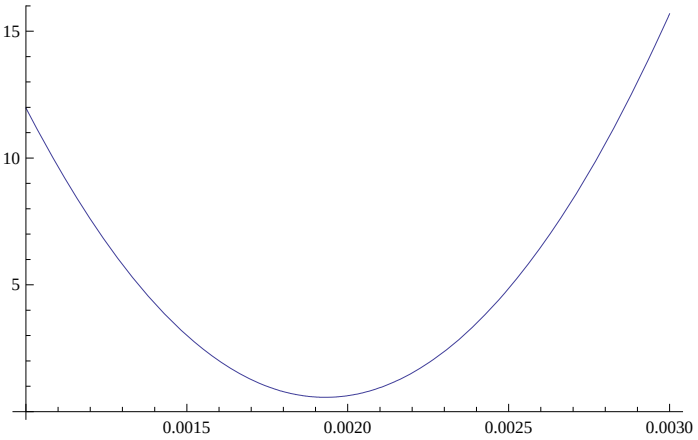
In[20]:=
```
Error[0.002, 260]
```

Out[20]=
```
0.627665
```

Study the SSE for values of k and d near k = 0.002 moles · m^{-2} · $s^{-1}$and d = 260 N · sec · m^{-3} graphically using Plot and Plot3D - it looks like there may be smaller SSE different choices of k and d!

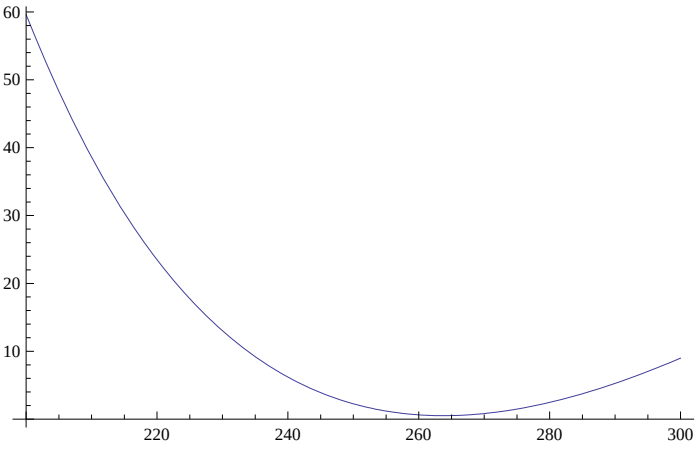
In[21]:=
```
Plot[Error[k, 260], {k, 0.001, 0.003}]
```

Out[21]=



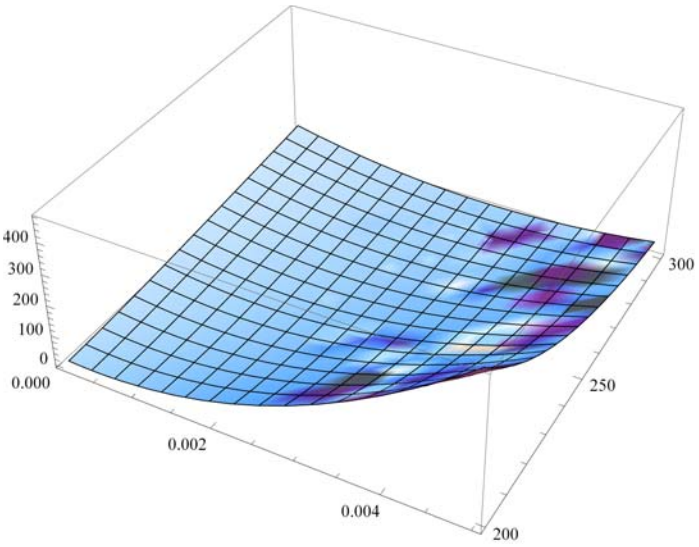
In[22]:=
```
Plot[Error[0.002, d], {d, 200, 300}]
```

Out[22]=



In[23]:=
```
Plot3D[Error[k, d], {k, 0.0001, 0.005}, {d, 200, 300}, PlotRange → All]
```

Out[23]=



Make a table of SSE values for choices of k and d, for k between 0.001 and 0.003 moles · m^{-2} · s^{-1} in steps of 0.0001 and for d between 255 and 275 N · sec · m^{-3} in steps of 1.

In[24]:=
```
ErrorData = Partition[
  Flatten[Table[{k, d, Error[k, d]}, {k, 0.001, 0.003, 0.0001}, {d, 255, 275, 1}]], 3]
```

Out[24]=
```
{{0.001, 255, 9.53067}, {0.001, 256, 10.0002}, {0.001, 257, 10.4798},
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```
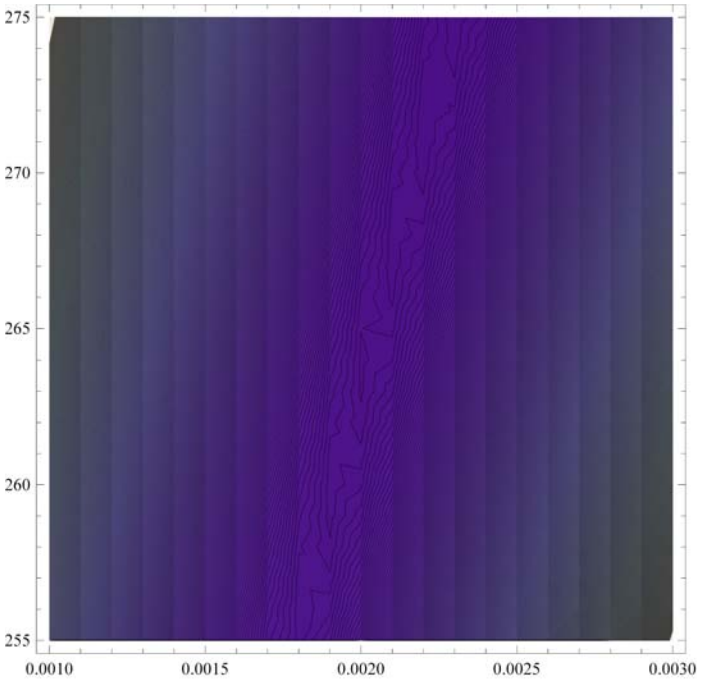
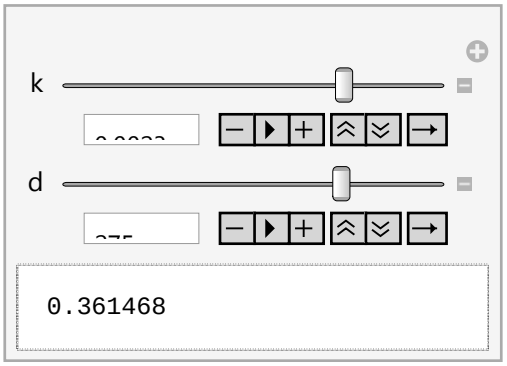

Use a ListContourPlot to study the SSE from the table we have produced (moving the mouse pointer over the table, one can see the SSE displayed).

In[25]:=
```
ListContourPlot[ErrorData, Contours → 500]
```

Out[25]=



Use a Manipulate command to study the SSE - one finds an SSE of 0.361468 cm^2 with k = 0.023 moles $\cdot m^{-2} \cdot s^{-1}$and d = 275 N $\cdot$ sec $\cdot m^{-3}$.

In[26]:=
```
Manipulate[Error[k, d], {k, 0.0001, 0.003, 0.0001}, {d, 200, 300, 1}]
```

Out[26]=