Project report

SFC Flow

D Malan
Department of Chemistry
University of Pretoria
5 December 2019

Introduction

The aim of this project is to get a feeling for how much the flow through the SFC is determined by the number of columns.

Experimental

The SFC pump was filled and set to a pressure of 200 atm. The flow trough the restrictor was measured.
"The choice was a simple linear restrictor and we trusted that heating the end of the restrictor would prevent discrimination. The final linear restrictor was 800mm long and had an internal diameter of 0.050mm."[1]
A different number of columns were connected in series, starting with one, and working up to 5. As a control, the flow without any columns connected were also measured.
"The SFC column we used in the SFC×GC system was ... HPLC columns (150mm × 4.6mm, 3μm particles) (Restek, Pinnacle DB Silica) connected in series."[2]
The time taken for 50 ml of gaseous carbon dioxide to flow through a bubble flow meter was measured with a hand-held stopwatch, and typed into an Excel spreadsheet.

Data analysis

Import the data:

In[1]:=
```
data = Import[
   "\\\\chemserv\\CHEMBACK\\HPLC-GC\\Varian-SFC-x-GC#R2-26\\ANAL\\EgmontR\\Niel\\Dropbox
     \\2019_12_04_SFC_Flow.xlsx", "DataLegacy"];
```

In[•]:=
```
data[[2]][[1 ;; 10]] // Grid
```

Out[•]=

Date	Time	Column A				
4/12/2019		Fed via	Link 1			
	Volume of gas	Time	Time	Flow		
	ml	s	min	ml/min	ml/min	1.
	50.	6.29	0.104833	476.948		1.
	50.	6.19	0.103167	484.653		1.
	50.	6.31	0.105167	475.436		1.
	50.	6.15	0.1025	487.805		1.
	50.	6.17	0.102833	486.224	482.213	1.

Data are in the following ranges. The list (a copy & paste from Excel[3]) gives the line number before the data starts, followed by the number of lines.

In[2]:=
```
datarange = Flatten[#[[1]] + Range[#[[2]]] & /@
    {{4, 5}, {13, 5}, {23, 5}, {34, 6}, {45, 6}, {56, 6}, {68, 6}, {79, 6}, {90, 6}, {102, 6}}]
```

Out[2]=
```
{5, 6, 7, 8, 9, 14, 15, 16, 17, 18, 24, 25, 26, 27, 28, 35, 36, 37, 38,
 39, 40, 46, 47, 48, 49, 50, 51, 57, 58, 59, 60, 61, 62, 69, 70, 71, 72, 73, 74,
 80, 81, 82, 83, 84, 85, 91, 92, 93, 94, 95, 96, 103, 104, 105, 106, 107, 108}
```

In[ ]:=
```
Length[datarange]
```

Out[ ]=
```
57
```

In[3]:=
```
flow = data[[2]][[datarange, {6, 8}]]
```

Out[3]=
```
{{476.948, 1.}, {484.653, 1.}, {475.436, 1.}, {487.805, 1.}, {486.224, 1.}, {480., 2.},
 {483.871, 2.}, {483.871, 2.}, {487.013, 2.}, {477.707, 2.}, {473.186, 3.}, {465.839, 3.},
 {467.29, 3.}, {468.019, 3.}, {474.684, 3.}, {463.679, 4.}, {461.538, 4.}, {465.839, 4.},
 {468.75, 4.}, {475.436, 4.}, {464.396, 4.}, {455.235, 5.}, {465.116, 5.}, {460.829, 5.},
 {473.934, 5.}, {472.441, 5.}, {464.396, 5.}, {449.775, 6.}, {459.418, 6.},
 {455.235, 6.}, {456.621, 6.}, {457.317, 6.}, {460.829, 6.}, {434.153, 7.},
 {436.681, 7.}, {432.9, 7.}, {436.681, 7.}, {436.047, 7.}, {430.416, 7.}, {465.116, 8.},
 {470.219, 8.}, {484.653, 8.}, {458.015, 8.}, {470.219, 8.}, {465.839, 8.}, {468.75, 9.},
 {460.829, 9.}, {471.698, 9.}, {467.29, 9.}, {469.484, 9.}, {474.684, 9.}, {420.757, 10.},
 {424.328, 10.}, {421.348, 10.}, {415.512, 10.}, {421.941, 10.}, {424.929, 10.}}
```

There are averages in the Excel sheet. The are at the last row of each range.

In[4]:=
```
avgrange = Flatten[#[[1]] + #[[2]] & /@
    {{4, 5}, {13, 5}, {23, 5}, {34, 6}, {45, 6}, {56, 6}, {68, 6}, {79, 6}, {90, 6}, {102, 6}}]
```

Out[4]=
```
{9, 18, 28, 40, 51, 62, 74, 85, 96, 108}
```

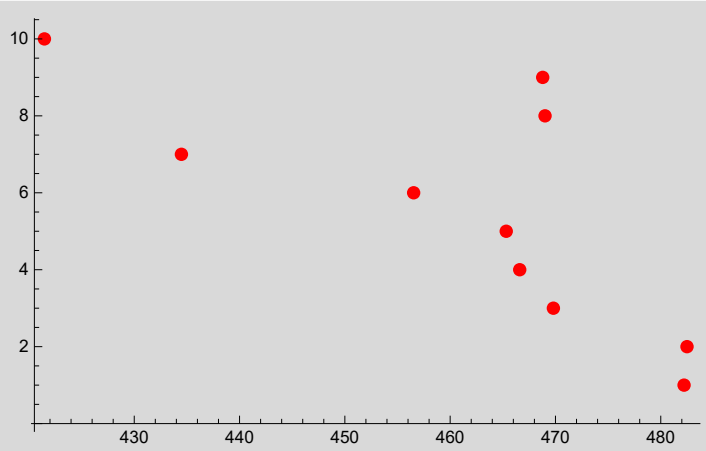
In[5]:=
```
flowavg = data[[2]][[avgrange, {7, 8}]]
```

Out[5]=
```
{{482.213, 1.}, {482.492, 2.}, {469.803, 3.}, {466.606, 4.}, {465.325, 5.},
 {456.533, 6.}, {434.48, 7.}, {469.01, 8.}, {468.789, 9.}, {421.469, 10.}}
```

In[ ]:=
```
ListPlot[{flow, flowavg},
 PlotStyle → {Blue, {Red, PointSize[0.02], ChartLabels → {0, 0, 1, 2}}}]
```

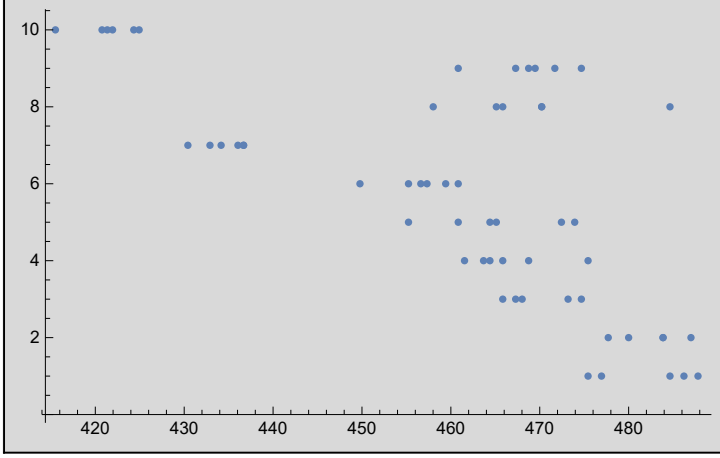
In[6]:=
```
flowavgplot = ListPlot[flowavg, PlotStyle → {Red, PointSize[0.02]}]
```

Out[6]=



In[7]:=
```
flowplot = ListPlot[flow]
```

Out[7]=



Prepare text for annotations:

In[8]:=
```
textlist = {"No. of columns", "1", "1", "2", "3", "3", "4", "5", "0", "0", "5"}
```

Out[8]=
```
{No. of columns, 1, 1, 2, 3, 3, 4, 5, 0, 0, 5}
```

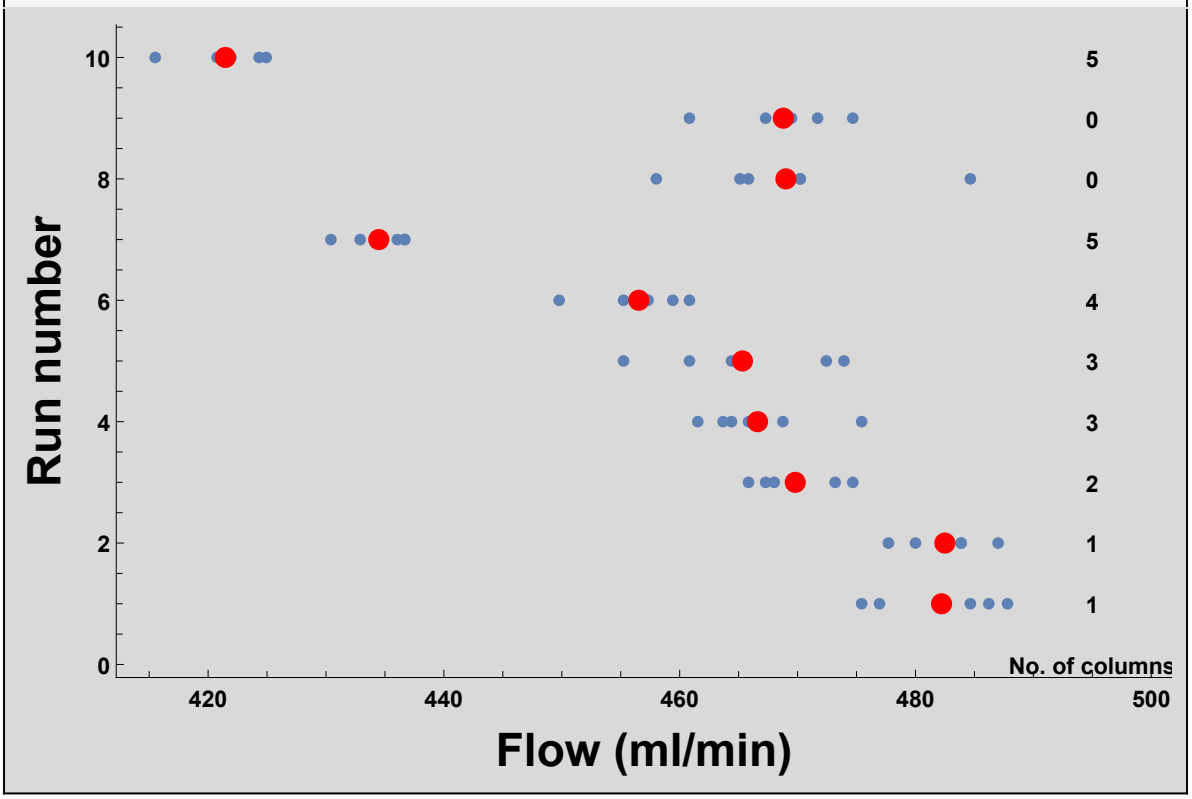
In[12]:=
```
textgraphics =
  MapIndexed[Graphics[Style[Text[#1, {495, #2[[1]] - 1}], Medium, Bold]] &, textlist];
```

Combine the graphics:

In[14]:=

```
Show[flowplot
 , flowavgplot
 , textgraphics
 , PlotStyle → {Automatic, {Red, PointSize[0.09]}}
 , Axes -> False
 , Frame → {True, True, False, False}
 , FrameLabel →
  {Style["Flow (ml/min)", Large, Black, Bold], Style["Run number", Large, Black, Bold]}
 , FrameStyle → Directive[Medium, Bold, Black]
 , ImageSize → 600
 , PlotRange → { {414, 500}, Automatic}]
```

Out[14]=



Results

The figure above summarizes the results. It is clear more columns leads to lower flow, but that inter-run repeatability is not very high. For runs 6 and 10 all five columns were in series, but there is a significant difference in flow. For runs 1 and two, with only one column connected, the flow is higher than the flow for runs 8 and 9, where there were no columns.
None of these observations suggest that the SFC separations will be significantly impacted with 5 columns in series.

Bibliography

A. [1] Malan, Daniel. 2019. "Fast temperature programmed chromatography coupled to supercritical fluid chromatography (SFC×GC)."

B. [2] Malan, Daniel. 2019. "Fast temperature programmed chromatography coupled to supercritica fluid chromatography (SFC×GC)."

C. [3] https://mathematica.stackexchange.com/questions/8997/cut-and-paste-data-from-a-spreadsheet