

```
1 #when F1=700
2
3 get_ipython().run_line_magic('reset', '-f')
4
5 import numpy as np
6 import pandas
7 import sympy
8 from termcolor import colored
9
10
11 ##### inputs
12
13 stream_direction = ["in","in","out","out"] # directions of streams
14 component_labels = ["Flow rate","Methene","Ethene","Propyne","Nitrogen","Oxygen","CO2"]
15 fraction_prefix = "y" # mass (x) or mole (y) fraction
16
17 ##### process relation
18
19 process_equation = ["F1=0.25*F2"] ## eg: "F1=0.25*F2" → 透過 list 隨意輸入 process relation
20
21 ##### input fraction , flow rate
22
23 #F1=700
24 y1M=0.33
25 y1E=0.29
26 y2N=0.79
27 y3M=0.1
28 y3P=0.3
29 y4E=0.06
30 y4O=0.07
31
32 y1N=0; y1O=0; y2M=0; y2E=0; y2P=0; y2C=0; y3N=0; y3O=0; y4P=0; y4C=0;
33
34 #####
```

```
37 Ns = len(stream_direction)
38 Nc = len(component_labels) - 1
39 Np = len(process_equation) → process_equation的長度就是Np數量
40
41
42
43 stream_labels = []
44 for i in range(Ns):
45     stream_labels.append("stream " + str(i+1) + "-" + stream_direction[i])
46
47
48 V_empty = np.empty([Ns, Nc+1], dtype=object)
49
50
51 df = pandas.DataFrame(V_empty, index=stream_labels, columns=component_labels)
52 print (df)
53
54
55 all_variables = []
56
57
58 for i in range(len(stream_direction)):
59     all_variables.append(component_labels[0][0] + str(i+1))
60
61
62 for i in range(len(component_labels[1:])):
63     for j in range(len(stream_direction)):
64         all_variables.append(fraction_prefix + str(j+1)
65                               + component_labels[i+1][0])
66
67
68
69 all_symbols = sympy.symbols(all_variables)
```

```

74 V_initial = V_empty.copy()
75
76 given_variables = []
77
78 unknown_index=[]
79 for i in range(len(all_variables)):
80
81
82     index_row = int(all_variables[i][1]) - 1
83
84     if all_variables[i][0] == component_labels[0][0]:
85         index_column = 0
86
87     else:
88         for j in range(len(component_labels)):
89
90             if all_variables[i][2] == component_labels[j][0]:
91                 index_column = j
92
93     if all_variables[i] in globals():
94
95         V_initial[index_row, index_column] = eval(all_variables[i])
96         given_variables.append(all_variables[i])
97     else:
98         V_initial[index_row, index_column] = all_symbols[i]
99         unknown_index.append([index_row,index_column])
100
101
102 print("\n")
103
104
105 df = pandas.DataFrame(V_initial, index=stream_labels, columns=component_labels)
106 print (df)

```

```
109 N_zeros = np.count_nonzero(v_initial == 0)
110 Nv = Ns*(Nc+1) - N_zeros + Np
111 Nd = Nv - Ns - Nc - Np
```

]  $\Rightarrow$  加入  $N_p$  後的  $N_v, N_d$

```
114 print ("\nThe number of total variables (zeros not included):", Nv)
115 print (colored("The number of design variables:", attrs=["bold"]), Nd)
116 print ("\nYou have given", len(given_variables)-N_zeros+Np, "variables")
```

```
120 if Np != 0:
121     print("\nThere are", Np, "process relations")
122     for i in process_equation:
123         print(i)
```

]  $\Rightarrow$   $N_p \neq 0$  時 print 出 process relation 的數量  
並將 process relation print 出

```
126 # Check if you have given too many or didn't give enough design variables
127 if len(given_variables)-N_zeros+Np > Nd:
128     print (colored("You have given too many input variables", "red"))
129 if len(given_variables)-N_zeros+Np < Nd:
130     print (colored("You didn't give enough input variables", "red"))
```

]  $\Rightarrow$  加入  $N_p$  後的判斷

```
133 u=0
134 for i in range(len(stream_direction)):
135     if all_variables[i] not in globals():
136         u+=1
137     if u==len(stream_direction):
138         print(colored("\nYou didn't provide any Flow information so can't solve the problem", "red"))
```

如果沒有定義任何  
Flow rate, 即顯示  
無法解

```

141 #####
142 sym_equations=[]
143
144 if Np!= 0:
145     function=process_equation
146     for i in range(len(process_equation)):
147         temp_eq=[]
148         n=0
149         for j in range(len(process_equation[i])):
150             if process_equation[i][j] == "=":
151                 n=1
152             if n>0:
153                 temp_eq.append("-("+process_equation[i][j+1:]+")")
154                 break
155             if n==0:
156                 temp_eq.append(process_equation[i][j])
157         function[i]="".join(temp_eq)
158
159 for i in range(len(process_equation)):
160     sym_equations.append(sympy.Eq((sympy.sympify(function[i])),0))
161
162 #####
163
164
165 unknown_variables = [element for element in all_variables if element not in given_variables]
166 number_unknowns = len(unknown_variables)
167 print ("\nThere are", number_unknowns, "unknown variables:")
168 print (*unknown_variables,sep=" ,")
169
170 signed_V = V_initial.copy()
171
172 for i in range(signed_V.shape[0]):
173     if stream_direction[i] == "out":
174         signed_V[i,0] = signed_V[i,0]*-1

```

當 $N_p \neq 0$ 時

整理 process equation

先尋找 process equation 中等號的位置  
並省略等號將等號右邊所有的東西  
括號起來並加上負號

最後放入 sym-equation 中

```

176 functions = []
177
178 for i in range(Nc):
179     functions.append(sum(signed_V[:,0]*signed_V[:,i+1]))
180
181 for i in range(Ns):
182     functions.append(sum(signed_V[i,1:]) - 1)
183
184
185 for i in functions:
186     sym_equations.append(sympy.Eq(i,0))
187
188
189 solutions = sympy.solve(sym_equations,unknown_variables)
190
191 solutions = eval(str(solutions))
192
193
194 Final_V = V_initial.copy()
195
196 if len(solutions)!=0:
197
198     print("\nThe solutions are:")
199
200     for i in range(len(unknown_variables)):
201         print(unknown_variables[i],"=",sympy.Float(solutions[0][i],5))
202
203     for i in range(len(unknown_variables)):
204         Final_V[unknown_index[i][0],unknown_index[i][1]] =sympy.Float(solutions[0][i],5)
205
206     for i in range(len(solutions[0])):
207         if int(solutions[0][i])<0:
208             print(colored("\nWarning !! The solution contains negative numbers","red"))
209             break

```

如果 process\_equation 中有已知項,最終的答案  
會得到解析解,所以還要將已知代入答案

如果 solution 中有負數  
將提出警告

210  
211  
212  
213  
214  
215  
216  
217  
218  
219  
220

```
elif len(solutions)==0 and len(given_variables)-N_zeros+Np == Nd:
```

```
    print(colored("\nWarning there should be existing dependent equations", "red", attrs=["bold"]))
```

```
print ("\n")
```

```
df = pandas.DataFrame(Final_V, index=stream_labels, columns=component_labels)
```

```
df
```

如果可以解但 solution  
為空集合代表有 dependant  
equation 存在