

Nonlinear least squares fitting: Use of 'Solver'

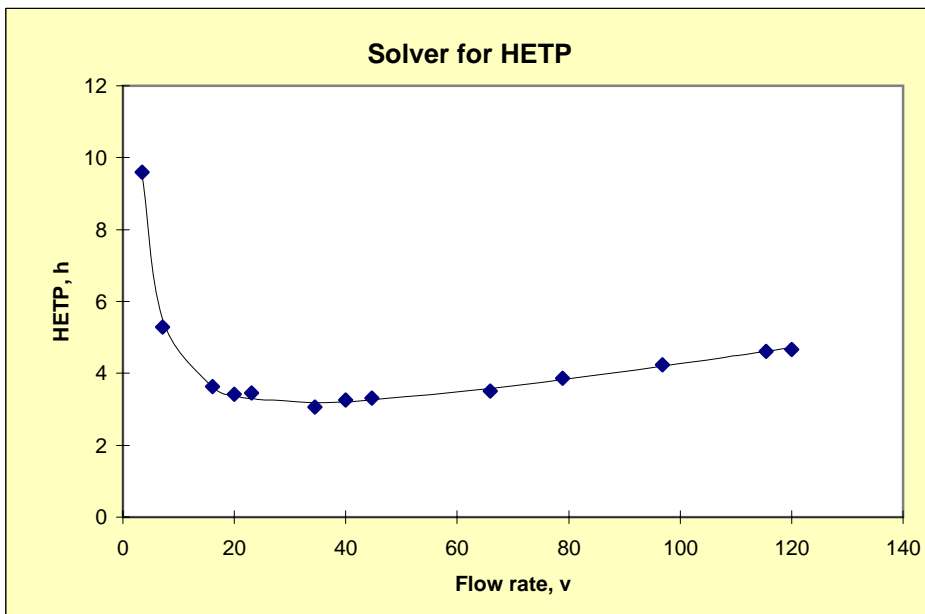
This is an example you should try to learn the SOLVER.

In separation chemistry, the height equivalent theoretical plate, h , of a column is dependent on the flow rate of mobile phase. The van Deemeter equation describes this relationship as

$$h = A + B / v + C v$$

where, A, B, and C are constants characteristics of the system related to eddy diffusion, longitudinal diffusion and speed of equilibrium, respectively. These constants are dependent on the solute-solvent, and solute-stat phase characteristics. Given the following data on $v - h$, the constants A, B, and C were estimated by using the 'Solver' program.

Obs#	Flow rate v , mL/min	HETP (mm) h -expt	Randomzd h -expt	Calculated h -calc	SQ-Resid $(h_e-h_c)^2$	Start with Guess values	Parameter	Optimized
1	3.4	9.59	9.548571	9.512027	0.00608	A=B=C=1		
2	7.1	5.29	5.288425	5.505509	0.046444			
3	16.1	3.63	3.625915	3.620365	9.28E-05		A	1.568078796
4	20	3.42	3.412824	3.391641	0.000804		B	26.72783956
5	23.1	3.46	3.48109	3.28781	0.029649		C	0.024358528
6	34.4	3.06	3.058986	3.182984	0.015125			
7	40	3.25	3.267739	3.210616	0.001551			
8	44.7	3.31	3.324423	3.254843	0.003042			
9	65.9	3.5	3.492008	3.578888	0.006223			
10	78.9	3.86	3.876448	3.828723	0.000978			
11	96.8	4.24	4.26214	4.202098	0.001437			
12	115.4	4.62	4.633442	4.610663	8.72E-05			
13	120	4.67	4.672605	4.713834	0.001921			
SSQR =					0.113435	<-- minimize this value		



NOTE: DON'T WORRY ABOUT RANDOMIZED VALUES
THEY ARE JUST FOR THE EXERCISE.

