VMGSim: Revisiting the Cavett Problem

By

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Introduction

VGMSim[1] (version 2.5.3) is a modern highly interactive steady state process simulation system It features auto determination of degrees of freedom and propagation of simulation data forward and backwards. Many of the developers were formerly associated with the HYSYS system.

VMGSim uses the Visio™ [2] system of MicroSoft (which must be purchased separately) to graphically input process flowsheets. However, VMGSim functions with or without Visio and the graphical component can be removed and replaced by a completely different package.

Among other powerful features of VMGSim is the integration of Excel at the unit operations level.

VMGSim has been used especially in the oil and gas, refining and petrochemical industries.

The Cavett Problem

The problem formulated by Cavett (1963) has been used to test tearing, sequencing and convergence procedures (Rosen and Pauls, 1977). The flowsheet (Seader and Henley, 1998) is equivalent to a four theoretical stage near isothermal distillation (rather than a conventional near isobaric type) for which a patent by Gunther[3] exists. An example, Gunther.vmp, is supplied as part of the VMGSim system.

Feed is fed to the four stage column at the second stage from the top. A partial condenser is the top stage and a partial reboiler is the fourth stage. Figure 3 specifies the feed conditions as well as the temperatures and pressures for each of the stages (named FL1, FL2, FL3 and FL4). The flow and composition of the two product streams are sought (P1 vapor stream from FL1 and P2 liquid stream from FL2 – see Figure 2).

Constructing the Flowsheet

Figure 1 is the drawing area upon which the flowsheet is constructed. The units and streams represented by the icons on the left are dragged one by one onto the drawing area. Clicking on the units and streams in the drawing area allows parameters to be specified.

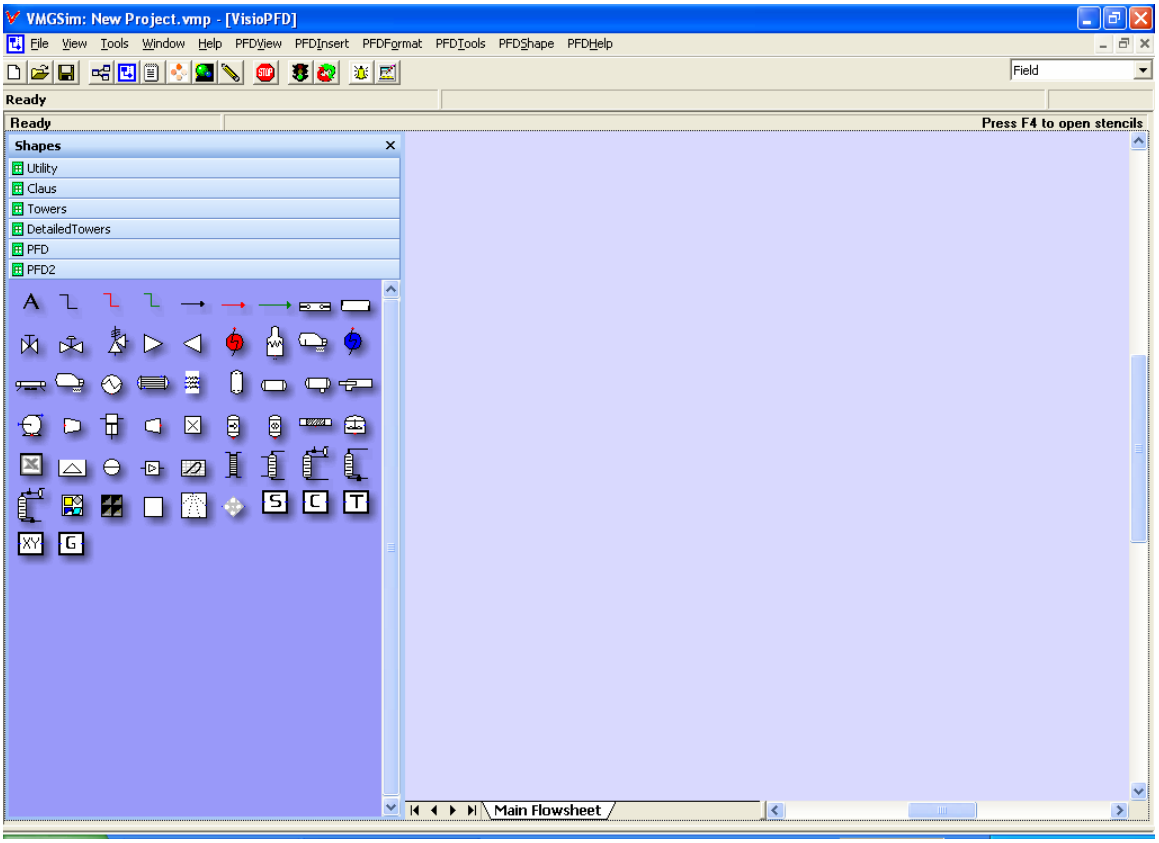

Figure 1. Stream, Unit Icons and the VMGSim Drawing Area

A degrees of freedom list for each unit is maintained. When the portion of the flowsheet that meets the degrees of freedom requirements has been input, the system automatically carries out the computations.

VMGSim does not have a separator for which temperature and pressure can be specified. Instead, compressors, valves, heaters and coolers must be used to simulate specified temperatures and pressures. Equilibrium flashes are enthalpy/pressure.

Figure 2 is the resulting flowsheet for the Cavett problem. When streams of different pressures are mixed (units AD1 and AD2), the outlet pressure is taken as the minimum. The unit names and key stream names follow that of Rosen and Pauls,1977.

During input, if an unknown stream (e.g. a recycle stream) is encountered, the stream is estimated (flow, temperature, pressure) utilizing a ~. The procedure is not unlike classical stream tearing.

Physical Properties

The physical properties available in the VMGSim system have been crafted to be applicable to the needs of the oil and gas, refining and petrochemical industries The default physical property system is an advanced Peng-Robinson. However, there are a large number of other options both for the vapor and liquid phases depending on the application.

Comparing Solutions

Figure 3 compares the VMGSim solution of the Cavett problem to that given by Rosen and Pauls, 1977.

The Rosen and Pauls, 1977 paper used FLOWTRAN to study the convergence properties of the problem and the speeding up of the otherwise slow convergence. Convergence was indicated when two successive iterations (scaled by the current value) of each component in the torn recycle streams (R1, R2, R3) was less than a small number (0.0005). An overall component balance was not used as a convergence criterion.

Figure 3 shows the inconsistencies in the overall component balance given in that paper. The ethane balance in particular is inconsistent (though this is more likely a typo in P1 and probably should be 2383.2 rather than 2883.2). Other than the ethane issue the largest inconsistency is in propane. Cavett, 1963 mentions the buildup of propane in all recycle loops (R1, R2, R3) which leads to slow convergence by direct iteration.

The VMGSim solution, however, rapidly converged and shows no such inconsistencies.

Other than the issues mentioned above, the two solutions compare favorably.

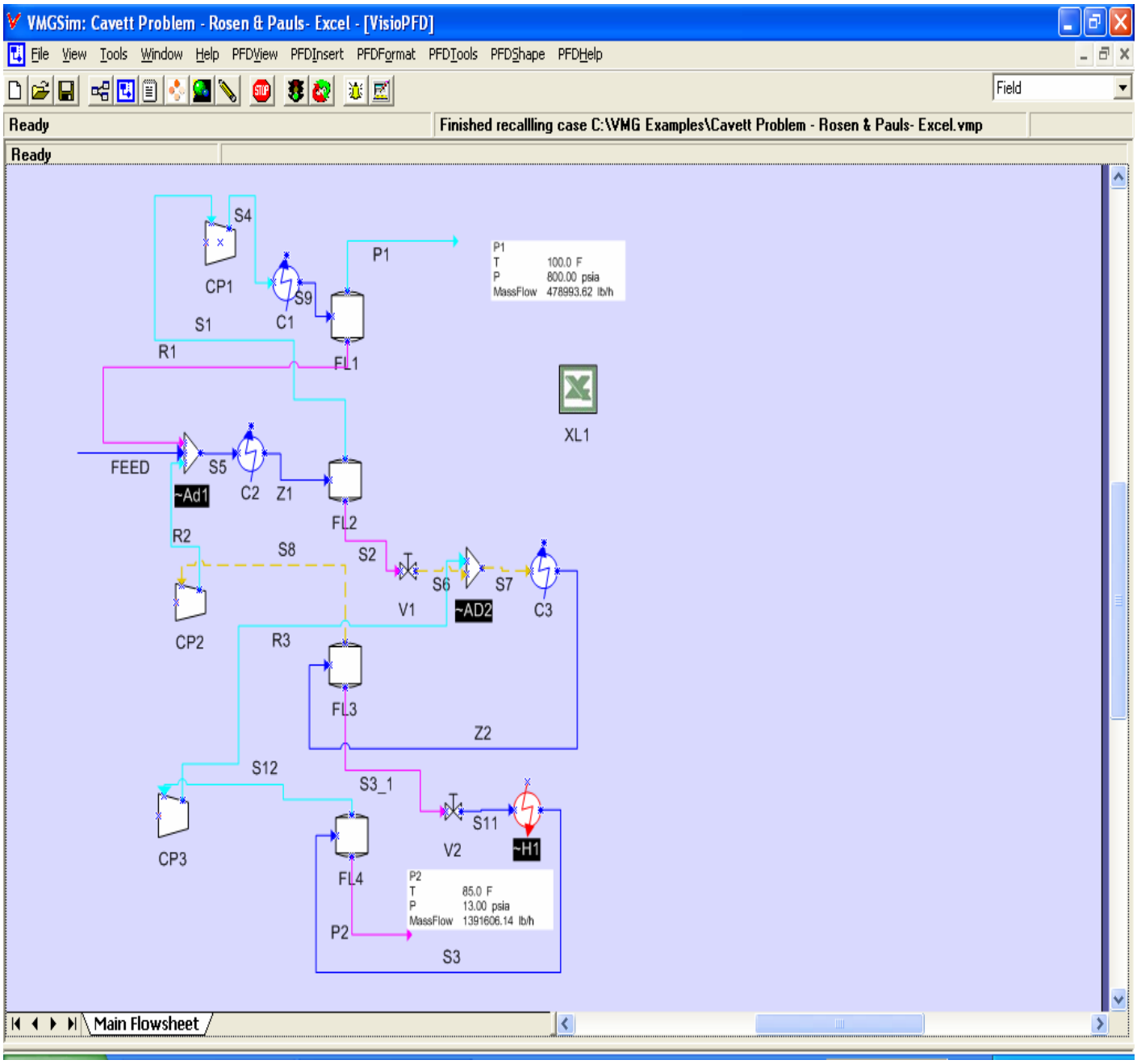

Figure 2. VMGSim Flowsheet of the Cavett Problem

Solution Comparisons VMGSim vs FLOWTRAN
Fixed Pressures in FL1, FL2, FL3, FL4 ==> 800, 270, 49, 13 psia
Fixed Temperatures in FL1, FL2,FL3, FL4 ==> 100, 120, 96, 85 F
Feed Temperature and Pressure ==> 120 F, 270 psia

	Feed	<===== ***P1***========>			<======= ***P2***======>			
	Flow Rate	***VMGSim***	***FLOWTRAN***		***VMGSim***	***FLOWTRAN***		***FLOWTRAN***
Component	mol/hr	APR*			APR*			***Imbalance***
Nitrogen	358.2	358.2	358.2		0	0.0009		0.0009
Carbon Dioxide	4965.6	4961.79	4964.7	#	3.81	4.73	#	3.83
Hydrogen Sulfide	339.4	334.95	334.7		4.45	5.22		0.52
Methane	2995.5	2995.35	2996.3		0.15	0.17		0.97
Ethane	2395.5	2378.28	***2883.2***	#	17.22	14.5	#	***502.2***
Propane	2291	1876.66	1899.1	#	414.34	404.2	#	12.3
Isobutane	604.1	197.73	198.2	#	406.37	410.3	#	4.4
n-Butane	1539.9	311.86	299.4	#	1228.04	1247.4	#	6.9
Isopentane	790.4	38.61	37.2		751.79	753.9		0.7
n-Pentane	1129.9	41.41	34.8		1088.49	1095.7		0.6
n-hexane	1764.7	11.14	10.5		1753.56	1754.6		0.4
n-heptane	2606.7	4.04	3.72		2602.66	2603.2		0.22
n-octane	1844.5	0.7	0.55		1843.8	1844		0.05
n-nonane	1669	0.15	0.12		1668.85	1668.9		0.02
n-decane	831.7	0.02	0.015		831.68	831.7		0.015
n-undecane	1214.5	0.01	0.007		1214.49	1214.5		0.007
								0
Total	27340.6	13510.9	14020.712	#	13829.7	13853.0209	#	533.1329

* APR - Advanced Peng-Robinson
# Imbalance in FLOWTRAN

Figure 3 VMGSim Solution Compared to FLOWTRAN
(FLOWTRAN Inbalance = P1+P2-Feed)

The icon for Excel in Figure 2 indicates that the spreadsheet of Figure 3 has been stored in Excel and can be accessed directly from the drawing area by clicking on the icon.

Conclusions

The VGMSim system provides a well formulated process simulation system when applied to the Cavett problem. It can successfully handle that problem with little difficulty. It did not display any particular convergence problems.

The Rosen and Pauls , 1977 study terminated the Cavett problem based on a looser convergence criterion than used by VMGSim. However, the focus of the Rosen and Pauls, 1977 study was on minimizing the number of iterations required for convergence.

VMGSim has many attractive features and does not have a particularly difficult learning curve.

Bibliography

1. Cavett, R. H., "Application of Numerical Methods to the Convergence of Simulated Processes Involving Recycle Loops", *American Petroleum Institute*, **43**, 57 (1963).

2. Rosen, E. M. and A. C. Pauls, "Computer Aided Chemical Process Design: The FLOWTRAN System", *Computers and Chemical Engineering*, **1**, 11-21 (1977).

3. Seader, J. D. and E. J. Henley, *Separation Process Principles*, John Wiley and Sons, Inc (New York) 1998, *Exercise* 10.35

Acknowledgement

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[1] See http://www.virtualmaterials.com
[2] See http://www.visio.com
[3] A. Gunther, U. S. Patent 3,575,077 (April 13, 1971)