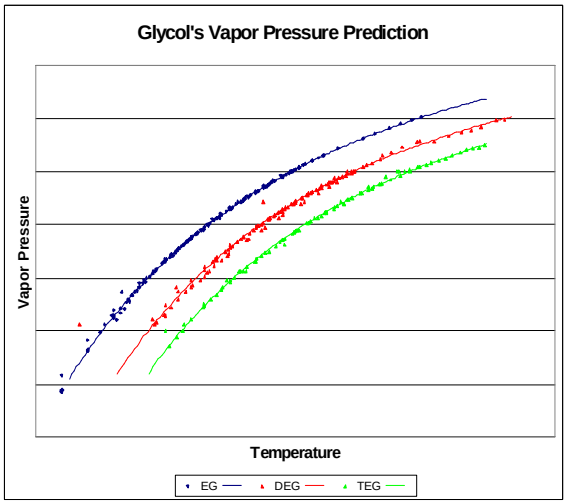
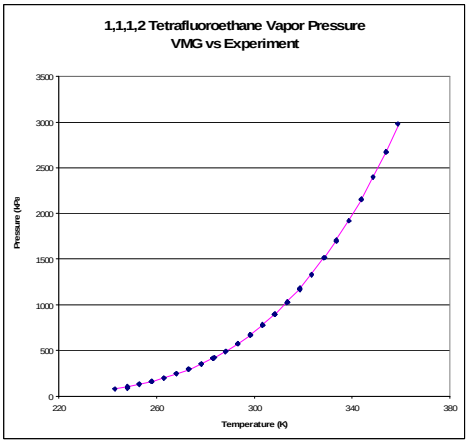
VMGThermo

Thermodynamics and Physical Property Software Component

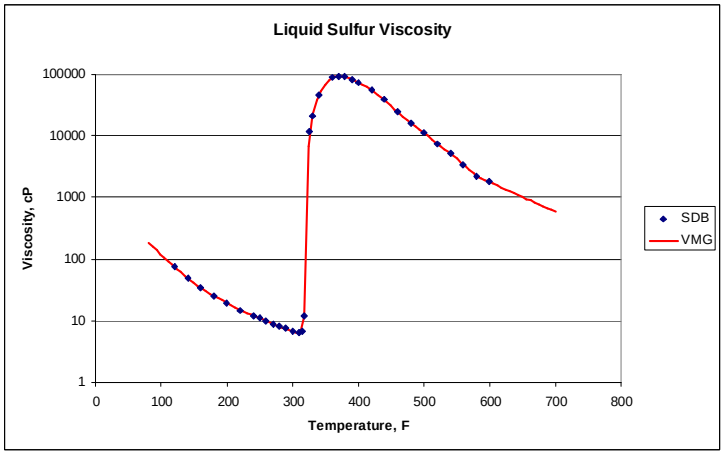
Accurate and reliable thermodynamics properties are essential for accurate and reliable process simulation and design of process equipment. Virtual Materials Group has invested many man-years of development and research into creating VMGThermo.

VMGThermo is a set of software components used for the calculation of thermo-physical properties as well as flash calculations. VMGThermo is a carefully crafted set of application programming interfaces, which can be used to power any application which can benefit from high quality physical properties. VMGThermo includes interfaces for EXCEL, Visual Basic, Delphi, Visual C++, C, C++ and FORTRAN. If you know how to use a spreadsheet, you can use VMGThermo.

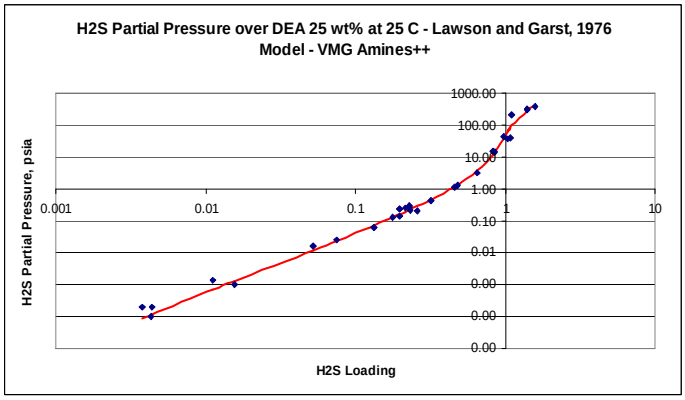


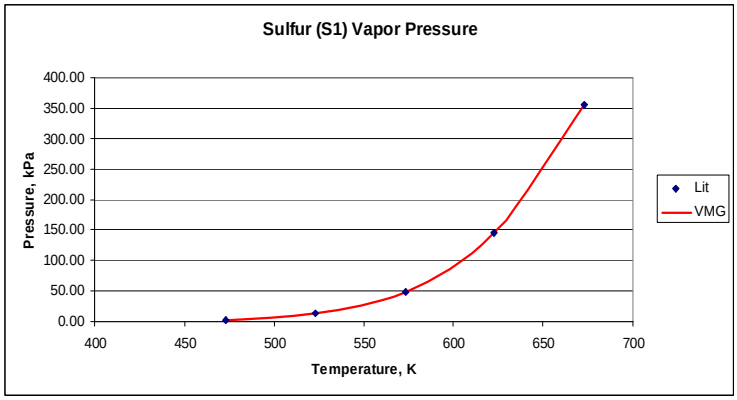


VMGThermo also ensures reliable and accurate process simulation modelling in VMGSim, the steady-state process flowsheet simulator.



VMGThermo provides a complete set of physical and thermodynamic properties for pure components and mixtures over a wide range of pressures, temperatures, compositions and phases. VMGThermo includes a comprehensive pure component database with nearly 5500 pure components, with more than 100 physical properties per component. These include important properties for environmental applications such as maximum exposure limits, adsorption capacity in activated carbon and solubility in water.





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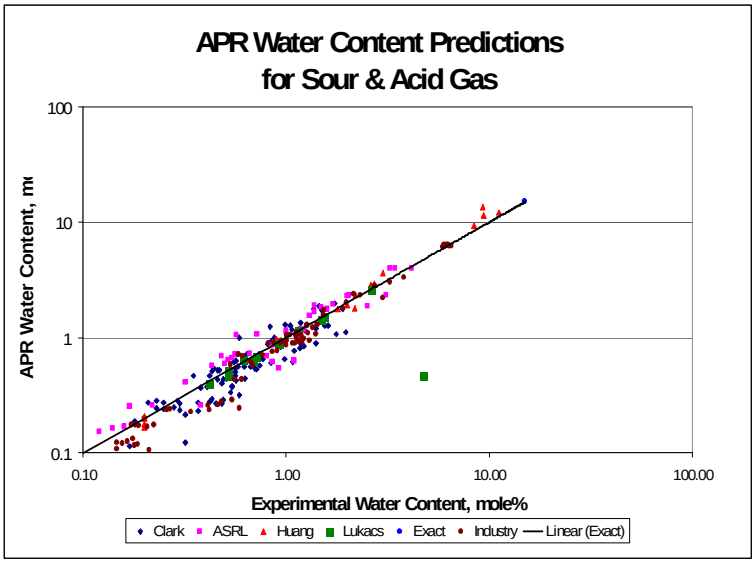
EOS++

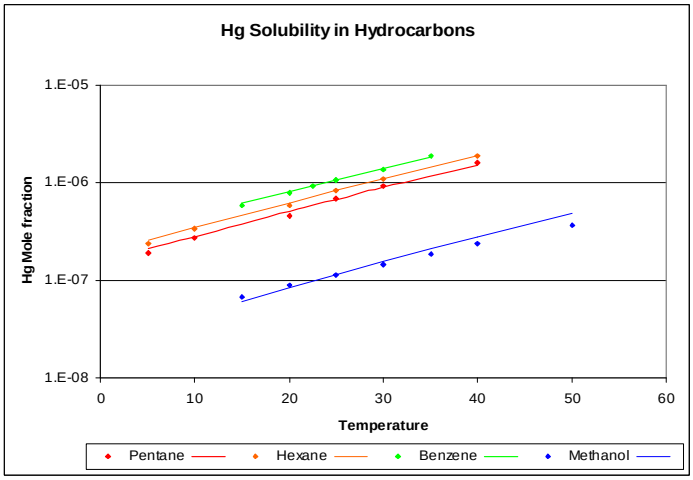
A subset of VMGThermo is called EOS++ and this includes a number of equation of state models. The EOS++ equations of state for hydrocarbon processing include more than 250 interaction parameters fitted for the wide range of process conditions found in the industry.

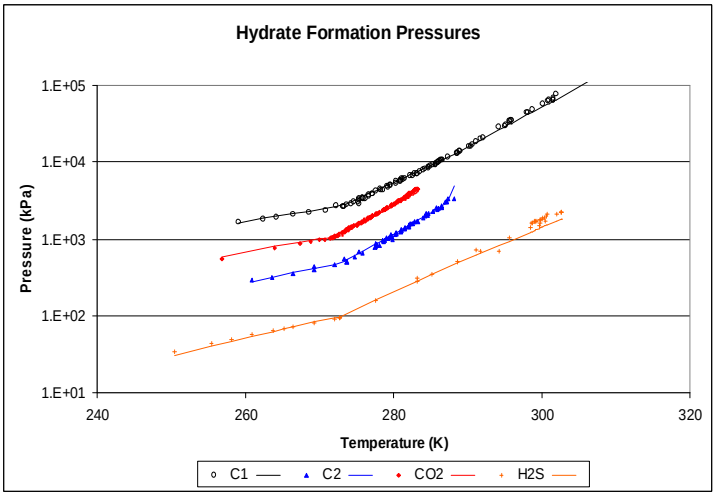
Unknown pure component physical properties are automatically estimated using a recommended set of models. Similarly, interaction parameters for systems where there is no data are estimated using a detailed routine which differentiates between hydrocarbon chemical types and accounts for the presence of water. The EOS++ Gibbs Excess Peng-Robinson model has its interaction parameters automatically estimated using UNIFAC. All estimated interaction parameters are documented and can be inspected by the user.

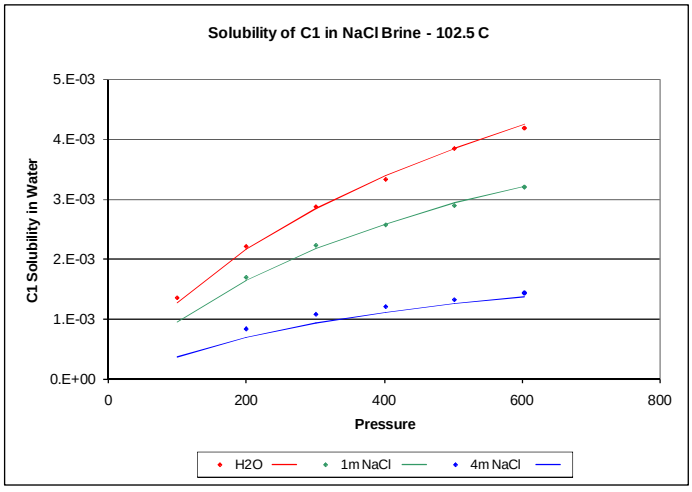
- Peng-Robinson
- Advanced Peng-Robinson
- APR-NG
- Natural Gas-Liquids Peng-Robinson
- Gibbs Excess Peng-Robinson
- Redlich-Kwong
- Soave-Redlich-Kwong
- Refinery Soave-Redlich-Kwong
- Natural Gas Compressibility Factor Soave-Redlich-Kwong
- Predictive Soave-Redlich-Kwong
- NIST Steam Tables
- BWR, BWRS
- Lee Kesler Plucker
- Virial Hayden-O'Connell



Hydrate predictions, water content and the solubilities of components such as mercury in LNG or methane in brine are important calculations in the natural gas industry.







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FATTY++

FATTY++ is a specific extension to VMGThermo designed to provide accurate property predictions for the design and simulation of the distillation of animal and vegetable fatty acids such as tallow, soybean oil, palm oil and coconut oil including compounds such as methanol, esters, tocopherols, tocotrienols and carothenes.

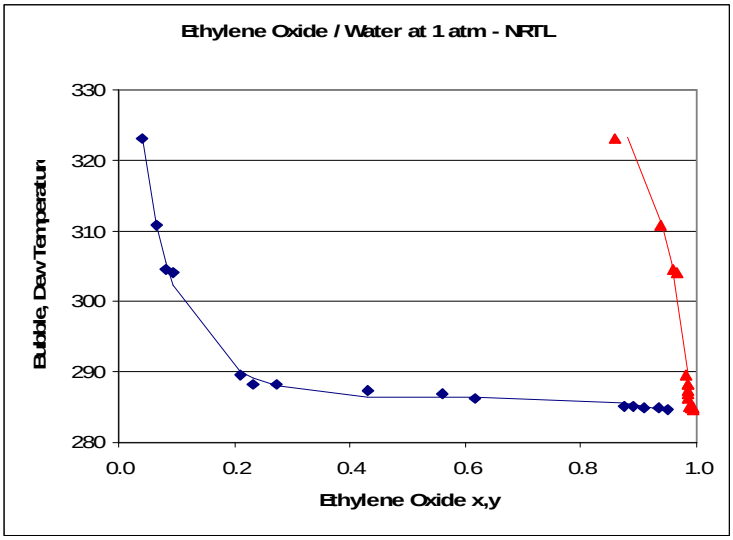
FATTY++ has all the necessary methods to accurately predict the volatility of heavy fatty acids at vacuum distillation down to pressures around 1 mmHg. Enthalpies of vaporization, solubility in water and other physical properties are calculated. In addition FATTY++ has 2,500+ specially calculated interaction parameters for VLE calculations determined by Virtual Materials, ensuring quality thermodynamic modeling.

ACTIVITY++

ACTIVITY++ is a carefully crafted set of models designed to provide thermodynamic properties for systems of interest for the chemical, fine chemical, petrochemical and pharmaceutical industries.

ACTIVITY++ provides a comprehensive set of activity coefficient models which can be used to model most processes found in the chemical industry:

- Ideal Solution
- Margules
- Margules4
- Monsanto van Laar
- Wilson
- Tsuboka-Katayama-Wilson
- Non-Random-Two-Liquids
- UNIQUAC
- UNIFAC
- Chao-Seader
- Grayson-Streed



The model parameters are a function of temperature for added flexibility when simultaneously modeling VLE and LLE.

The vapor phase may be modeled using several different equations of state such as Ideal Gas, Redlich-Kwong, Soave-Redlich-Kwong, Peng-Robinson, Virial

Important non-condensable industrial gases such as Nitrogen, Oxygen, Hydrogen and Carbon Dioxide are included and automatically handled using Henry's law modified for handling of multi-component mixtures.

ACTIVITY++ offers one of the most comprehensive interaction parameter databases in the industry. Based on extensive, high quality data collected by the Thermodynamics Research Centre, there are 100,000+ high quality interaction parameters in the VMG databases. This unique, high quality set of interaction parameters comes with extensive statistical quality assessment and can be used for a wide variety of industrial conditions.

Accessing VMGThermo

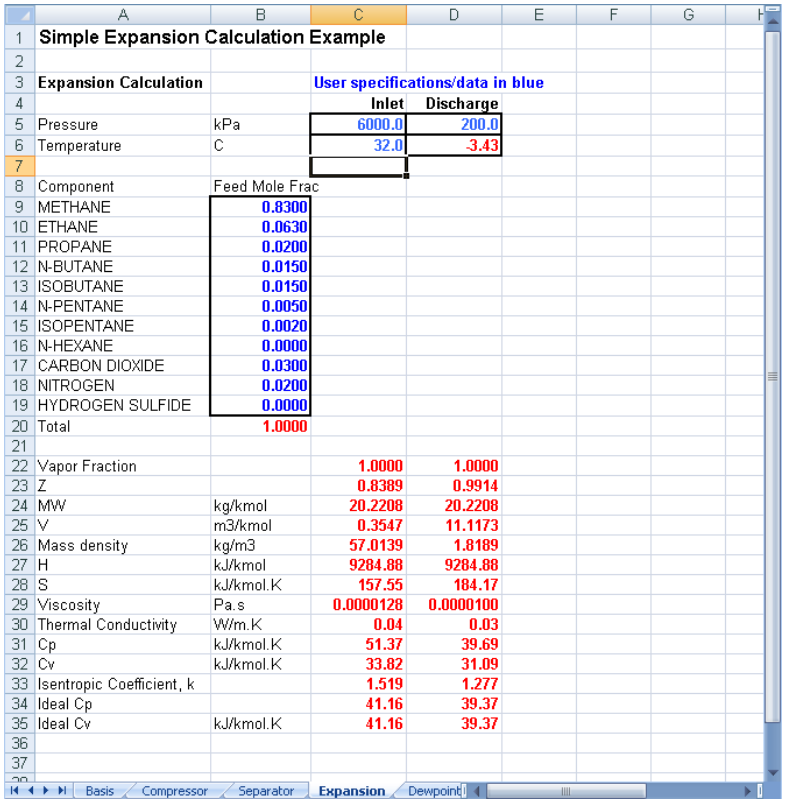
VMGThermo may be executed from Excel via a VBA interface or a user's own calculation program as a callable DLL or within VMG's own flowsheet simulation program VMGSim. VMGThermo is being used as an operator advisory tool. VMGThermo is also CAPE-OPEN enabled and can thus be interfaced to software at this interface level.

References

VMGThermo is the thermodynamics engine for a number of design and modeling software solutions in the Process industries. Some example customers include HTRI, Farris, Berwanger, Ariel, Schmart, Ideas Simulation, General Physics, Batch Process Technologies, GE, RollsRoyce and Neotec.

Comprehensive Estimation

Missing pure component physical properties are automatically estimated using a recommended set of models. Missing interaction parameters for activity coefficient models are automatically estimated using UNIFAC. All estimated interaction parameters are documented and can be inspected by the user.



	A	B	C	D
1	**Simple Expansion Calculation Example**			
2				
3	**Expansion Calculation**		**User specifications/data in blue**	
4			**Inlet**	**Discharge**
5	Pressure	kPa	6000.0	200.0
6	Temperature	C	32.0	-3.43
7				
8	Component	Feed Mole Frac		
9	METHANE	0.8300		
10	ETHANE	0.0630		
11	PROPANE	0.0200		
12	N-BUTANE	0.0150		
13	ISOBUTANE	0.0150		
14	N-PENTANE	0.0050		
15	ISOPENTANE	0.0020		
16	N-HEXANE	0.0000		
17	CARBON DIOXIDE	0.0300		
18	NITROGEN	0.0200		
19	HYDROGEN SULFIDE	0.0000		
20	Total	1.0000		
21				
22	Vapor Fraction		1.0000	1.0000
23	Z		0.8389	0.9914
24	MW	kg/kmol	20.2208	20.2208
25	V	m3/kmol	0.3547	11.1173
26	Mass density	kg/m3	57.0139	1.8189
27	H	kJ/kmol	9284.88	9284.88
28	S	kJ/kmol.K	157.55	184.17
29	Viscosity	Pa.s	0.0000128	0.0000100
30	Thermal Conductivity	W/m.K	0.04	0.03
31	Cp	kJ/kmol.K	51.37	39.69
32	Cv	kJ/kmol.K	33.82	31.09
33	Isentropic Coefficient, k		1.519	1.277
34	Ideal Cp		41.16	39.37
35	Ideal Cv	kJ/kmol.K	41.16	39.37
36				
37				

Basis | Compressor | Separator | Expansion | Dewpoint

VMG Software Products

VMGThermo is VMG's thermodynamic package available for use in flowsheet simulation models and other software packages such as Excel and HTRI's heat exchanger programs. VMGSim is VMG's new fully interactive, steady-state process flowsheet simulation program.

References and Validation Materials

References and detailed validation material for VMG customers are available from your local VMG Associate. Please call:

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