

Virtual Materials Group

Overview and Products

www.virtualmaterials.com



Introduction

Virtual Materials Group (VMG) is focused on developing high quality and cost-effective software for the Process Industries. VMG provides its clients with proven, validated and robust thermo-physical property prediction packages for the hydrocarbon, chemicals and petrochemical industry. VMG's thermodynamic models are backed by extensive experimental data and development support provided by the VMG technical support team.

More recently, VMG developed a new steady-state, process flowsheet simulation called VMGSim. This simulator uses the same interactive calculation principles of non-sequential, unit operation calculations with partial data flow, which were developed in the late 1970's in Calgary and which are used today by most process engineers in the oil & gas production industry. The steady-state process simulator integrates a state of the art steady state process simulation kernel combined with Microsoft Visio for extensive graphics capabilities and Excel for spreadsheet calculations. VMGSim provides affordable steady-state process simulation with uncompromising quality.

Virtual Materials Group also provides high level consulting in custom process simulator development, custom process model building, operator training simulator development and thermodynamic model development.

Background to VMG People

Most of the people involved in VMG have had extensive (15-25 years each) experience in thermodynamics and process simulation. One of the VMG partners founded Hyprotech and another developed and wrote most of HYSIM and then the original basis of HYSYS. The VMG development group has many years of writing, teaching and applying thermodynamic models to process simulation.

VMG's development team have been involved in thermodynamic modelling and creation of the software packages associated with thermodynamic modelling. VMG also has a close working relationship with the thermodynamic research group at NIST in the USA.

The basis of the flowsheet simulation program incorporates new ideas in flowsheet simulation relating to integrated tower models and sub-flowsheeting.

VMG's Associates around the world were all involved in marketing of, support of and user-training for HYSIM and HYSYS during the past 15-20 years. Most were involved in pioneering the move of process engineering software to personal computers and have remained involved as personal computers became the standard computer used for engineering calculations in the process industries. VMG's European Associate introduced PC-based process engineering to the European oil & gas industry in late 1984. The first

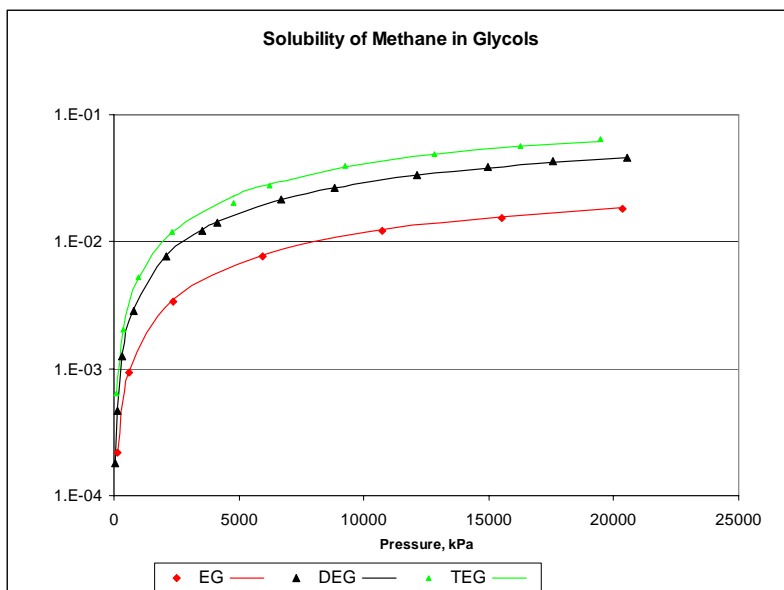
licenses of such software in Europe were delivered in 1984. VMG's Associates in the USA, Japan, Far and Middle East were all involved in pioneering PC-based and interactive process simulation in their respective countries.

Oil & Gas Industry Applications

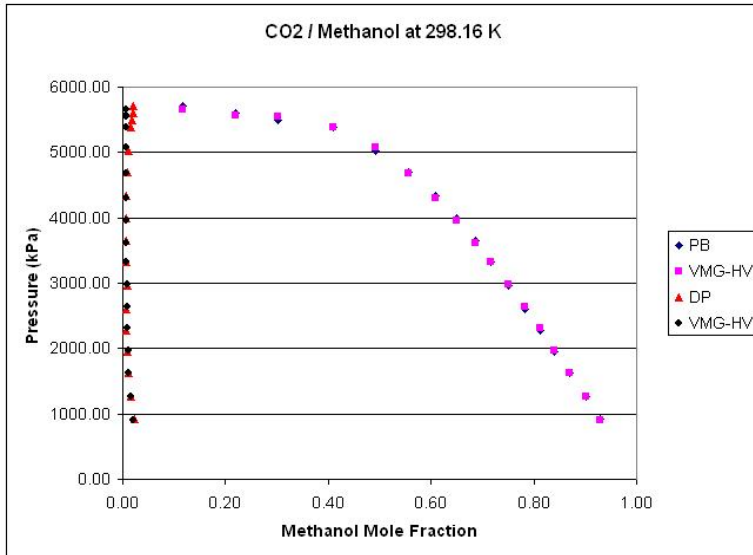
VMG have developed an advanced Peng-Robinson model within their thermodynamic package VMGThermo and initial work on VMG's steady-state process flowsheet simulator called VMGSim has been concentrated on the oil & gas production industry.

In addition to modelling "standard" hydrocarbon systems, VMG have recently paid special attention to extending their thermodynamic models towards accurate modelling of acid gas, mercury, glycols and hydrocarbons dissolved in glycols over wide operating ranges as well as taking salinity into account in the water phase for hydrate and hydrocarbon solubility predictions. The intention is to provide the oil & gas production industry with more accurate thermodynamic modelling than has been possible up to now.

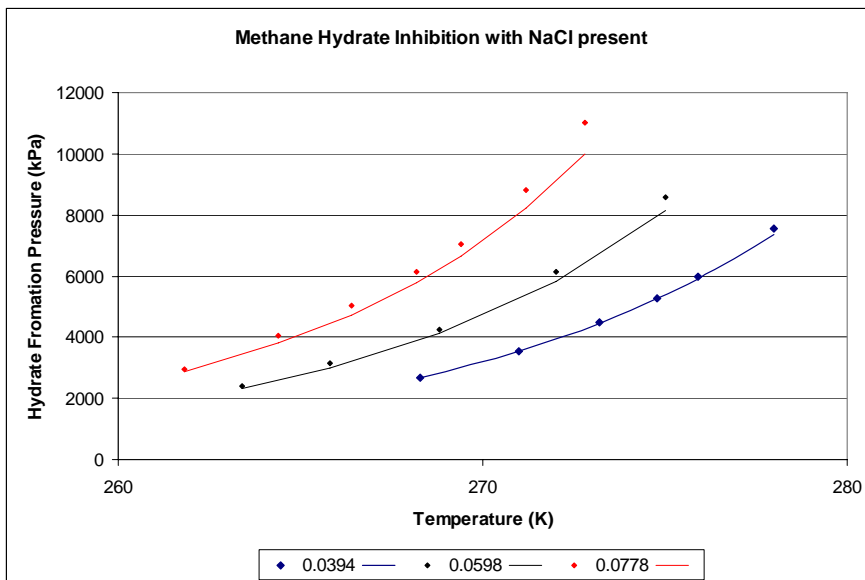
An example showing the experimental versus calculated values for solubility of methane in various glycols is shown below. This has been achieved by accurate fitting of vapour pressures for the components over wide ranges of temperatures then collection and validation of binary data which was then used to determine the thermodynamic model parameters.



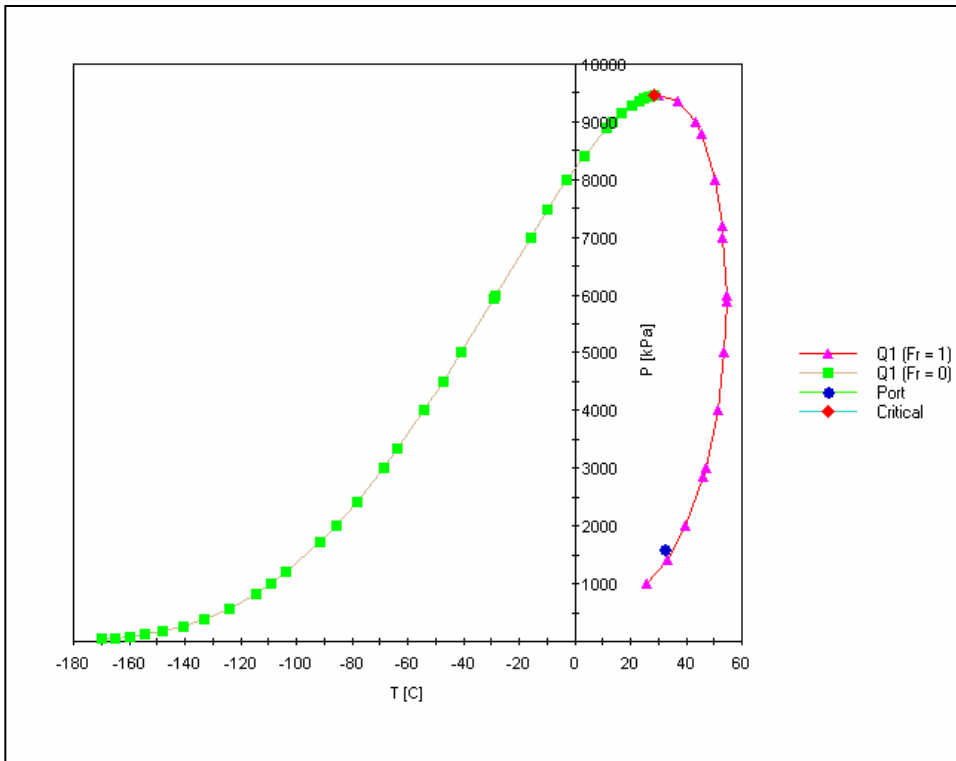
The Peng-Robinson model was extended to include a free energy term by Huron-Vidal and VMG's version of this powerful model is identified as GE-PR within the VMGThermo package. Calculation of the phase behaviour of CO₂-methanol at 25°C over a range of pressures is shown in the diagram below with comparison to literature data.



Gas hydrates form in natural gas systems if water is present. The salinity of the water affects the hydrate formation temperature as the water activity is altered by the presence of salt. It is possible to predict this effect as shown below.



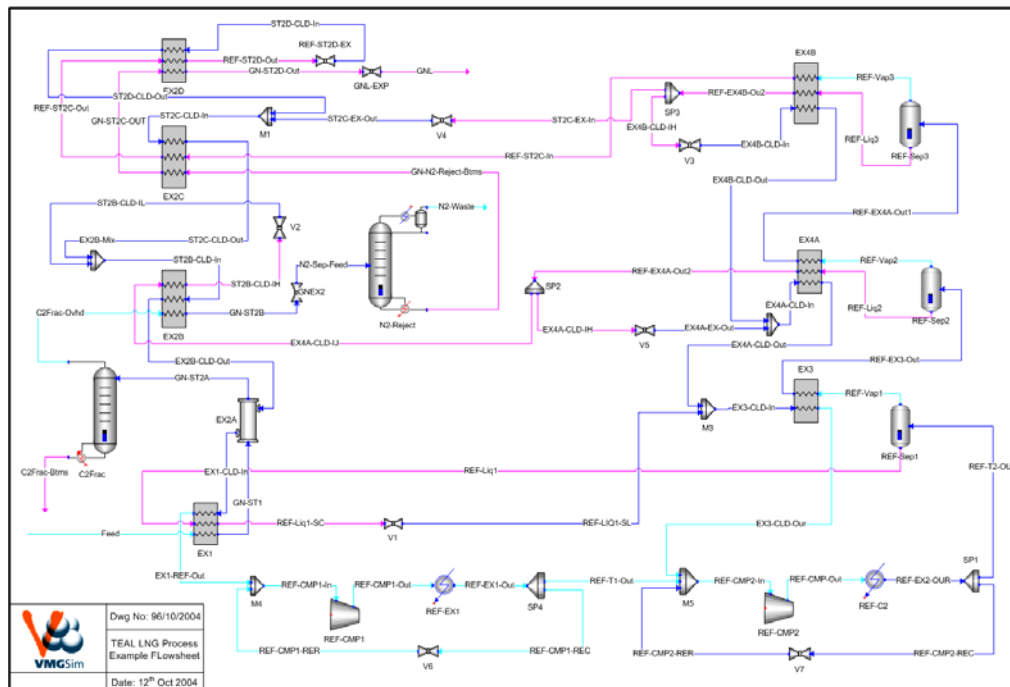
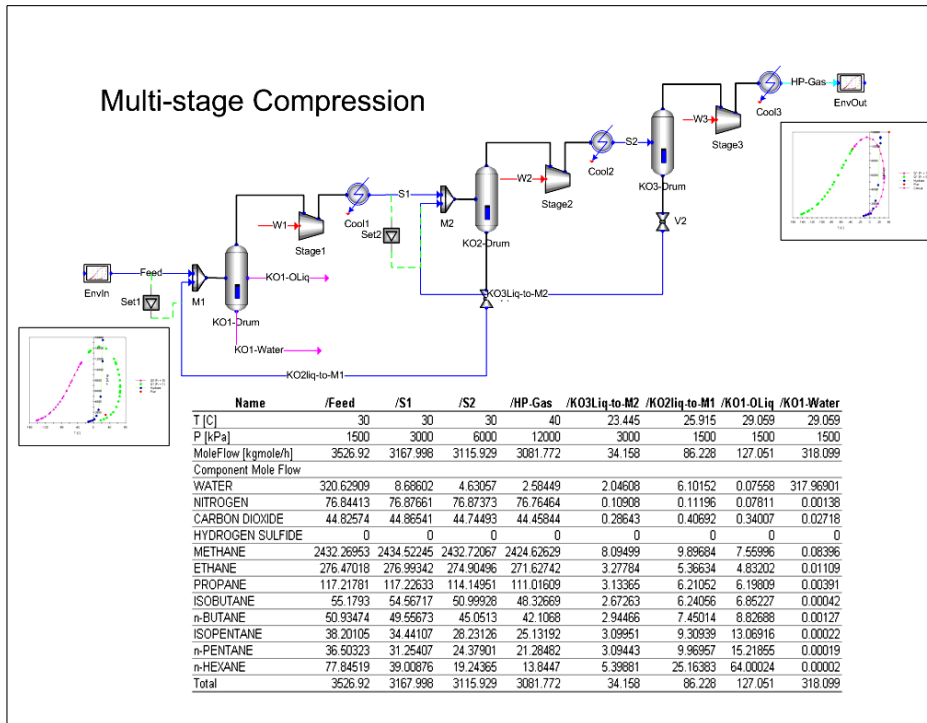
A phase envelope showing the dew and bubble point lines of a stream being produced from a reservoir is shown below. This was calculated within VMGSim using VMG's Advanced Peng Robinson thermodynamic model.



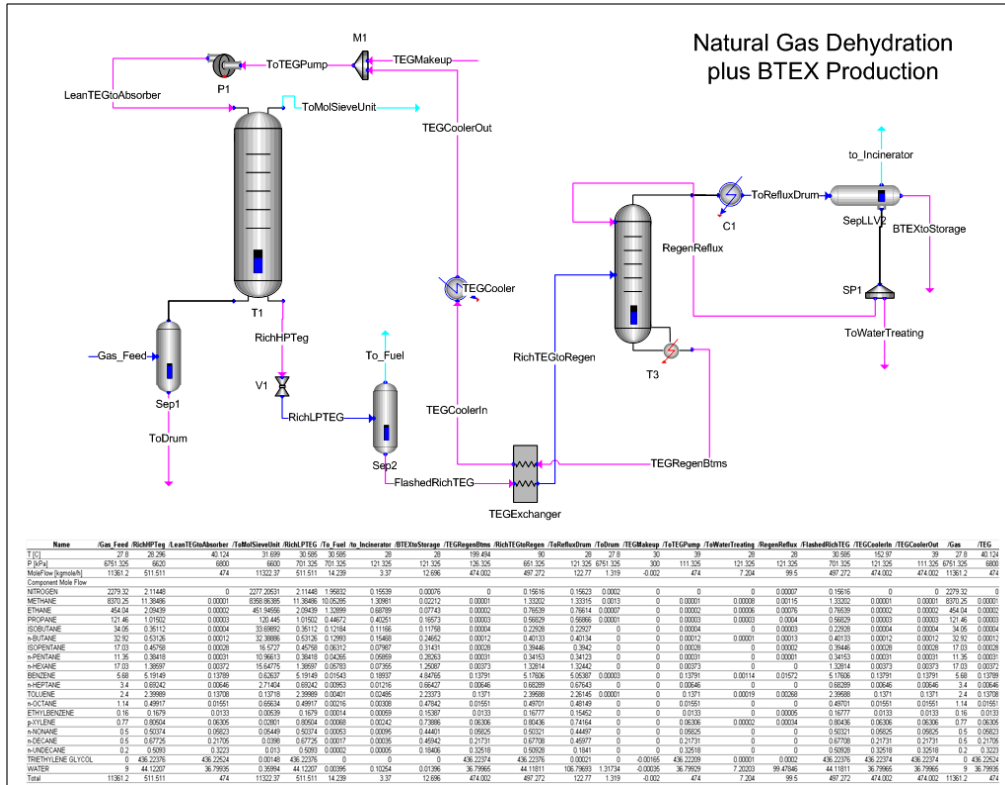
The true critical temperature and pressure of the stream as well as the cricondenbar and cricondenthem are also calculated and reported and shown below.

	P [kPa]	T [C]
Cricondenbar	9466.3	30.09
Cricondenthem	5886.9	54.44
Crit_P	9455.2	
Crit_T		28.34

Using the graphic tool Microsoft Visio has enabled VMG to add PFD visualization to the simulation program. MS Visio can then be used outside the simulation program to enhance the PFD by addition of comments or graphic pictures such as phase envelopes as shown below.



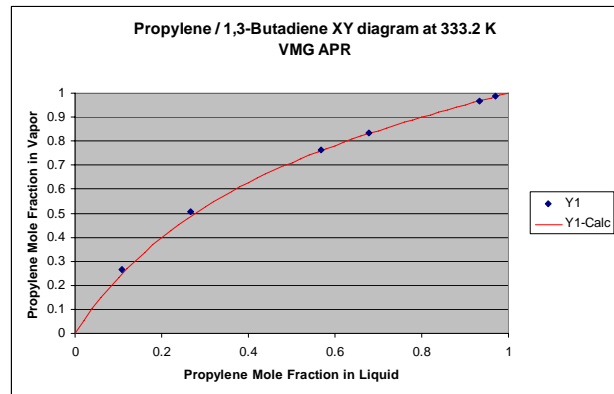
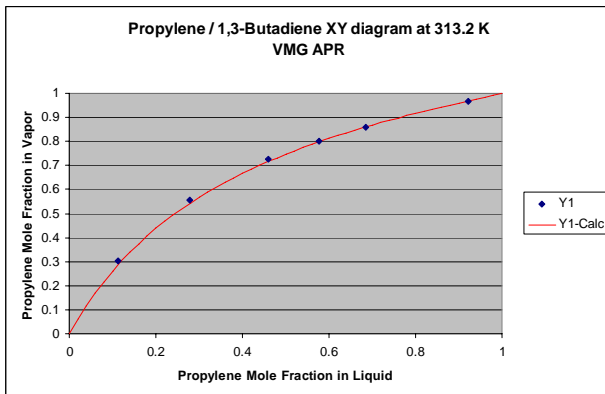
Further work on the thermodynamics has enabled accurate modelling of hydrocarbons dissolved in TEG so that modelling of a gas dehydration system specially designed for a high BTX content gas production system becomes possible. A schematic of the model with stream results is shown below.



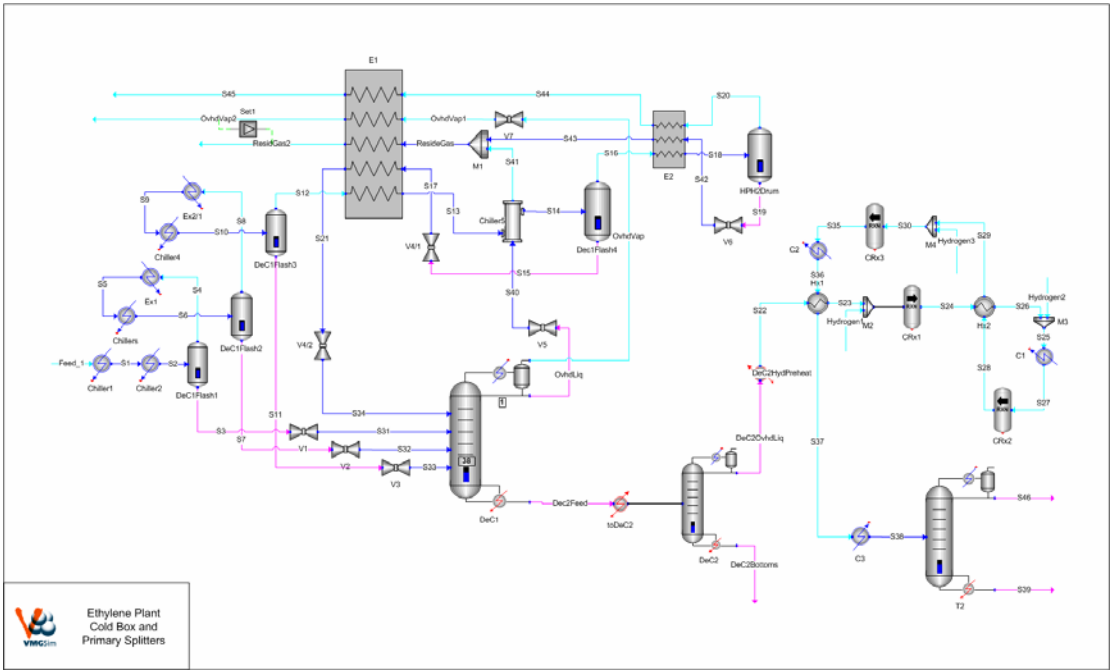
Petrochemical Applications

VMGThermo and VMGSim have also been applied to petrochemical applications such as modelling of ethylene and propylene plants.

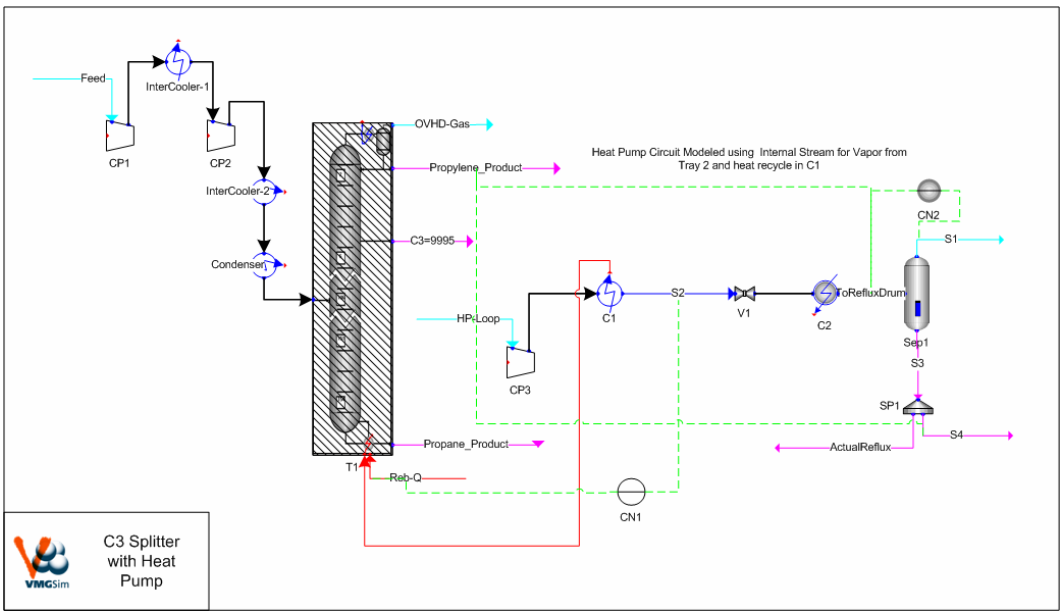
An accurate phase behaviour prediction for the fractionation in such plants is vital to achieve correct prediction of the compositions of products, particularly in mixtures such as propylene and butadiene. A couple of validation curves (XY diagrams) at two different temperatures are shown below.



The gas from the cracked gas compressor section is fed to the demethanizer section then the C2 components are split from the C2-rich liquid and in turn split into ethane and ethylene.



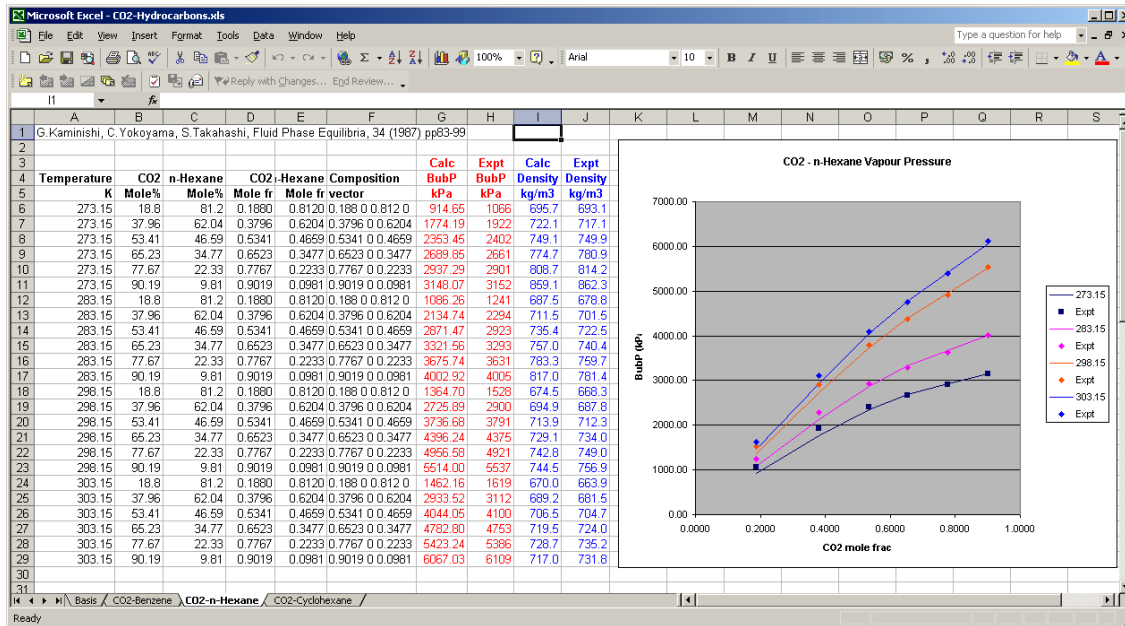
A simulation model schematic of a propane-propylene splitter with a heat pump system used to provide energy for the tower reboiler is shown below.



Other Applications of VMGThermo

VMGThermo is now being used by a number of software vendors in the process industries for thermodynamic property calculations within their own software. The vendor list includes HTRI (heat exchanger design), Ariel Compressors, Schmart (relief valves) and Neotec (multiphase flow and production forecasting).

VMGThermo may also be run directly from Excel. An example showing the calculation of vapour pressure of a range of CO₂-n-Hexane mixtures for a series of temperatures is shown below.



VMG will be developing a CAPE-OPEN interface for VMGThermo so that VMGThermo will be available for use with any CAPE-OPEN software package.

VMGThermo is also linked to IDEAS from IDEAS Simulation and formed the thermodynamic engine for a very large operator training system for an oil sands extraction plant in Alberta, which used a new solvent-based bitumen recovery process. During the process of development of the OTS the customer was also to check out the large process control system as well as identify and resolve problems in design of the control philosophy.

Conclusion

VMGThermo is a general thermodynamic package which applies to mixture of components found in the oil & gas, petrochemical and chemical process industries as well as certain specialised processes such as fatty acid production, sulphuric acid manufacture and urea fertilizer plants. VMGThermo is wrapped in a generalised callable package and may be used from programs written in FORTRAN, C++, Python and Visual Basic as well as having a direct link to Excel.

VMGThermo has been extensively tested and validated by VMG and a number of partner companies. VMGThermo has been used in many industrial applications. VMGThermo is linked to several equipment design programs to provide accurate thermophysical properties for use in design calculations.

VMGSim is a new interactive steady-state flowsheet simulator driven by VMGThermo. VMGSim offers some interesting new features, flexibility and capabilities to process engineers in the process engineering industry.