GPA MIDSTREAM PROJECT 111: COMPARISON OF GPA MIDSTREAM DATA TO SIMULATION SOFTWARE PREDICTIONS

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ABSTRACT

Over the decades projects sponsored by GPA Midstream has generated thousands of data points that have helped characterize the equilibria and other characteristics of chemical systems that are important in the gas industry. The industry is also reliant on the use of process simulation software and the evaluation of how well the GPA data and the results of simulation software compare is important. GPA established Project 111 in order to evaluate GPA-generated data and compare it to simulation-generated data. A portion of the GPA data in specific areas of interest were selected for analysis: hydrocarbon vapor-liquid equilibrium (VLE), hydrocarbon and acid gas VLE/solubility/hydrate formation with water, solubility of hydrocarbons and acid gas in glycols and amines, methanol concentration in gas phase, sulfur compound distribution glycols and amines, and effect of inhibitors on hydrates. Flash calculations and other simple methods were used to generate predictive data to compare to the experimental data, using simulation software commonly used in the gas processing industry. The level of agreement between the experimental data and the simulation software results can be used by GPA member companies as a guide in the evaluation and interpretation of simulation results, and can also be used by the GPA to determine cases where additional experimental data may be necessary. The results of this project are currently under review and revision, and have not yet been released for publication. This paper focuses on summarizing the objectives, scope, and methods used in the study. Complete results will be published in the Project 111 Research Report that will follow.

1. Introduction and Objectives

For decades the GPA Midstream has sponsored projects to collect experimental data that are important to their member companies. Thousands of data points have been generated covering all facets of the gas processing industries, and include physical property, phase equilibria, reactions, and other topics. One of the more common data categories is phase equilibria, where composition data for phases at equilibrium are measured at defined conditions (temperature, pressure, etc.). These type of data are valuable to GPA member companies, and are used to compare with operating data and predict process performance. One of the most important uses of equilibrium data is in the creation and tuning of thermodynamic models used in simulation software and other mathematical models.

Simulation software is routinely used in numerous industries, including gas processing, to characterize and design processes. Engineers in the industry are highly reliant on the use of process simulation software, and it is therefore critical that the engineer be aware of how the simulation software represents the equilibrium of chemical systems and how those predictions compare to the results of the GPA-sponsored research. The GPA data is one of the data sources used by the creators of process simulation software to generate physical property models that are key features of the software.

GPA Midstream established Project 111 to analyze data that has been created by GPA-sponsored projects over the years and compare that data with predictions generated by process simulation software. This will be helpful in evaluating GPA data while also providing software users and vendors useful guidance. Additionally, the project provided GPA members with useful insights on simulation properties basis selection and data comparison techniques. The experimental data were drawn from a large number of GPA projects, and this project covered a small fraction of those data and were confined to specific areas of interest that were defined by the GPA.

One of the goals of the project was to use all of the process simulation software most commonly used in gas processing. Due to “benchmarking” restrictions contained in many software licensing agreements, it was not possible to include all software packages in this study. Negotiations with four of the software vendors resulted in agreements that would allow for the use of their software in this study.

2. Scope of the Study

The software packages used in this study are BR&E ProMax, Schneider Electric SimSci Pro/II, Virtual Materials Group VMGSim, and WinSim DESIGN II. The GPA defined six specific

areas from which GPA data would be selected and compared to simulation-generated data. These six subject areas are:

Set 1: Hydrocarbon vapor-liquid equilibrium (VLE)

Set 2: Hydrocarbon and acid gas VLE/solubility/hydrate formation with water

Set 3: Solubility of hydrocarbons and acid gas in glycols and amines

Set 4: Methanol concentration in gas phase

Set 5: Sulfur compound distribution glycols and amines

Set 6: Effect of inhibitors on hydrates

Only experimental data that was created by GPA-sponsored projects was selected for comparison. The types of experimental data selected were confined to phase equilibria and other basic thermodynamic data. Data pertaining to the rates of reactions, mass transfer, and transport properties were excluded. As of the publication of this report there were more than 230 Research Reports available from the GPA. As part of this project, all of the Research Reports were examined for data that fit into the aforementioned six subject areas. Experimental data were selected from those areas from the Research Reports, the four software packages were used to simulate the experimental data, and the results of the software were compared with the experimental data.

3. Methods

The procedure used in this study is summarized below:

1. Select representative data from each subject area
    - Only original data published in GPA Research Reports were used
    - Only equilibrium data selected, kinetic and transport data were ignored
    - Some newer reports present data in the same range as some older reports, in which case the newer data was used
    - Selected about 10% of > 6,000 candidate data points
    - Data is necessarily “sparse”, doesn’t cover any one area extremely well
2. Review and understand data, consider if the data is valid for use
    - Eliminated data that doesn’t represent a complete equilibrium data set
    - Eliminate data with unusually high self-reported error levels, and data with any other apparent inconsistencies or obvious typographical errors

- Eliminated data that is not entirely experimental (there are some data sets where some phase information is provided by process simulation or other predictive technique)
- Eliminated data that were not generated in the GPA-sponsored project
- Eliminated data where implied equilibrium compositions (e.g., stating that a feed phase composition is essentially equivalent to the equilibrium concentration of the same phase) could not be verified by study of experimental methods

3. Develop experimental error estimates when possible
    - Documented experimental error
    - If a derived (not directly measured) quantity was included in the analysis, such as K-values, the error in the derived quantity was calculated.
4. Get advice from simulation software vendors
    - Thermodynamic package recommendation
    - Specific advice on how to run simulation
5. Run simulations and document results
6. Share data with simulation vendors for review
    - Correct errors as necessary

Simulation Vendor Input

In order to minimize errors due to inappropriate use of the simulation software, the advice of the simulation software vendors was sought, and the vendors were also allowed to review the outcome of the simulations prior to finalizing the work. In addition to providing valuable advice in proper use of their software, there were some cases where the vendor was able to detect errors in the use of their software, inconsistencies in the approach used to compare the simulation data to the GPA data, and inconsistencies in the source GPA data. Some data were eliminated from this work, or corrections made, as a result of the vendor reviews.

As part of the process of seeking advice from the simulation software vendor for each data set, the software vendor sometimes stated that their software was not well-suited for a particular type or range of data. Simulation software was excluded from use for certain data points and sets whenever advised by the vendor.

In order to improve simulation results some software vendors may occasionally advise users to input experimental data, such as binary VLE data, into the software and use the software to model these data. Frequently the data modeling is used to create binary interaction parameters (BIP) in the software, which can improve the accuracy of the simulation. Simulation software usually contain a data base of BIP and other parameters for various chemical systems, and the

entry of new experimental data and creation of new parameters is usually only done when modeling unusual conditions, unusual chemical mixtures, or there is a specific need for greater-than-normal accuracy in a certain region.

It is recognized that the entry of experimental data into some process simulation software and the use of the software to model the data to improve simulation accuracy is a valuable technique that users should be aware of and be prepared to do when necessary. But for this project this practice was not allowed. The chemical systems and range of conditions included in this project are (with some exceptions) within the range normally experienced in gas processing, and the GPA preferred to compare the simulation software to the GPA data based on the software results on an "out of the box" basis; i.e., relying only on the BIP and other parameters that the vendor has included with their software. Also it was rationalized that the input of the GPA data into the software followed by the generation of the data from the software model would not necessarily be meaningful for this project.

Methods Used to Generate Comparative Data in Simulation Software

A variety of methods were used to generate comparative data in simulation software. Different data sets included information that required different approaches in simulation, and also the software used have differences which result in the need to tailor the simulation approach to each software to some extent. The method used to analyze and simulate each set of data was done on a case-by-case basis. All of the methods used to analyze the data cannot be provided in this paper, but two of the more typical methods are summarized below.

One common method used in this work, particularly for simpler (e.g., fewer components, two phases) was to set up a flash block at the temperature and pressure of the experimental data, and feed in the components until the bulk compositions of the one of the phases closely matched that of the experimental data. The composition of the other phase generated by the software could then be directly compared with the experimental phase composition.

Systems that were more complex – many components and/or more than two phases – often required a different approach since it was often difficult to match an equilibrium phases exactly in the simulations, or the assumption that one of the phases was unchanged from feed to the equilibrium products was not certain. For some of these cases, when sufficient data was available from the research report the simulations would not be based on mimicking one of the phases at equilibrium, rather it would be based more on mimicking the experiment, where the flash of the experiment-specified feed stocks would be simulated at the experimental temperature and pressure.

4. Representation of Results

The primary mode of the comparison of experimental data and simulation results is the direct examination of the resulting data. For example, for a data set containing VLE data at a fixed temperature and pressure, typically the composition of one phase was closely matched in the simulation and the predicted composition of the other phase could be compared directly with the GPA data. In addition to directly comparing the phase composition data, it was considered useful to have other ways of considering the data. This included the use of derived quantities – typically a K-value – and graphs.

K-values were often calculated to provide another method for considering and comparing phase equilibrium data. In addition to the calculation of K-values for vapor-liquid equilibrium data (yi/xi), K-value and also calculated for some liquid-liquid equilibrium data (x_{1i}/x_{2i}). K-values are particularly useful when trying to make use of a GPA data point to draw conclusions regarding a similar condition of interest. In a limited range of composition variation, it may be reasonable to use a K-value to estimate equilibrium outside of the measured composition from which the K-value was derived. Additionally, the calculation of K-values allowed for the creation of more meaningful graphs of data, because K-values derived from data may not have as great a variation range as the source data itself.

Because the data selected for this study are typically sparse – scattered across a wide variety of compositions, types of equilibria, and conditions – it is difficult to show the data in more convenient forms than a data table. However, graphs of the data were produced when reasonable. For many data sets it was reasonable to create parity plots displaying most or all of the data from the set. The parity plots were created using the GPA data as the reference line. The use of the GPA data as the reference line is not intended to imply that the GPA data in necessarily more correct.

In many of the graphs of results the accuracy of the experimental data is represented on the graphs as error bars. For a derived quantity, such as a K-value, the error bars implicit in the GPA source data can be calculated from the stated error of the source x and y compositions by the propagation of error equation:

$$\frac{\sigma_K}{K} = \sqrt{\left(\frac{\sigma_x}{x}\right)^2 + \left(\frac{\sigma_y}{y}\right)^2}$$

Where σ_K is the calculated standard deviation of the K value.

5. Results

Because this project is not complete, the results are considered preliminary and are therefore not included in this paper. The forthcoming Research Report for this project will include all of the results – the GPA source data and the data from the simulation runs. In general, for most of the more common chemical systems at more common operating conditions there tended to be very good agreement between the GPA data and the simulated results. For equilibrium of systems often not considered as common or important in gas processing, and/or at unusual operating conditions, the agreement between the simulation data and the GPA data was more variable.

6. Conclusion

The differences between the experimental data and the simulation software results can be used by the reader as a guide in the evaluation and interpretation of simulation results. It is not implied that when there is significant disagreement between experimental data and the simulation results that the GPA experimental data are always correct and the software results are always not correct. It is possible that some portion of the GPA data contained in the Research Reports are not highly accurate. The data in the GPA Research Reports are a common source of experimental data upon which some software vendors base their physical property models, but there are many other experimental data sources that have also been used to develop physical property models, and it is likely that some of the other experimental data may not always agree with the GPA experimental data. Software vendors may sometimes choose the data source that they believe best suited to their needs. Overall, the study demonstrates that the user of process simulation software should check results against outside data; this should be considered a common best practice.

Please see the Research Report to be issued later for complete results.

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