

# **BTEX EMISSIONS FROM ETHYLENE GLYCOL CIRCULATION IN NATURAL GAS REFRIGERATION PLANTS: A PROCESS SIMULATION STUDY**

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## **ABSTRACT**

Monoethylene Glycol (EG) is widely used as a hydrate inhibitor in low-temperature refrigerated gas plants. One of the main environmental issues with the operation of glycol units is the release of BTEX (benzene, toluene, ethylbenzene, xylenes) emissions, which are controlled by federal and/or local regulatory agencies. Although the vast majority of glycol units use Triethylene Glycol (TEG) to remove water from natural gas, there are a significant number of refrigeration plants that rely on EG to ensure hydrate-free operation. Earlier reports have shown that the main process simulation tools used in the sector to predict BTEX emissions from TEG systems provide reasonably similar results and adequately match the available experimental data. EG systems however have not been extensively studied and it is well-known among practitioners that the simulation software tools generally used can produce widely different results, and in some cases even fail to produce results at all.

In North America, HYSYS<sup>TM</sup>, ProMax<sup>TM</sup> and GRI-GLYCalc<sup>TM</sup> are the most common simulation tools used to predict BTEX emissions from glycol units. For HYSYS, a more recently added “Glycol” property package was developed with good results for predicting BTEX emissions from glycol units. ProMax has also been widely used with the recommended SRK equation of state incorporating fitted interaction parameters. GLYCalc has also been used in industry, but relies in part on simplified methods to calculate emissions.

In this work, a set of refrigeration plants operating in Western Canada were simulated using these different approaches; results are presented in this report.

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## Executive Summary

A previous study [1] reviewed the prediction of BTEX emissions in Triethylene Glycol (TEG) dehydration units using HYSYS and GLYCalc. This report reviews the accuracy of BTEX emission predictions for ethylene glycol (EG) systems using AspenTech HYSYS, BR&E ProMax and GRI GLYCalc. In this study, the predictions of these simulators were compared using a set of operating data corresponding to several refrigeration plants in Western Canada and concluded the following:

- The Peng Robinson property package in HYSYS (HYSYS-PR) should not be used for the prediction of BTEX emissions in refrigeration plants. The Peng-Robinson property package predicts negligible amounts of BTEX in the aqueous phase of low temperature separators, resulting (incorrectly) in predicting zero emissions.
- For the prediction of BTEX emissions in refrigeration plants, the Glycol property package in HYSYS (HYSYS-Glycol) is recommended by AspenTech and is significantly better than HYSYS-PR for this purpose. Of the three reviewed simulators, HYSYS-Glycol tended to predict the highest BTEX emissions. However, HYSYS-Glycol should be used with caution at lower LTS pressures (less than 2,500 kPa).
- BR&E has published much information related to TEG dehydration facilities and BTEX emissions but very little related to EG (refrigeration). Of the three simulators reviewed in this study, ProMax consistently predicted BTEX emissions higher than GLYCalc but lower than HYSYS-Glycol.
- It was found that GLYCalc often fails to predict a hydrocarbon liquid phase in the low temperature separator, resulting in very high predicted BTEX emissions in those cases. The user must be careful when using GLYCalc for EG (refrigeration) units. When GLYCalc calculates “reasonable” results, it consistently predicts the lowest amount of BTEX emissions among the three simulators reviewed.
- While VLE data has been published for BTEX-hydrocarbon systems at cold separator conditions, VLLE data is not available in the literature, which would be crucial in understanding how much BTEX would be soluble in the hydrocarbon liquid and aqueous phases, respectively.
- Field data was obtained and the results of the simulators were compared to this data. For two of the three units, HYSYS-Glycol had the closest results to the data for the combined BTEX predictions. For these units, the results of ProMax were about 50-60% of the original data, and GLYCalc significantly overpredicted the results due to the inability to properly predict a hydrocarbon liquid phase in the cold separator. For a third unit, HYSYS significantly overpredicted BTEX emissions, understood to be a thermodynamic issue at lower pressures (less than 2,500 kPa). In this third case, the ProMax results were very close to the data, while GLYCalc results were about 40% of the original data. While these conclusions could be obtained for BTEX overall, individual component predictions were much less comparable to the field data.
- Some effort was made to fit thermodynamic parameters to field data; while it was found that a reasonable match could be made to the field data, it did not extrapolate well to the wide range of conditions required.
- While GLYCalc has been successfully used in industry to calculate BTEX emissions in EG units, there are limitations. Customizable simulation platforms such as HYSYS or ProMax can be used to improve thermodynamic calculations as well as improve on data transfer and modeling aspects, especially when combined with knowledge of the range of applicability of each simulator.

## Introduction

The objective of this study is to evaluate the accuracy of GRI GLYCalc, AspenTech HYSYS, and BR&E ProMax in calculating BTEX emissions in EG units. All of these tools are frequently used to predict BTEX emissions from EG units. In Canada, HYSYS and GLYCalc are recognized by:

- The ERCB (Alberta Energy Resources Conservation Board), in Directive 39 - Revised Program to Reduce Benzene Emissions from Glycol Dehydrators), *and*
- CAPP (Canadian Association of Petroleum Producers), in “Best Management Practices – Control of Benzene Emissions from Glycol Dehydrators”

The ERCB also recognizes BR&E PROSIM as a suitable simulation tool. There are other simulation platforms which could also be used for this application, including Virtual Materials Group VMGSim, SimSci ProII and proprietary tools. These other simulators were not reviewed in this paper.

In Canada, ERCB Directive 39 (and similar directives from other provinces) as well as the CAPP Best Management Practice, clearly outline the accepted procedures for estimating the *benzene* emissions in dehydration and refrigeration facilities. These documents do not specifically address toluene, ethylbenzene and xylene emissions (the “TEX” in BTEX), but other guidelines in Canada do address these component emissions (i.e., National Pollutant Release Inventory or NPRI). In other jurisdictions, BTEX emissions are regulated, such as in the United States where the Environmental Protection Agency (EPA) does address these emissions.

Therefore the scope of this report considers the accuracy of the simulators in predicting BTEX emissions in EG units, specifically reviewing GLYCalc, ProMax and HYSYS as the most common simulation tools used in North America for this purpose.

## Calculation Basis

Some details regarding the calculation basis for the three reviewed simulators are discussed in this section.

### GLYCalc

GLYCalc has been available since the early 1990’s and in North America is likely the most commonly used tool used to calculate BTEX emissions from refrigeration units due to its low cost and ease of use. However, it is known to have some difficulties estimating BTEX emissions in EG refrigeration units, as discussed further in this report. One of the drawbacks of GLYCalc is that it is not possible to adjust thermodynamic parameters and as it is currently not supported it is unlikely that further improvements will be made.

The thermodynamic calculations in GLYCalc are described in detail as part of the documentation provided with the GRI GLYCalc software. For EG systems, the most important flash calculations occur in the low temperature (cold) separator, flash tank, still and condenser.

According to the GLYCalc manual [2]:

“The input data for the wet gas and lean EG are used to perform a three-phase vapor-liquid-liquid equilibrium (VLLE) flash calculation at the specified contactor temperature and pressure to represent the

combined contactor, chiller, and cold separator. That is, the gas-EG contactor and three-phase separator are considered as one block in the program. Because a one-stage equilibrium flash calculation is used for the contactor, the user does not enter an estimate for the number of equilibrium stages or the dry gas water content. The gas and hydrocarbon liquid phases are considered to be product streams, and the rich EG stream is used as input to the glycol pump.”

The following data sources were used to fit interaction parameters [2]:

Parameter	Interacting Compounds	Data Source
UNIQUAC Binary Interaction Parameters	TEG - BTEX	<i>The Solubility of Selected Aromatic Hydrocarbons in TEG</i> . GPA Report RR-131. DB Robinson Research, 1991.
	TEG - Aliphatic Hydrocarbon	Preliminary GRI experimental work.
	BTEX - Water	<i>Mutual Solubilities of Hydrocarbons and Water at 0 and 25 deg C</i> . Polak and Yu, 1973; review of existing literature.
	TEG - Water	<i>Water Equilibrium in the Dehydration of Natural Gas with Triethylene Glycol</i> . Rosman, 1973.
Henry's Law Constants	Acid Gas - TEG; Methane-TEG	<i>Vapor-Liquid Equilibria for Acid Gases and Lower Alkanes in Triethylene Glycol</i> . Jou, Mather, et. al., 1987.
UNIQUAC Binary Interaction Parameters	DEG - BTEX	Various literature sources (see Sources of Additional Information).
	DEG - Aliphatic Hydrocarbon	Hutton, P.G. and J. H. Jones. <i>J. Chem. Eng. Data</i> . 8 (1963) 617. (DEG/n-hexane).
	DEG - Water	Formulated Glycol Additives Study. GRI Contract 5091-221-2366.
Henry's Law Constants	Methane - DEG	D.B. Robinson Research, Ltd. <i>Equilibrium Phase Compositions for Systems Containing Methane, Benzene, and Water in DEG</i> . GRI Contract 5093-260-2578.
UNIQUAC Binary Interaction Parameters	EG - BTEX	<i>The Solubility of Selected Aromatic Hydrocarbons in Ethylene Glycol</i> . GPA Report. DB Robinson Research, 1993.
	EG - Aliphatic Hydrocarbon	Preliminary GRI experimental work.
	EG - Water	Data of Trimble (1935) and Sokolov (1967) from <i>DECHEMA</i> compilation; <i>DOW Gas Conditioning Fact Book</i> , 1958.
Henry's Law Constants	Acid Gas - EG	<i>Vapor-Liquid Equilibria of H<sub>2</sub>S and CO<sub>2</sub> and Ethylene Glycol at Elevated Pressures</i> . Jou, Mather, et. al., 1990.
	Methane - EG	<i>The Solubility of Selected Aromatic Hydrocarbons in Ethylene Glycol</i> . GPA Report. DB Robinson Research, 1993.

**Figure 1 – Data sources used to fit interaction parameters (From GLYCalc manual)**

Of critical importance are the EG-BTEX parameters (from GPA Report 137 – discussed in further detail in this report), and the EG-Aliphatic hydrocarbon parameters. Little information is provided with respect to the “EG-Aliphatic Hydrocarbon” interaction parameters, calculated from “preliminary GRI experimental work”. GPA Report 137 helps to determine the vapour-liquid equilibrium, but it does not address the solubility of BTEX in the hydrocarbon liquid and aqueous phases (LLE) at the low temperature separator.

As mentioned in a previous report [1], the manual [2] notes that for the regenerator (still) “to avoid the complex heat and material balances that would be needed if the regenerator were rigorously modeled, a simple empirical calculation is used.”

## HYSYS

HYSYS is a general-purpose process simulator which has been widely used in the oil and gas industry since its first inception when it was introduced as HYSIM in the early 1980's. However, it wasn't until the “Glycol” property package was introduced in version 2004.1 that AspenTech focused specifically on BTEX emissions in Glycol units. It is noted that in later versions (2006, 2006.5, v7.1, v7.2, v7.3), successive improvements were made in the interaction parameters. The differences in calculations between these versions are significant and the basis for this report was version v7.1, which introduced many additional fitted binary parameters. It is also noted that the Peng Robinson (PR) property package has historically been used as the recommended simulator for gas facilities, and is briefly reviewed in this report.

The Glycol package is based on the “TST” equation of state which has the following characteristics [3]:

“The TST cubic equation of state improves the representation of the pure component vapour pressures by the introduction of a three parameter alpha function. TST uses Cubic Equation of State/Excess Helmholtz energy (CEoS/AE) mixing rules [3] that permit a smooth transition of the mixing rules [*author addition*: from  $A^E$  models] to the conventional van der Waals one-fluid mixing rules. It also uses an excess Gibbs Energy (GE) model, which when combined with the CEoS/AE mixing rules allows both a van der Waals fluid and highly non-ideal mixtures to be described over a broad range of temperatures and pressures in a consistent and unified framework.”

It is finally noted that the column models in HYSYS utilize rigorous stage-by-stage mass and energy balances (not using shortcut methods as in GLYCalc).

## ProMax

ProMax is a process simulator used in the oil and gas industry which was introduced in the early 1980's (as PROSIM). BR&E does not have a specific “Glycol” property package, but recommends using an Equation of State Property Package (SRK or Peng-Robinson). These property packages have been specifically fitted to predict BTEX emissions in dehydration and refrigeration units. For this study, the “SRK” property package was used.

The column models in ProMax utilize rigorous stage-by-stage mass and energy balances (not using shortcut methods as in GLYCalc).

## Data Comparison

For the prediction of BTEX emissions in refrigeration units, the flash calculation in the cold separator (also called the low temperature separator or LTS) is of critical importance. Also important, but not as critical, are the calculations in the flash tank and regenerator still. The reason for the relative importance of the cold separator flash is that the vast majority of BTEX absorbed in the aqueous phase of this separator is ultimately emitted from the flash tank and/or still overhead.

A significant challenge in this study was that the reviewed simulators had widely varying predictions as to how much BTEX would be soluble in the aqueous phase of the cold separator.

A number of reasons for this variation are proposed:

- There are typically three phases in the cold separator – hydrocarbon vapour, hydrocarbon liquid and an aqueous (EG/water) phase. Little, if any, VLLE data is available for BTEX-H<sub>2</sub>O-EG-hydrocarbon systems at cold separator conditions.
- The flash calculation needs to apply over a wide range of temperatures and pressures; typical ranges would be:
  - -35 C to -10 C (-31 F to 14 F)
  - 2,000 – 7,000 kPa (290 – 1,015 psi)
- The simulators must not only accurately predict the BTEX phase split, but must also accurately predict other aspects of the flash, for example the hydrocarbon vapour/liquid split and losses of components such as EG to the vapour and hydrocarbon liquid phases.

A significant amount of effort has been made to accurately predict BTEX emissions in dehydration units (TEG being the most common glycol); however the available information for refrigeration units (EG) is much more limited.

Perhaps the most important data source for BTEX solubility in EG systems is the Gas Processors Association (GPA) Research Report RR-137 – “The Solubility of Selected Aromatic Hydrocarbons in Monoethylene Glycol” [4]. It is an important paper since a good deal of data is available at conditions expected in the low temperature separator, flash tank and regenerator of a typical EG system. In a previous paper [1] it was shown how a related study, GPA Research Report RR-131, could be used to determine the accuracy of the simulators to predict BTEX emissions in TEG units.

However, a significant limitation in the available data in RR-137 is that only VLE measurements were made for Methane/BTEX/EG systems. This is a limitation since it does not help to understand how much BTEX will be soluble in the hydrocarbon liquid vs. aqueous phases. No VLLE data for BTEX / hydrocarbon / EG / water systems at cold separator conditions has been identified in the open literature.

It is useful to know how the three reviewed simulators compare to each other, even if VLLE data is not available to compare the BTEX solubility in the cold separator. Therefore, a set of ten facilities for which operating data was available were selected and the amount of BTEX absorbed in the aqueous phase of the low temperature separators for each of the reviewed simulators was compared. This is discussed in the sections *Facility Comparison: Low Temperature Separator* and *Facility Comparison: Flash Tank and Regenerator*. The section *Comparison to Plant Data* details comparisons made to data collected from three facilities.

## Facility Comparison: Low Temperature Separator

Ten facilities were selected with varying characteristics for which sufficient data was available, and for each of the simulators the solubility of the BTEX components was calculated in the LTS aqueous phase. As previously mentioned, the solubility of BTEX in the aqueous phase of the LTS is critical in accurately estimating the BTEX emissions for the facility.

Earlier it was noted that for HYSYS, the Peng Robinson (PR) equation of state has historically been used as the “general purpose” simulator for gas facilities and it is therefore possible that engineers would consider using this property package to predict BTEX emissions in refrigeration units. The Peng Robinson package *is not* recommended for this purpose, as no emissions would be predicted due to the negligible amount of BTEX predicted to be soluble in the aqueous phase at the cold separator. AspenTech clearly recommends that the Glycol package be used for the purpose of predicting BTEX emissions in refrigeration units.

### Benzene

The following figure compares the amount of benzene predicted by each of the simulators to be in the aqueous phase of the cold separator for each of the ten facilities. To make it easier to compare the simulators, all the results are normalized to one standard (the results of the HYSYS-Glycol package). This does not imply a recommendation of HYSYS-Glycol as the standard but is merely the convention used. Specifically, the mass flow rate of benzene in the aqueous phase was calculated and divided by the mass flow rate of aqueous-phase benzene predicted using HYSYS-Glycol (mass flow rate was selected since BTEX emissions are typically reported on a mass basis).

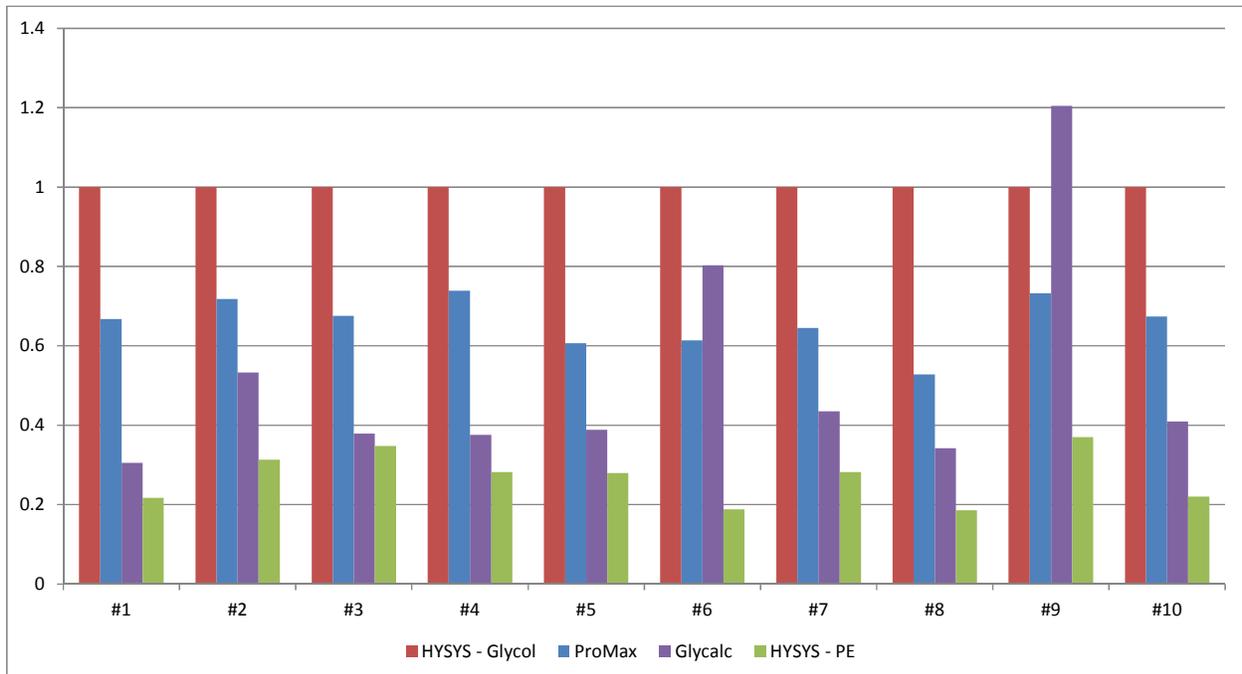


Figure 2 – Comparison of benzene in LTS aqueous phase (HYSYS-Glycol = 1)

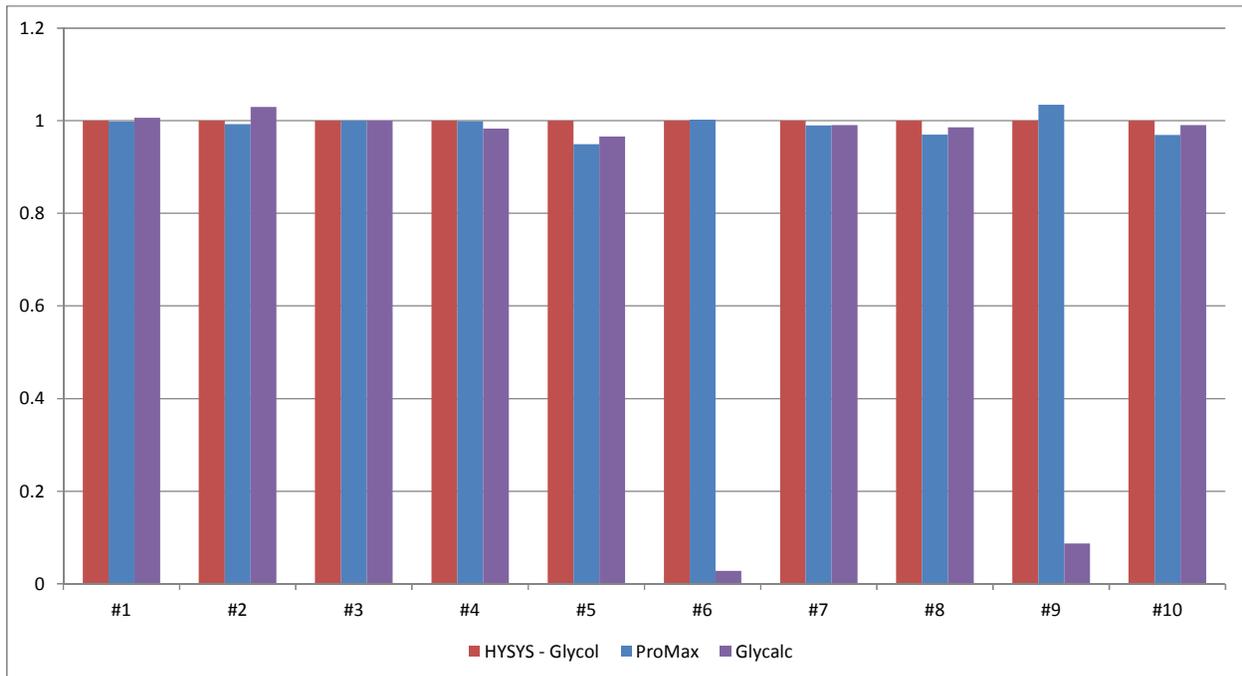
The results of the simulators are quite different, but are at the same time surprisingly consistent in terms of the relative predictions. In each of the ten systems reviewed:

- The HYSYS-Glycol package typically predicted the highest benzene solubility in the aqueous phase.
- ProMax typically predicted the second-highest benzene solubility in the aqueous phase.
- GLYCalc typically predicted the lowest benzene emissions. However, for datasets #6 and #9, GLYCalc incorrectly predicted the absence of a hydrocarbon liquid phase and therefore calculated a much higher benzene concentration in the aqueous phase.

It is important to note that for the BTEX components, the simulators predicted that benzene was the component with the highest concentration in the aqueous phase (>50% of the BTEX components), ultimately resulting in the highest proportion of emissions.

### *Benzene in combined Aqueous and Hydrocarbon Liquid phases*

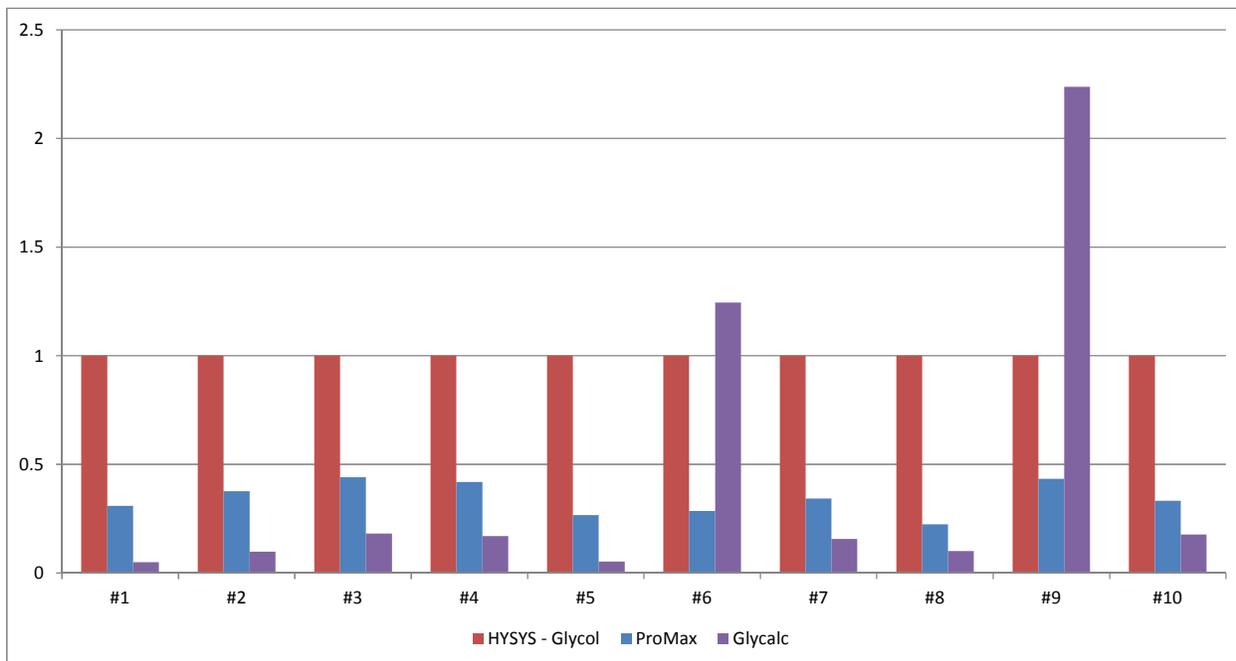
The following figure illustrates why it is critical to understand the vapour-liquid-liquid equilibrium (VLLE), and not just the vapour-liquid equilibrium (VLE). In general, the simulators offer very similar predictions regarding the amount of benzene in the combined aqueous and hydrocarbon liquid phases (overall the VLE is similar) but as evidenced in the previous section can clearly deviate significantly in terms of how much benzene goes to the individual liquid phases (VLLE). It is noted that the simulators predict that the vast majority of benzene (usually 95%+) goes to the hydrocarbon liquid phase.



**Figure 3 – Comparison of benzene in combined LTS hydrocarbon liquid and aqueous phase (HYSYS-Glycol = 1)**

## Toluene

As before, the mass flowrate of the reviewed component (toluene) in the aqueous phase was calculated and divided by the mass flow rate of aqueous-phase toluene predicted using HYSYS-Glycol to obtain normalized results as shown in the following figure.



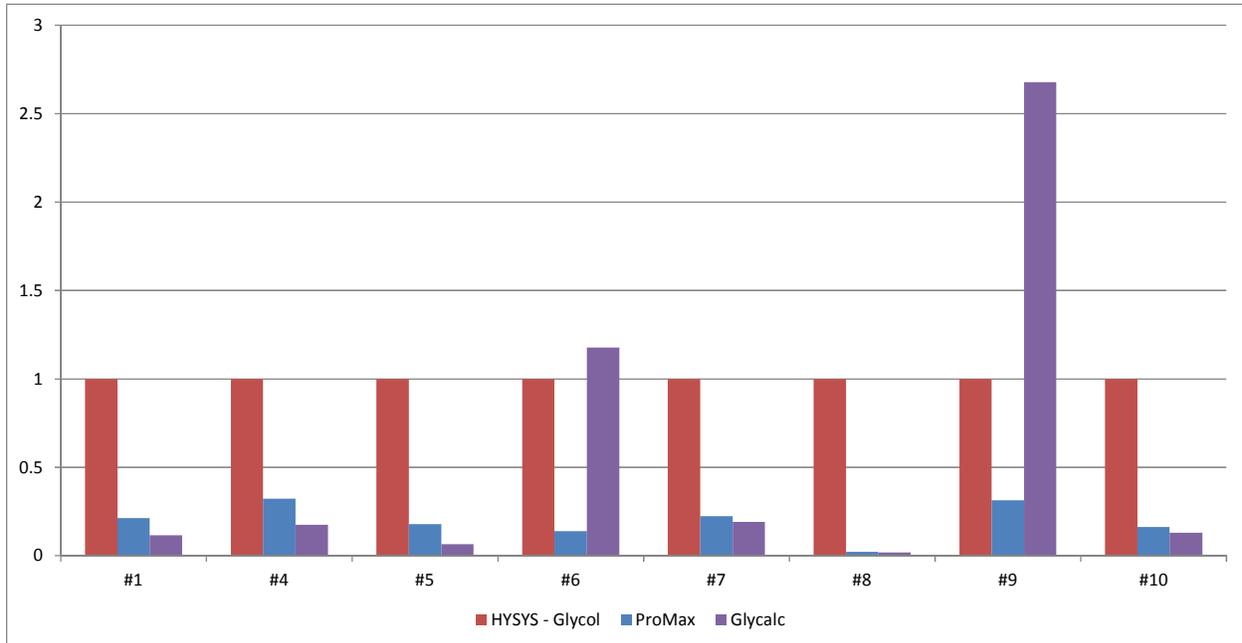
**Figure 4 – Comparison of toluene in LTS aqueous phase (HYSYS-Glycol = 1)**

For the 10 systems reviewed:

- The HYSYS-Glycol package typically predicted the highest toluene solubility in the aqueous phase by far.
- ProMax typically predicted the second-highest toluene solubility in the aqueous phase.
- GLYCalc typically predicted the lowest toluene emissions. However, for datasets #6 and #9, GLYCalc incorrectly predicted the absence of a hydrocarbon liquid phase and therefore calculated a much higher toluene concentration in the aqueous phase.

## Ethylbenzene

As before, the mass flow rate of the reviewed component (ethylbenzene) in the aqueous phase was calculated and divided by the mass flow rate of aqueous-phase ethylbenzene predicted using HYSYS-Glycol to obtain normalized results as shown in the following figure.



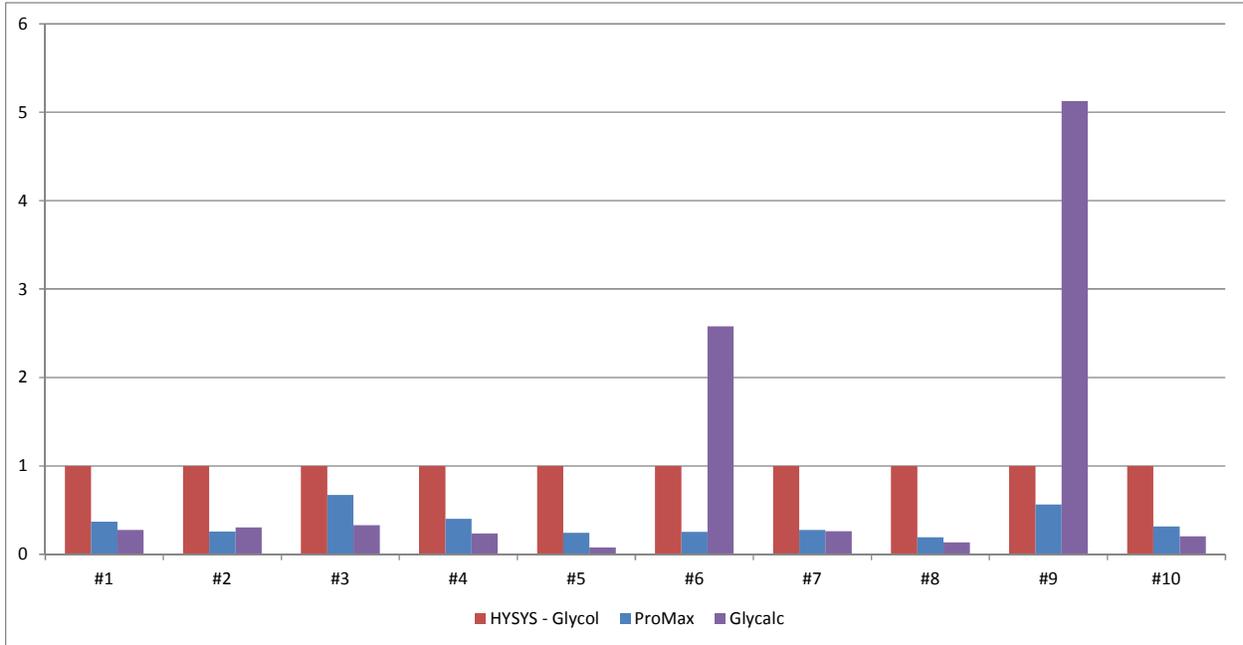
**Figure 5 – Comparison of ethyl-benzene in LTS aqueous phase (HYSYS-Glycol = 1)**

For the 10 systems reviewed:

- Two systems (#2 and #3) did not contain ethylbenzene and are therefore not shown in Figure 5.
- The HYSYS-Glycol package typically predicted the highest ethylbenzene solubility in the aqueous phase by far.
- ProMax typically predicted the second-highest ethylbenzene solubility in the aqueous phase.
- GLYCalc typically predicted the lowest ethylbenzene emissions. However, for datasets #6 and #9, GLYCalc incorrectly predicted the absence of a hydrocarbon liquid phase and therefore calculated a much higher ethylbenzene concentration in the aqueous phase.

## Xylenes

As before, the mass flow rate of the reviewed components (xylenes) in the aqueous phase were calculated and divided by the mass flow rate of aqueous-phase xylenes predicted using HYSYS-Glycol to obtain normalized results as shown in the following figure. It is noted that the xylenes (o-, m-, and p-xylene) were lumped together as “xylenes” since GLYCalc does not differentiate between them.



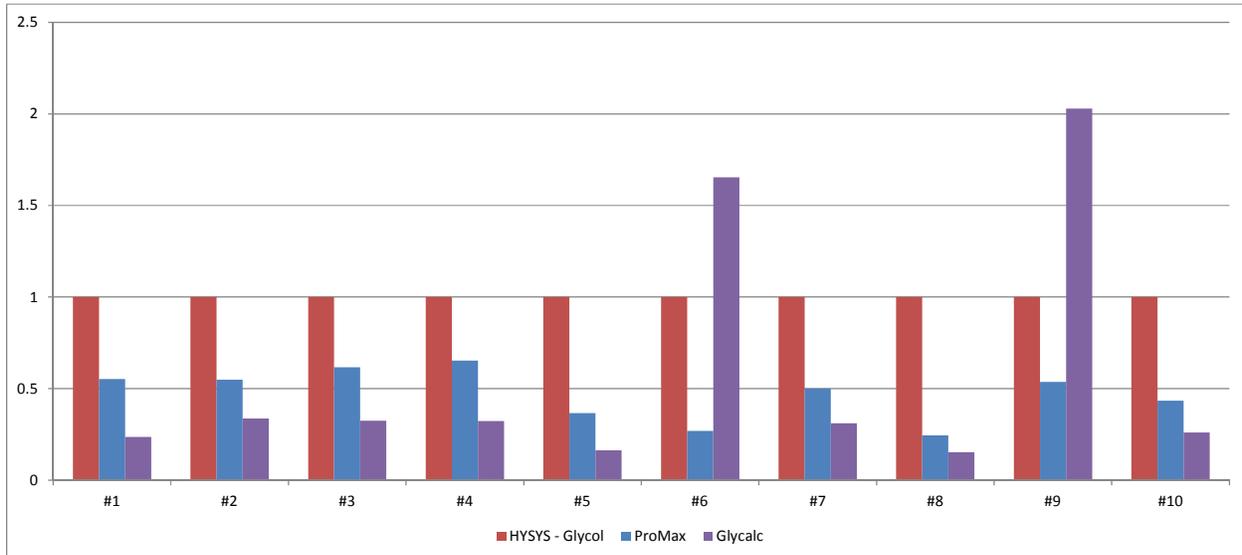
**Figure 6 – Comparison of xylenes in LTS aqueous phase (HYSYS-Glycol = 1)**

For the 10 systems reviewed:

- The HYSYS-Glycol package typically predicted the highest xylenes solubility in the aqueous phase.
- ProMax typically predicted the second-highest xylenes solubility in the aqueous phase.
- GLYCalc typically predicted the lowest xylenes emissions. However, for datasets #6 and #9, GLYCalc incorrectly predicted the absence of a hydrocarbon liquid phase and therefore calculated a much higher xylenes concentration in the aqueous phase.

## BTEX

As before, the mass flow rate of the reviewed components (BTEX) in the aqueous phase was calculated and divided by the mass flow rate of aqueous-phase BTEX predicted using HYSYS-Glycol to obtain normalized results as shown in the following figure.



**Figure 7 – Comparison of BTEX in LTS aqueous phase (HYSYS-Glycol = 1)**

The results for each of the individual BTEX components presented in the previous sections are very similar in terms of the relative predictions of each of the simulators. Therefore, the overall BTEX results show the same trend:

- The HYSYS-Glycol package typically predicted the highest BTEX solubility in the aqueous phase.
- ProMax typically predicted the second-highest BTEX solubility in the aqueous phase.
- GLYCalc typically predicted the lowest BTEX emissions. However, for datasets #6 and #9, GLYCalc incorrectly predicted the absence of a hydrocarbon liquid phase and therefore calculated a much higher BTEX concentration in the aqueous phase.

## Facility Comparison: Flash Tank and Regenerator

The solubility of BTEX in the low temperature separator aqueous phase is most critical in estimating the BTEX emissions in refrigeration systems. ProMax and HYSYS predicted that in excess of 99.8% of the BTEX in the LTS aqueous phase ends up being emitted from the flash tank overheads or still tank vent (the remainder staying in the lean glycol).

However, the relative emissions for the flash tank and still overhead are important if these overheads are handled differently. For example, the flash tank vapour (being mainly hydrocarbons) may end up as fuel gas, while the still overheads are vented. In this respect, ProMax and HYSYS-Glycol were very similar, with the results from GLYCalc being significantly higher:

Simulator	Benzene K factor (y/x)	Toluene K factor (y/x)	Xylenes K factor (y/x)
ProMax	1.14	0.76	0.27
HYSYS-Glycol	0.97	0.58	0.27
GLYCalc	2.76	1.66	0.71

**Figure 8 – Flash Tank Comparison – K factors for benzene, toluene, xylenes**

It is noted that K-factors are used for this analysis due to the differences in the inlet composition to the flash tank for each of the simulators; in addition, it is not possible to directly specify an inlet composition in GLYCalc for direct comparison. K-factors are highest for GLYCalc meaning that it will predict more benzene going to the flash tank overheads than the other simulators.

Detailed analysis of the still was not completed in this report. The reader is invited to refer to reference [1], where it is stated:

The HYSYS-PR and HYSYS-Glycol compare favorably to the data. [However,] it is difficult to make a direct comparison of the GLYCalc results to the data given the empirical nature of the GLYCalc regenerator model. One would expect that the K-values calculated by GLYCalc would be greater than the experimental K-values based on a typical assumption of 2 equilibrium stages above the reboiler; however a check in HYSYS indicates that the K-values there do not increase by this magnitude. It is also clear that the methane K-value in GLYCalc is far too large.

A question that could be asked is, if the match is very good at the contactor but possibly poor at the regenerator, what will be the overall impact on BTEX emissions? Based on our experience, the match is usually reasonable – as both HYSYS and GLYCalc predict that *most* of the BTEX at the inlet of the regenerator goes to the vent; it is more critical to ensure that there is a good match at the contactor to ensure prediction of BTEX concentration in the rich glycol phase.

The same conclusion applies to the EG still – while there may be significant discrepancies, it is not so important in the context of predicting BTEX emissions.

Finally, it is noted that the still overheads are occasionally routed to a condenser to reduce the BTEX emissions; we have anecdotally found that GLYCalc sometimes failed to properly predict the hydrocarbon liquid phase in the condenser, a problem which we earlier noted for the cold separator.

## Comparison to Plant Data

Inlet extended gas and lean/rich glycol analyses for three facilities were obtained, along with corresponding operating data. The rich glycol analyses can be used to directly compare the amount of BTEX absorbed in the cold separator aqueous phase. Both the extended gas and rich glycol analyses report the BTEX concentration.

The basic facility data is as follows:

Parameter	Unit #1	Unit #2	Unit #3
Inlet Benzene	54 ppm	38 ppm	58 ppm
Inlet Toluene	42 ppm	62 ppm	29 ppm
Inlet Ethylbenzene	< 10 ppm (assumed 5 ppm)	< 10 ppm (assumed 5 ppm)	< 10 ppm (assumed 5 ppm)
Inlet Xylenes	13 ppm	35 ppm	19 ppm
Inlet Temperature	23 C (73 F)	11 C (52 F)	25 C (77 F)
Inlet Pressure	2,400 kPag (348 psig)	5,850 kPag (848 psig)	4,700 kPag (682 psig)
Inlet Gas Rate	507 E3m3/d (17.9 MMSCFD)	812 E3m3/d (28.7 MMSCFD)	155 E3m3/d (5.5 MMSCFD)
LTS Temperature	-21 C (-6 F)	-22 C (-7 F)	-17 C (1 F)
LTS Pressure	2,300 kPag (334 psig)	5,800 kPag (841 psig)	4,600 kPag (667 psig)
Glycol Circulation	3.11 USGPM	1.49 USGPM	3.8 USGPM

**Figure 9 – Facility Data**

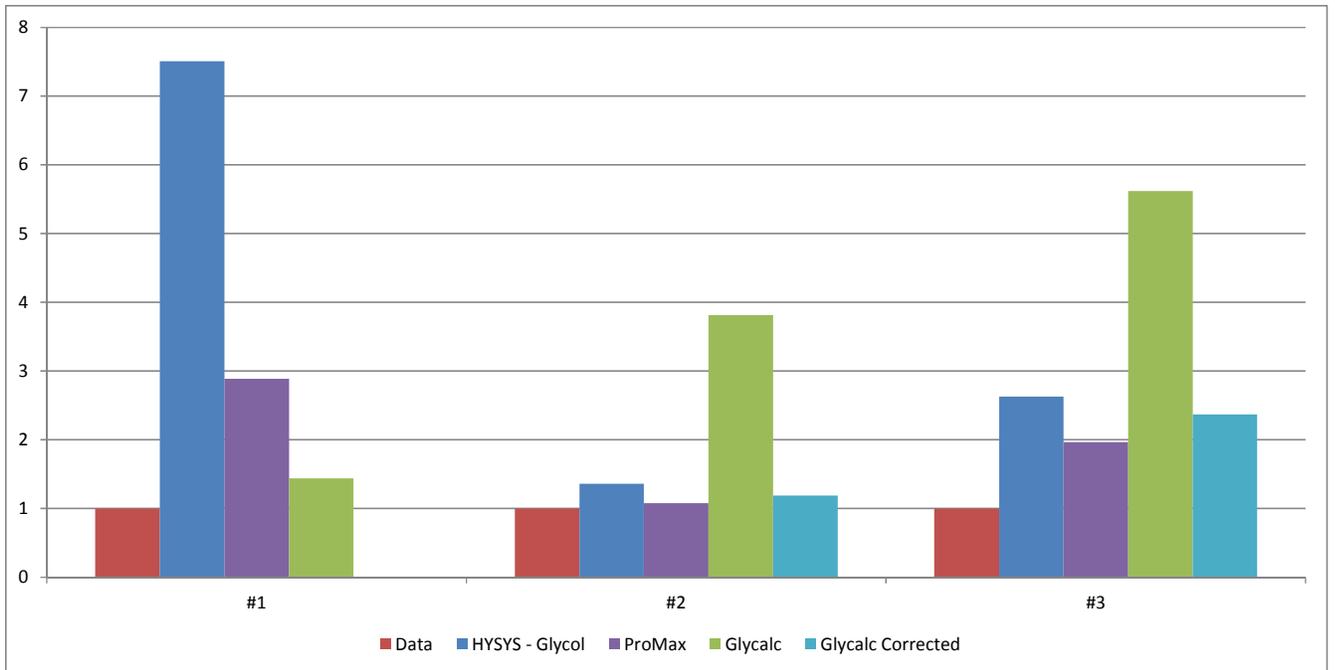
The data for ethylbenzene showed “<10 ppm” for all three locations. This is not sufficient accuracy for comparing the ethylbenzene emissions predictions. For the purpose of predicting overall BTEX emissions (of which ethylbenzene is a minor contributor) 5 ppm was assumed.

It is important to note that the field data is prone to error in measurement; significant possible sources of error are:

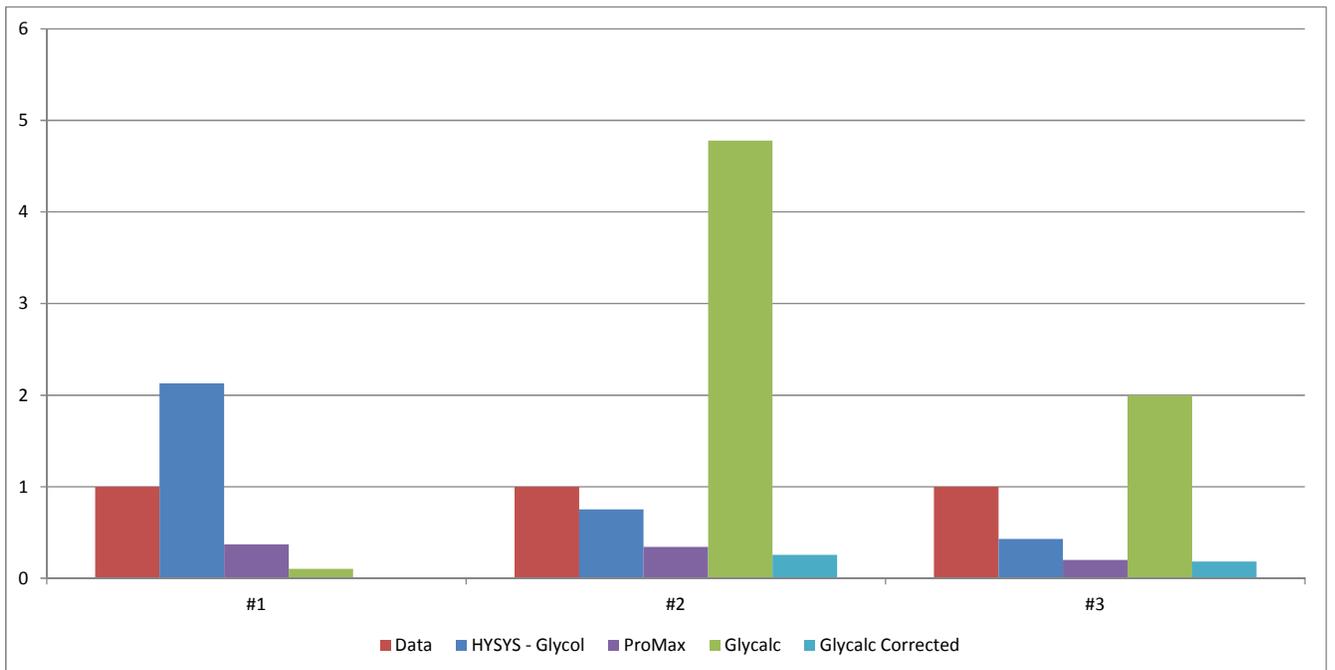
- Inlet gas analysis – minimum detectable limit of individual components is under 10 ppm. According to the analysis company, accuracy above 10 ppm is about  $\pm 1.5$  ppm up to 100 ppm.
- LTS temperature – BTEX solubility is very sensitive to this temperature. It is anticipated that actual temperature should not differ by more than 1-2 C, which would change BTEX solubility by  $\pm 10\%$ . Measurement of other reported conditions – LTS pressure, gas rate, glycol circulation rate can also introduce error in the calculations.
- Rich glycol analysis – reportable detection limit (RDL) is 0.5  $\mu\text{g/mL}$  (this would be 0.5 ppm if the density is 1000  $\text{kg/m}^3$ ).
- The actual gathering of the samples is prone to error (sampling, transportation, measurement).

For each of the simulators (including a “corrected” GLYCalc result), the following figures are presented:

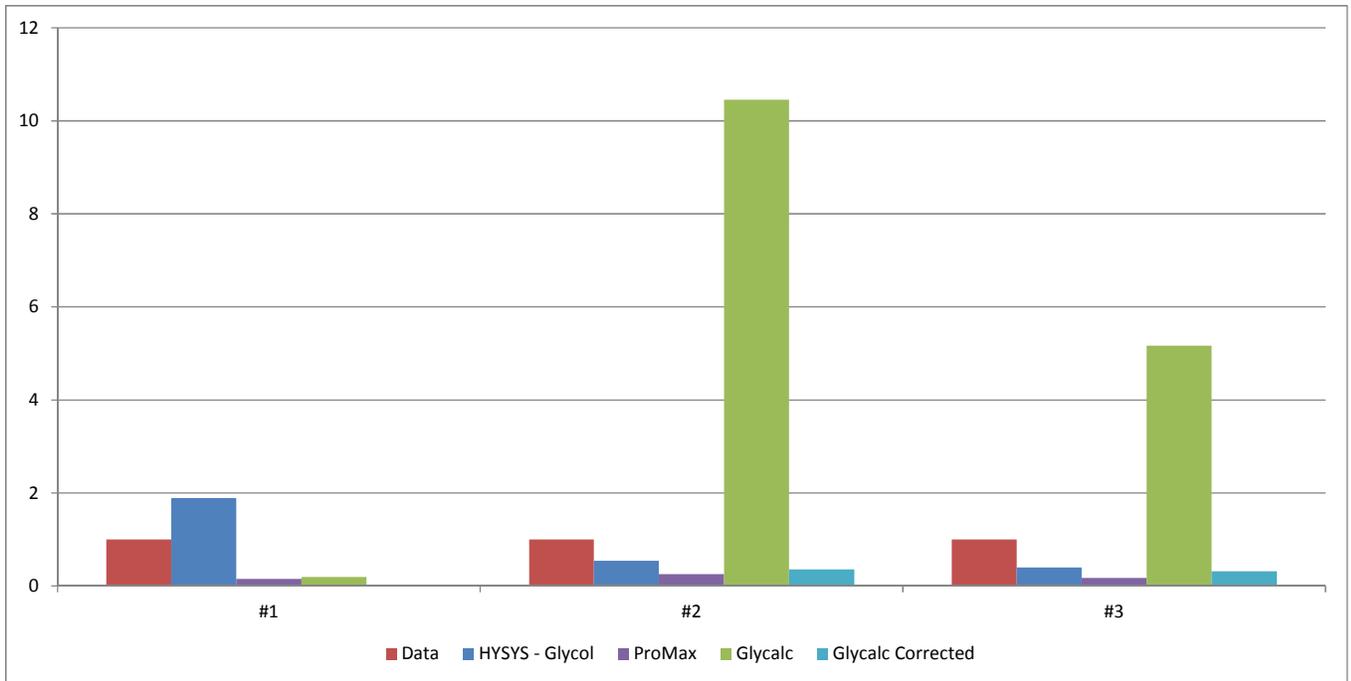
- Figure 10: Benzene in the aqueous phase of the LTS (normalized to the data).
- Figure 11: Toluene in the aqueous phase of the LTS (normalized to the data).
- Figure 12: Xylenes in the aqueous phase of the LTS (normalized to the data).
- Figure 13: BTEX in the aqueous phase of the LTS (normalized to the data).



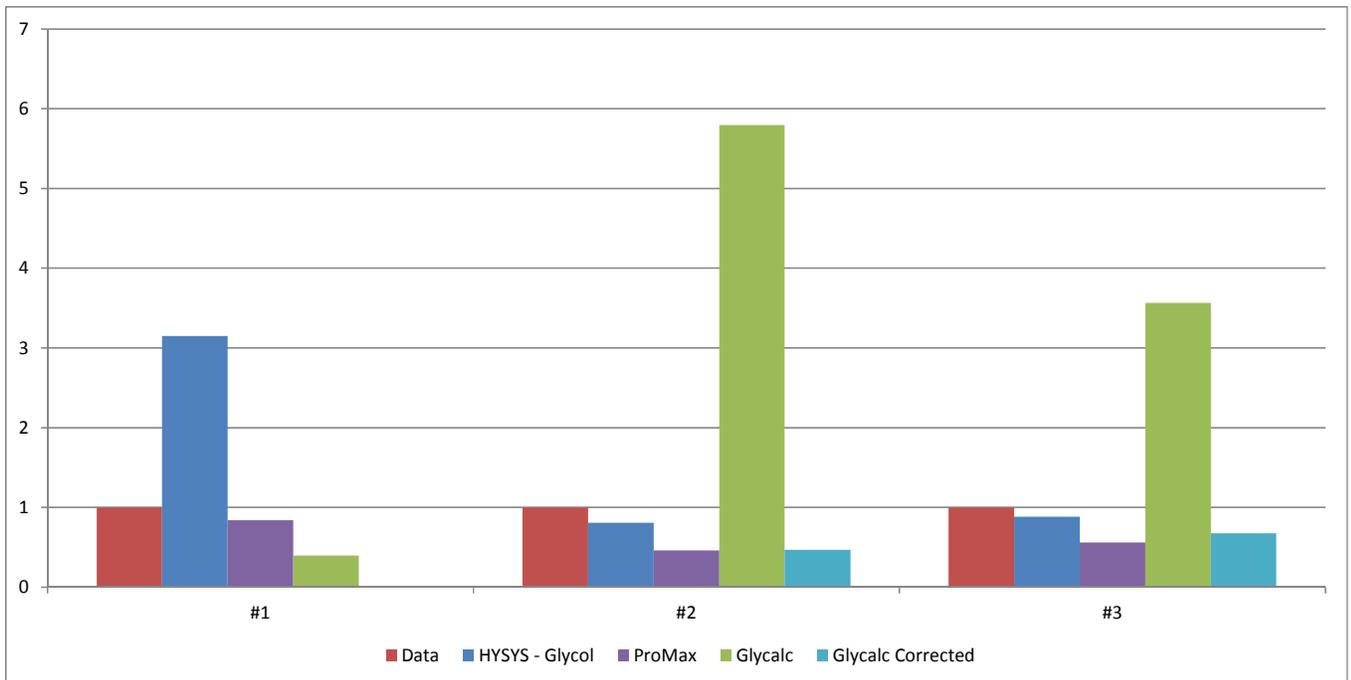
**Figure 10 – Comparison of Benzene in LTS aqueous phase (Data = 1)**



**Figure 11 – Comparison of Toluene in LTS aqueous phase (Data = 1)**



**Figure 12 – Comparison of Xylenes in LTS aqueous phase (Data = 1)**



**Figure 13 – Comparison of BTEX in LTS aqueous phase (Data = 1)**

The calculations for the individual BTEX components were individually quite different from the data in many cases, with the exception of Location #2 benzene. The overall predictions of BTEX were much better, except for HYSYS location #1 which overpredicted BTEX by 3 times and GLYCalc locations #2 and #3 which overpredicted BTEX by 3-6 times.

### **Location #1**

This is a relatively low pressure unit (2,400 kPag) for which HYSYS-Glycol predicts BTEX emissions 3 times higher than the data; ProMax predicts BTEX solubility close to the reported total, and GLYCalc is less than half of the reported total. It is recommended that caution be used when predicting BTEX emissions using HYSYS for units at lower pressures (< 2,500 kPag).

### **Location #2**

GLYCalc did not predict a hydrocarbon liquid phase (incorrectly) and therefore calculated a much higher BTEX concentration in the aqueous phase. HYSYS predicts BTEX solubility close to the reported total, and ProMax solubility was about half of the data. When GLYCalc was “corrected” by adding enough C8+ to create a hydrocarbon liquid phase, the results for GLYCalc were also similar to ProMax.

### **Location #3**

GLYCalc did not predict a hydrocarbon liquid phase (incorrectly) and therefore calculated a much higher benzene concentration in the aqueous phase. HYSYS-Glycol predicted BTEX solubility close to the reported total, and ProMax predictions were about 56% of the data. When GLYCalc was “corrected” by adding enough C8+ to create a hydrocarbon liquid phase, the results for GLYCalc were about 67% of the data.

## **Recommendations for Further Review**

Some further work can be done to improve our understanding of the various simulators’ ability to predict BTEX emissions in EG facilities. Areas to focus on include:

- Comparison with facility data: It would be helpful to obtain more plant data, ensuring a close review of the procedure for collecting data and samples.
- Comparison with experimental data: Although GPA RR-137 is very useful, a VLLE study would improve on this work and be very useful in understanding the solubility of BTEX in the aqueous and hydrocarbon liquid phases of cold separators.
- Efficiency of condensers in removal of BTEX: This was not specifically addressed in this report but would be a useful area of study.

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