Experimental and Modeling Results for Rich Gas Absorption of HCl in Caustic Solutions

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Developing a modeling capability and providing performance data in the area of absorbing "rich gas" fills a long-standing technical gap in separations technology. The term "rich gas" is used in this context to denote an application in which a substantial portion or a majority of the gas is absorbed from the incoming gas mixture. Closing this gap can lead to more efficient designs of scrubbers, resulting in lower cost and smaller footprints for our processes. Ultimately, the goal is to work toward the more fundamentally predictive methods of calculating mass transfer which rely on the individual mass transfer coefficients, k_g and k_l, along with the effective area for mass transfer across the packing or tray, a. However, since the present state of the predictive methods is not adequate even for the more typical cases encountered, this work must become a part of the total understanding of the larger picture.

As noted above, the term "rich gas" is used in this context to denote an application in which a substantial portion of the gas is absorbed from the incoming gas mixture. It can be easily visualized that under the conditions where a substantial fraction of the incoming gas is absorbed into the liquid mixture, the gas volume diminishes across the tower. Along with the reduction in gas volume is the commensurate reduction in the associated dimensionless numbers, particularly the gas Reynolds number. Where the point "rich gas" applies is a matter of some judgment, but it can certainly be seen that the prediction of the mass transfer coefficient, which is dependent in part on the Reynolds number, is especially problematic in the prediction of the individual mass transfer coefficient. The prediction of "total scrubbers", or rich applications, is especially problematic because of complications from the hydraulic behavior as well as the fact that the controlling mass transfer resistance is not clearly understood.

The system of absorbing HCl in caustic is a classic system that can be used to quantify and test correlations for gas phase mass transfer coefficients because the ionic reactions of HCl_{aq} with excess $NaOH_{aq}$ are extremely rapid. While the statement is true of the HCl / NaOH system as an effective test system, it is not widely reported in literature. The difficulties of handling HCl and NaOH in an academic or university laboratory would make the system uninviting as a "normal" test system. In general, only industrial laboratories or specially equipped laboratories are in a position to handle such reactive and corrosive systems on a routine basis. If we add to this the fact that industrial practitioners are far more likely to have an interest in absorbing rich gas streams that may result from process upsets, it is not surprising to find that there is very little information available in the literature on this type of problem.

An experimental apparatus for rich gas absorption was built, consisting of a 2" (5.08 cm) packed tower with ¼" (0.635 cm) ceramic saddles. This experimental unit was used to measure the absorption performance of hydrogen chloride gas in aqueous sodium hydroxide absorbent. Increasing concentrations of HCl in nitrogen were absorbed across limited packed bed heights to produce meaningful data for absorption performance evaluation. Concentrations of HCl in the incoming feed gas were varied from 5% to 90%. The results of this experimental program are presented in this report.

The results of the experiments on HCl can be viewed below in Table 1. Seven experiments were carried out, varying the concentration of the gas feed from 5 to 90 mole % HCl in the inlet gas. The experiment conducted at 10 mole % concentration was carried out three times. The first experiment seems to be in disagreement with the second two duplicate experiments, but all of the data gathered is presented below. All of the experiments were performed with 10 wt% caustic solution, and arranged such that there was always an excess of caustic over stoichiometric requirements for reaction of HCl and NaOH.

Table 1. Experimental results for several HCL gas concentrations

HCl Concentration Feed Gas Mole %	**HCl Concentration Vent Gas Mole %**	**Gas Feed Rate SCCM**	**Liquid Feed Rate ml/min**	**Percent Absorption %**
5	0.0429	26463	550	99.1
10	0.0311	26068	550	99.7
10	0.1376	26068	550	98.6
10	0.1775	26068	550	98.2
25	0.3593	25680	550	98.6
50	0.8857	27840	550	98.2
75	0.656	24090	550	99.1
90	1.4088	23640	550	98.4

The experimental conditions were modeled using the rate based modeling tool in Aspen Version 2004 known as RateSep. While it is certainly true that RateSep is a better tool from a modeling standpoint than previous tools and that it constitutes a vast improvement from the user's perspective, one must not confuse ease of use with improvements in the fundamental correlations. At the heart of the rate based modeling effort are still the same fundamental correlations, whether the correlations are those of Onda, Billet and Schultes, or Bravo and Fair. The ultimate goal of this entire work is to improve the correlations that are available by generating new data and regressing existing data in order to provide better, more robust correlations that can be delivered in RateSep.

The experimental configuration was modeled using an electrolyte NRTL model that has been developed for use in Dow applications. The model has been tested a number of times, and gives excellent results across a broad spectrum of HCl concentrations. The tower was modeled with 12 segments (not stages) that represent the 15.2 cm. of packing. Finer discrimination of the grid (more segments) resulted in no numerical changes in the outlet gas result, but did result in decreased stability of the numerical solution. The correlations that were used in this study were the Onda correlations and the Bravo and Fair correlation. The correlations of Billet and Schultes require packing specific parameters for application to a specific type of packing, and so were not utilized in this comparison.

There are several general comments that are appropriate regarding the ability to predict the performance of these types of systems, and lessons that can be learned from the experimental data. The results of the comparison between the simulation and the experimental results can be seen in Figure 1. Note that outlet gas concentration is presented on a logarithmic scale.

- In general, our ability to accurately predict the outlet gas concentration from an absorber is limited. If we were to be tasked with predictive modeling of a system such as this, and the requirement of this is the safety of our facilities and our environment, then these approaches are not yet good enough to employ without resorting to experimental data.

- The older correlation of Onda under predicts the performance of the absorption tower, and the correlation of Bravo and Fair over predicts the performance. Obviously, there are other correlations that can be applied, but none of the available correlations in an unaltered form adequately modeled the system.

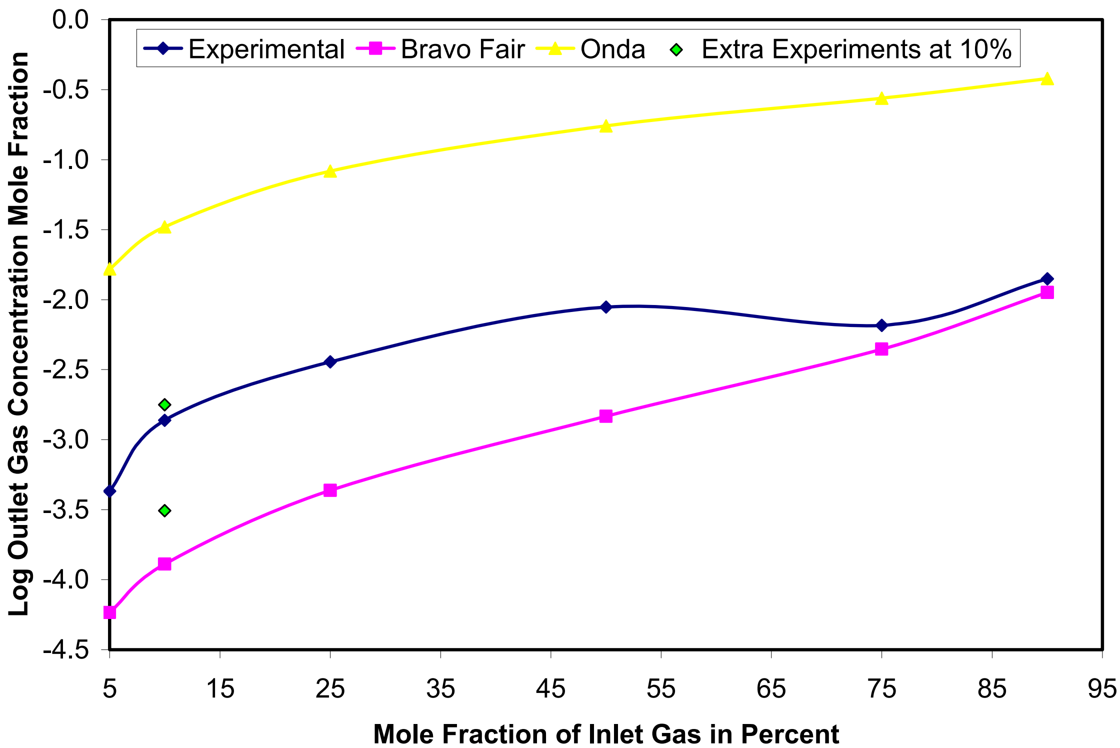

Figure 1. Comparison of experimental outlet concentration of HCl in the gas with the models of Bravo-Fair and Onda.