CHAPTER 7:

CONCLUSIONS, RECOMMENDATIONS AND OBSERVATIONS

7.1 Modeling and ASPEN Plus Computer Simulation

The engineer cannot check his/her knowledge and experience at the door when it comes to computer simulations. "Garbage in-garbage out" remains true in the computer industry especially when it comes to chemical process modeling. Simulation engineers still require critical problem-solving skills.

7.1.1 Modeling NOx Absorption

Conversion-reaction models with vapor-liquid equilibrium provide satisfactory information for the development of mass-balance simulations of NOx absorption. However, they give little insight into the response of the system to changes in process variables. We have shown that equilibrium-reaction models with vapor-liquid equilibrium match experimental results in the literature for NOx absorption for mass balance as well as process changes. We have also shown that kinetic effects for general NOx absorption remain minimal under normal circumstances. Therefore, we see the use of kinetic modeling as superfluous in most cases. Cases involving the use of reactants such as ozone, hydrogen peroxide, and where NO forms a preponderance of the NOx load increase the relevance of kinetic modeling.

7.1.2 Modeling SCR

Conversion modeling of the SCR, as in the case of NOx absorption, give satisfactory results for mass-balance information. This is of less use, however, because no vapor-liquid equilibrium exists in the SCR. We have shown equilibrium modeling of the SCR to be highly unstable and inaccurate. Apparently, ASPEN Plus experiences mathematical limits and artifacts for calculating results for equilibrium reactions near completion. Kinetic modeling is the only acceptable route for modeling the SCR. For such modeling, accurate and consistent kinetic data must be found or determined experimentally to achieve meaningful results.

7.2 Process Improvements

For the specific case study of NOx absorption and SCR at RFAAP, we found little improvement possibility for the SCR as it was running near optimum. We recommend the testing of the catalyst to determine its viability. Replacement or cleaning may be needed. However, the astronomical cost of SCR catalyst may cast favorable light on research of other technologies and methods of NOx reduction. Also, because new catalyst, even when treated properly, deteriorates at a steady rate, replacement cannot be seen as a long-term solution. Resources for the catalyst replacement schedule could fund supplemental processes or modifications to the existing NOx absorption process.

The lack of options for the SCR is counterpoint to the plentiful opportunities to improve NOx absorption by the scrubber/absorber. We have explored fully, through computer simulation and research of the literature, the key process variables that improve the performance of this process. We have also studied the economic implications of implementation of these improvements through equipment retrofit. The most promising adjustments include cooling the fume stream, adding side-water streams, adding a flash drum in the waste acid stream, and using supplemental reactants such as ozone and hydrogen peroxide. We have also discussed the "non-economic" merits of these options including ease of control, stability of operation, and relief for downstream waste neutralization operations.

It is clear that improvements must be made in the foreseeable future to keep pace with the tightening governmental restrictions on controlled effluents. The choice now is simply which direction to pursue.