COMPUTER SIMULATION AND OPTIMIZATION OF THE NOx ABATEMENT SYSTEM AT THE RADFORD FACILITY AND ARMY AMMUNITION PLANT

by

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(ABSTRACT)

This thesis discusses findings gained through work with the NOx abatement system at Radford Facility and Army Ammunition Plant (RFAAP). Removal of harmful substances from flue-gas emissions has garnered increased priority in the chemical industry in preceding decades, as governmental restrictions on these substances become more stringent and as national awareness concerning environmental quality and resource utilization continues to grow. These reasons make the study of NOx abatement an important and challenging endeavor.

This work concerns itself specifically with reduction of NOx in flue-gas emissions from stationary sources. First we present an overview of current technology and approaches to controlling NOx for stationary sources. Next, we focus in on one particular approach to control of NOx within the context of a case study of the technology used at the Radford Facility and Army Ammunition Plant. RFAAP employs a scrubber/absorber tower followed in series by a selective catalytic reduction (SCR) reaction vessel in their NOx abatement system. We use as the method of study computer simulations within ASPEN Plus, a process simulation software package for chemical plants.

We develop three different models with which to characterize NOx abatement at RFAAP, a conversion model, an equilibrium model and a kinetic model. The conversion-reaction model approximates the absorption and SCR reactions with constant percentage extent-of-reaction values. Though useful for initial investigation and mass balance information, we find the conversion model's insensitivity to process changes to be unacceptable for in-depth study of the case of NOx absorption and SCR. The equilibrium-reaction model works on the assumption that all the reactions reach chemical equilibrium. For the conditions studied here, we find the equilibrium model accurately simulates NOx absorption but fails in the case of SCR. Therefore, we introduce a kinetic-reaction model to handle the SCR. The SCR reactions prove to be highly rate-dependant and the kinetic approach performs well.

The final evolution of the ASPEN Plus simulation uses an equilibrium model for the absorption operation and a kinetic model for the SCR. We explore retrofit options using this combined model and propose process improvements. We end this work with observations of the entire project in the form of conclusions and recommendations for improving the operation of the NOx abatement system through process-parameter optimization and equipment-retrofit schemes.

By leading the reader through the process by which we arrived at a successful and highly informative computer model for NOx absorption and SCR, we hope to educate the reader on the subtleties of NOx abatement by absorption and SCR. We attempt to break down the numerous complex processes to present a less daunting prospect to the engineer challenged with the application of current NOx removal technology. In addition, we introduce the reader to the power and usefulness of computer modeling in instances of such complexity. The model teaches us about the details of the process and helps us develop concrete information for its optimization. Ideally, the reader could use a similar approach in tackling related operations and not confine the usefulness of this thesis to NOx absorption and SCR.

The audiences that we think would benefit from exposure to this thesis are the following:

- Environmental engineers with a NOx problem;
- Process engineers interested in optimization tools;
- Design engineers exploring flue-gas treatment options;
- Combustion engineer desiring to learn about SCR;
- Chemists and mathematicians intrigued by the complexities of NOx absorption chemistry.

For Melissa, my love, my inspiration, my reason, my wife…

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