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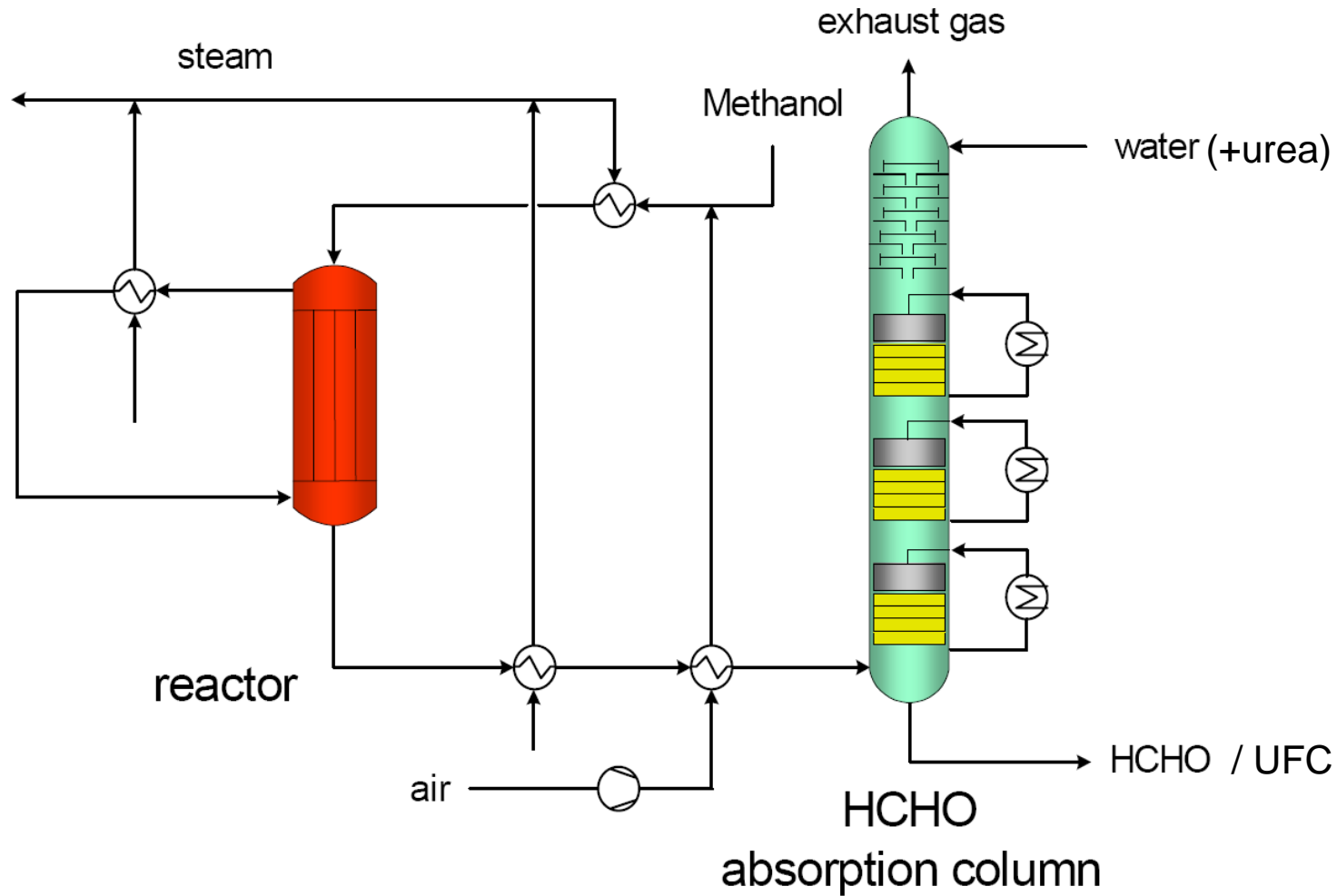
Chimar Hellas S.A.



Modeling of Formalin & UFC Production in Absorption Columns

FORTH/ICE-HT – CHIMAR HELLAS SA

Typical Formaldehyde/UFC production scheme



Process Modeling

Modern Tools

- Modeling of the absorption process utilizing the latest know-how on materials, reactions, physical and thermodynamic data libraries.
- Validation of model predictions using experimental data from the literature and typical absorption units.
- Investigation of the potential to simulate process conditions at several scales (lab, pilot, and industrial scale).

Formalin

- Latest experimental and theoretical data were collected through an extensive literature survey, and used for the simulation of the dissolution of formaldehyde under the presence of methanol in aqueous solutions (formalin) in model reactors, and in model adsorption columns.
- The thermodynamic description and the reaction kinetics for the ternary system formaldehyde – methanol – water are relatively complex, however they were successfully implemented in the present simulator. The conversion reactions into heavier substances, such as hemiformal and poly(oxymethylene) hemiformals, methylene glycol and poly(oxymethylene) glycols, were taken from state-of-the-art studies in modern literature.
- For validation purposes, a comparison of the performance of the absorption simulation in a model reaction under various operating conditions with relative published work was performed.

Conclusions

- The results showed that the accuracy of the physicochemical equilibriums and reaction rate models used in the simulation of the above system developed and used here is highly satisfactory.
- The increased predictional capabilities of the developed simulator, compared to existing experimental and theoretical studies, is also very encouraging for the next level of simulations, namely the UFC production.

Urea Formaldehyde Condensate

- After a comprehensive literature and state-of-the-art survey, data for the physico-chemical equilibrium, reactions and kinetics for the conversion of formaldehyde and urea to UFC complexes were obtained and implemented in the absorption model.
- The “Methylation” system of reactions, the dissolving reactions, the Cannizzaro and the neutralization reactions were properly modeled, using reaction rates and parameters that are not constant throughout the column (crude assumption), but vary and depend on the local operating conditions, such as temperature, pressure, concentrations, and pH (refined assumption).
- All parameters and values corresponded to typical operating conditions of standard HCHO absorption columns.

Conclusions

- The UFC production results, with respect to the conversion rates and the solids produced, were very realistic, when compared to independent measurements in typical HCHO units.
- The UFC production simulator has enabled the immediate and inexpensive, yet trustworthy calculation of various conditions for alternative scenarios that can facilitate future optimization of formaldehyde plants.