

## Model of a Formaldehyde Absorption System

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In the current context, where the increase in energy costs and environmental regulations have proven to be a great challenge for chemical industries to maintain their product quality and secure their profit and market share, process modelling and optimization are powerful tools for a better understanding of the physico-chemical phenomena of the systems installed in industrial units. The present work is inserted in a project to optimize an industrial formaldehyde production unit. One of the objectives of this work was to develop a first-principles model of a system of absorption columns used in the removal of the formaldehyde present in a gas stream coming from a methanol oxidation reactor to form aqueous solutions (formalin) with concentrations of 35 to 55 w%.

The modelling and simulation of formaldehyde absorption columns is very challenging, mainly due to the reactions occurring in the liquid phase, and the exothermicity of the process. When in contact with water, formaldehyde reacts immediately to form methylene glycol that then polymerizes to poly(oxymethylene) glycols in a series of reversal reactions, additionally, formaldehyde also reacts with methanol forming hemiformals, which in turn polymerize to poly(oxymethemiformals).

The absorption system subjected to study involves a column composed of two sections of random packing with a section of trays in between and a second tray column that includes internal cooling coils. A rate-based model was developed and implemented in *gPROMS® ModelBuilder* and validated with industrial data. The model is based on a description of a single stage, which relates to either a tray or a packing segment, where the gas and liquid phase balances are calculated separately, and the mass and heat transfer resistances are considered according to the film theory, combining the film model equations with the relevant reaction and diffusion kinetics. The vapour-liquid equilibrium data of the formaldehyde-methanol-water system was obtained from Albert et al. [1] to account for the nonidealities of the system.

The absorption model was simulated using data supplied by the licensor of an industrial unit for formaldehyde production as input values of the model. The results show a good agreement with the industrial data and the model will be further used together with a previously developed model of a methanol oxidation reactor [2] in the simulation and optimization of the complete formaldehyde production unit.

[1] M. Albert, B.C. García, C. Kuhnert, R. Peschla, G. Maurer, 2000, Vapor-Liquid Equilibrium of Aqueous Solutions of Formaldehyde and Methanol. *AIChE Journal*, 46, 8, 1676-1687.

[2] C.G. Braz, H. A. Matos, A. Mendes, J. Rocha, R. Alvim, 2017, *Computer Aided Chemical Engineering*, 40, 121–126.