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## A simulation model of an Ethylene Oxide reactor

Hanna Perzon

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*There are high demands on companies today to survive when competition is high and that also applies to companies that manufacture ethylene oxide. The raw material in the production of ethylene oxide is ethylene and oxygen where ethylene is the largest cost. To facilitate the reaction a catalyst, which increases the reaction rate, is used. The catalyst has a major influence on the efficiency and economics of the production of ethylene oxide. Catalysts used in commercial ethylene oxide processes contain silver on an alumina oxide carrier with addition of promoters and moderators to improve selectivity towards ethylene oxide and stabilize activity. For an ethylene oxide company to be competitive in the market, it is important to follow catalyst development and to investigate the possibilities of using catalysts that increase stability and selectivity towards ethylene oxide. When a change of a catalyst to another type of catalyst is considered, it's important to investigate the change of process parameters that will be a result of another type of catalyst. A simulation model in the commercial program Aspen Plus<sup>®</sup> has here been performed as a tool for future catalyst evaluations.*

Ethylene oxide was first prepared in 1859 by Wurtz using potassium hydroxide solution to eliminate hydrochloric acid from ethylene chlorohydrin. This led to an industrial production of EO (Ethylene Oxide) which began in 1914. The direct catalytic oxidation of ethylene, discovered in 1931 by Leffort, was gradually replaced by the chlorohydrin process. Today EO is produced by direct oxidation of ethylene with air or oxygen.

In the production of ethylene oxide, oxygen and ethylene reacts over a silver catalyst on an alumina oxide carrier and the main reactions are:



The reactions are exothermic which means that heat is created. As the catalyst is used, its selectivity and activity decreases due to deactivation of the catalyst. Deactivation occur from impurities in the reactor inlet, changing of silver particles (silver sintering) and blocking of pores in the catalyst. To minimize the deactivation of the catalyst it's important to control the impurities in the inlet of the reactor and to minimize the temperature in the reactor.

One of the first steps when creating a simulation model of an ethylene oxide reactor in Aspen Plus<sup>®</sup> is to choose a thermodynamic model that correlate with the system. In this simulation a model by Soave-Redlich-Kwong was used and the reason was that the model is known to give a better fit of a system, which includes condensation of water. This will occur when the simulation is expanded and the heat exchangers downstream of the reactor are included. In this simulation three operating conditions were studied, start of run (SOR), middle of run (MOR) and end of run (EOR). As a starting point kinetic parameters from the literature were used and fine-tuned to correlate with process parameters for SOR collected from process flow diagrams (PFDs) at AkzoNobel. The second step was to adjust the kinetic parameters from SOR to correlate with process parameter for MOR collected from PFDs at Akzo Nobel. The third step was to adjust the kinetic parameters from MOR to correlate with process parameters from EOR collected from PFDs at AkzoNobel.

As the catalyst ages the selectivity decreases and the reason for this is deactivation of the catalyst. The activation energies for both reactions (1) and (2) are increased over time and this is compensated with higher temperature in the reactor. When selectivity decreases, more ethylene is totally oxidized to CO<sub>2</sub> and water and a result from this is that more heat is produced since reaction (2) has a higher enthalpy of reaction.