Optimum Design of Ethyl Acrylate Process with Coupled Reactor/Columns Configuration

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Ethyl acrylate (EA) is widely used in industry as a precursor for varnishes, adhesive, and finishes of papers and textiles. This important ester can be produced directly from ethanol (EtOH) and acrylic acid (AA) via esterification reaction with the presence of sulphuric acid as homogeneous catalyst. Only in a very recent paper (Witczak, et al., 2004), the kinetics of this esterification reaction has been given. There is no paper in the literature on the subject of the production of ethyl acrylate. In this study, the optimum design of this process with coupled reactor/columns configuration will be studied. The principal behind the coupled reactor/columns configuration, similar to reactive distillation, is that the continuous removal of products from the esterification reaction mixture by distillation reduces the backward reaction rate. The advantage of the coupled reactor/columns configuration over reactive distillation also include: the existing reactor/columns in the plant can be retrofitted for this usage; easy maintenance of the overall system; larger reactor holdup and different reaction temperature can easily be designed; etc.

There are total of four azeotropes in this system including two homogeneous azeotropes of EtOH+H_2O and EtOH+EA and two heterogeneous azeotropes of EA+H_2O and EtOH+EA+H_2O. Thermodynamic model parameters set of NTRL-HOC has been found to fit well the VLE and LLE of binary and ternary mixtures in the system. The predicted azeotropic temperatures and compositions of the four azeotropes also agree with the experimental data. Since the two products (ethyl acrylate and water) of this esterification reaction are neither the lightest nor the heaviest component in the system, the complete designed process will need to be more complex in comparison with the other reactive distillation papers in the literature.

The proposed design of this process including a CSTR reactor coupled with a rectifier (without heat source). The heat input in the CSTR totally vaporizes the reactor outlet stream to vapor phase and enter the rectifier from the bottoms. The bottom liquid stream from the rectifier containing mostly heavy boiler AA is recycled back to the CSTR. The composition of the top vapor stream from the rectifier is close to the light boiler of ternary azeotrope of EtOH+EA+H_2O. This stream after sub-cooling to 40 ºC can be naturally separated inside a decanter to form organic and aqueous phases. Extra water is added in the decanter to maintain suitable composition inside of the liquid-liquid boundary. The water purity of the aqueous phase is quite high, thus is suitable for discharge. The organic phase composition by natural liquid-liquid separation has the benefit of crossing the distillation boundary into a desirable region to obtain pure ethyl acetate product. This organic phase stream is partly refluxed and is partly designed to feed into another stripper with reboiler for further purification into the final EA product. The top vapor of this stripper with composition near the top vapor of the rectifier is also condensed and then fed into the decanter. The bottom stream of the stripper is the final EA product with stringent specifications of less than 0.1wt% EtOH and 0.005wt% AA impurities in this product stream.

The optimal design is selected based on the maximization of Total Annual Profit (TAP) for the overall system. This TAP includes: the product value minus the costs of two feed streams, minus annualized capital costs, minus total utility costs, and minus the waste water treatment cost. The design and operating variables that need to be determined include: AA/EtOH feed ratio, CSTR holdup, total stages of the rectifier, total stages of the stripper, and the water addition rate into decanter. An iterative optimization procedure is proposed to find the optimal flowsheet of the overall system. In the design of the process flowsheet, pure AA feed composition is assumed while the EtOH feed stream is practically to assume containing 82.2 mol% ETOH and 17.8 mol% H_2O. The optimum pure AA and pure EtOH feed ratio is not exactly equal molar, but with the ratio of AA:EtOH to be 1:1.27. The optimized process flowsheet can be seen in the following Figure 1. The result of this optimum process design will be used in a later control study to hold the stringent product specifications despite feed flow rate and feed composition disturbances.

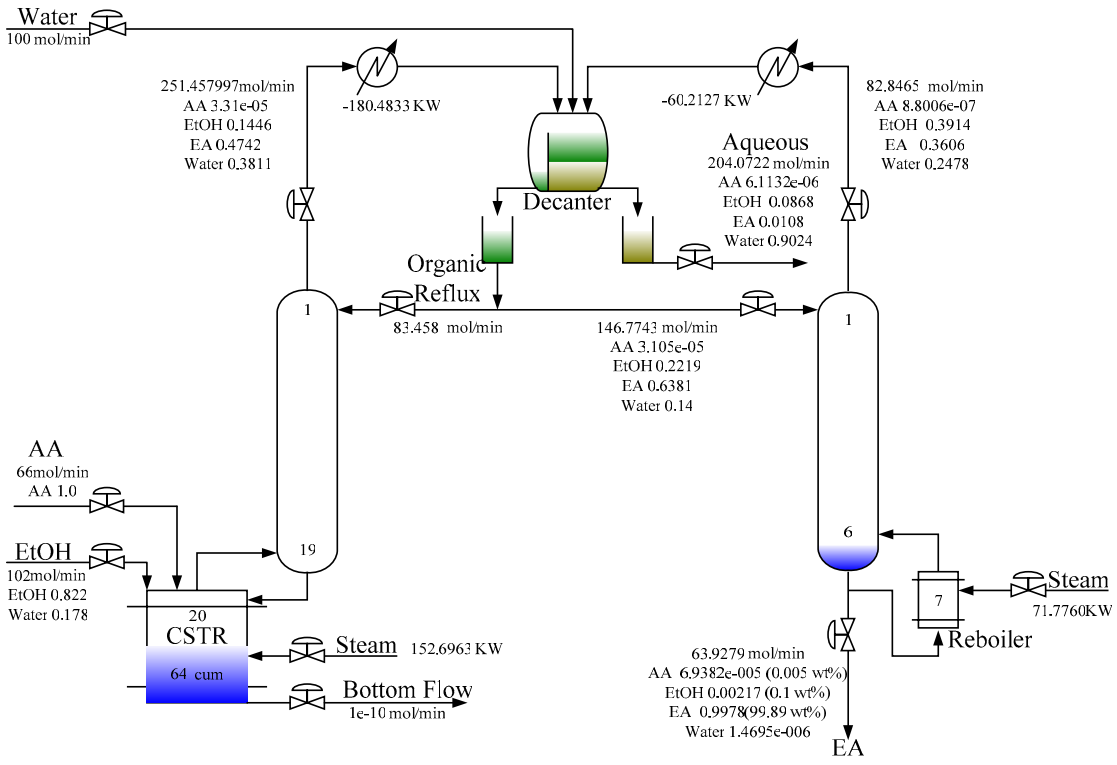

Figure 1: Optimum process flowsheet for the production of ethyl acrylate.

Literature Cited

Witczak, M.,, Grzesik, W., and Skrzypek, J., “Kinetyka Estryfikacji Kwasu Akrylowego Nizszymi Alkoholami Alifatycznymi” *Inzynieria Chemiczna I Procesowa*, 25, 331-340 (2004).

Keywords: Ethyl Acrylate, Esterification Reaction, Reactive Distillation, Coupled Reactor/Columns, Optimum Design.