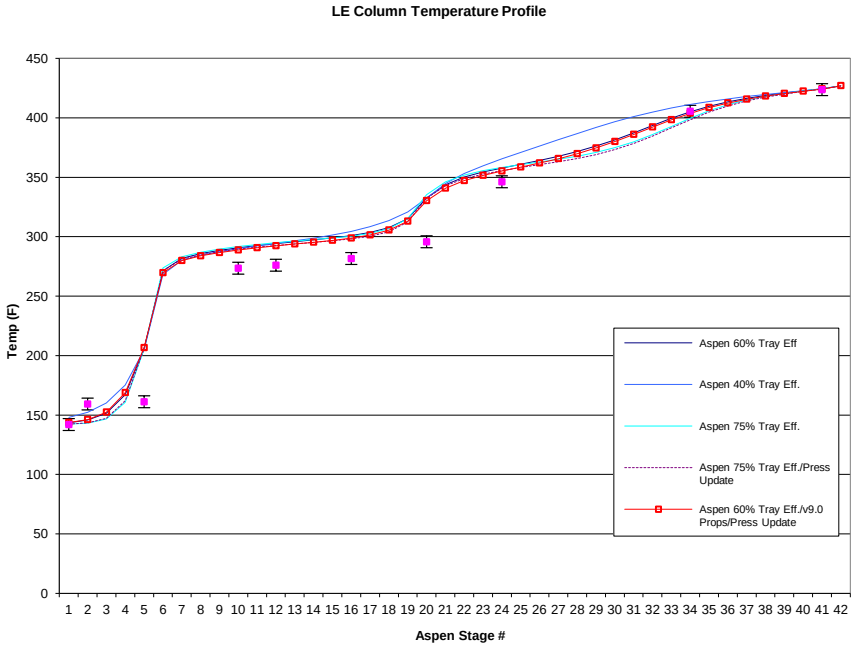
Case Study 10 – Detergent Alcohol Plant Design

To develop the heat and material balance for the detergent alcohol plant design, this consultant (with assistance from other individuals and groups) used Aspen Plus® to generate a flowsheet model of the carbon 16 and 17 branched alcohol reaction and finishing processes. This consultant developed the original flowsheet in Aspen Plus®. Others extended and improved the model, resulting in the basis for the final heat and material balance. The entire reaction and finishing process is represented in a single flowsheet model, simplifying the model operation and interpretation.

The client developed the physical property data for this model, which was no small task for this system. Even though the detergent alcohols process is a 'chemical' process by definition, the branched alcohols product, the branched olefin feedstock, and all the intermediate compounds and impurities had to be handled more like a refinery stream. The olefins feedstock contains a 'smear' of linear and multi-branched olefins ranging from C11 to C19, but predominantly containing C15 and C16 branched olefins. Each carbon number is further graduated into 5 to 6 isomers representing a somewhat Gaussian distribution of mono- and di-branched olefins. After generating corresponding paraffins, aldehydes, and other impurities, the simulation component slate numbers 146 components. This component slate results in large calculation matrices in the model, which can adversely affect model convergence time.

Prior to completely developing the pure component and binary interaction data, this consultant spent considerable time validating the property approach. Using existing plant data for a similar product run (identified by the solid squares with upper and lower confidence limits representing the statistically stable daily averaged process data), the existing model and property approach were validated with reasonable agreement. Because of its complex nature, validating against the light ends column data in the finishing section proved particularly useful. Applying this and other validation results to the branched system, the client and this consultant chose SR-POLAR (Schwartzentruber and Renon method, a coefficient-aided equation of state model) to represent the high pressure vapor/liquid equilibria (VLE) in the reaction and degassing systems and an activity coefficient model (Non-Random Two Liquid, NRTL) to represent the low pressure VLE and LLE in the remaining system.



Based on this physical property definition, other models were developed to help during the air permitting and preliminary design processes, including a stand-alone evaporator model (using the information provided in the adjoining figure), and a comprehensive kinetic reactor model applying the Langmuir-Hinshelwood kinetic equation forms within Aspen Plus® (not described here).