Process modelling issues in the design of a continuous flow process for the production of ibuprofen

Antonio Tripodi[1], Rocco Martinazzo[2], Gianguido Ramis[3], and Ilenia Rossetti[1]

[1]Affiliation not available
[2]Università degli Studi di Milano
[3]DICCA

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Abstract

The continuous flow synthesis of ibuprofen is simulated taking into account the main process modelling issues. The most appropriate thermodynamic models were revised to account for the properties of the unconventional reactants and complex molecules. Furthermore, in some reaction steps ionic properties may be needed rather than those of the neutral molecules. All these points need a careful optimisation of the methods for the estimation of the properties, with possible huge discrepancies of the results. The products separation and purification steps in continuous mode was also added, but, again, the key issue is the correct selection of the thermodynamic package, relying on very complex cases where experimental equilibrium data are missing. Improper previsions can neglect important issues, such as the unpredicted precipitation of salts, not predicted during the simulation, but observed experimentally by us

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