A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design

The manufacture of emulsified products is of increasing interest in the consumer oriented chemical industry. Several cosmetic, household and pharmaceutical products are in the emulsified form when sold and/or they are expected to form an emulsion when used. Therefore, there is a need for the development of a methodology and relevant tools in order to spare time and resources in the design of emulsion-based chemical products, so that the products can reach the market faster and at a reduced cost. The understanding and modeling of the characteristic behavior of emulsions and their peculiar ingredients is consequently necessary to tackle this problem with computer-aided methods and tools. A comprehensive framework for the selection and design of surfactants, the main responsible for the formation and the stability of emulsions, is presented here together with the modeling of the cloud point, a key-property of nonionic surfactants, with a group-contribution model. The mathematical formulation of a standard product design problem is presented, together with the list of both the pure component properties (related to nonionic surfactants) and the mixture properties (relevant to the overall products as an emulsion) needed for the solution of the design algorithm. These models are then applied together with established predictive models for pure component properties of ionic surfactants and for standard mixture properties such as the density, the viscosity, the surface and the interfacial tension, but also the type of emulsion expected (through the hydrophilic–lipophilic balance), and its stability (through the hydrophilic–lipophilic deviation), forming a robust chemical product design tool. The application of this framework is highlighted for the design of some emulsion based chemical products.