Property Prediction for Emulsion based Chemical Product Design

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PROPERTY PREDICTION FOR EMULSION BASED CHEMICAL PRODUCT DESIGN

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New Processes, New Products: Development of New Products. Fine Chemistry.

The chemical industry is changing, shifting from the manufacture of commodities towards higher value added products. Because of this major change in the chemical industry and consequently in the chemical engineering, chemical product design is gaining more and more importance[1]. The goal of chemical product design is to find a product that exhibits a set of desirable or specified behavior, by first establishing a list of chemical formulations satisfying the defined needs, and then selecting the most advantageous option among those generated[2]. A systematic step-by-step methodology is then necessary to reliably solve a chemical product design problem. This consists in a first model-based stage, in which computer-aided techniques are employed to determine the base case formula, followed by a second experimental stage, in which experiments are performed to verify or revise the final product formula[3]. Most of the higher value added products gain their value from a molecular or micro structure which gives them better performance. The principal issue of the first type of these products is the selection/evaluation of the active ingredient, while the second category refers to a chemical organization on the scale of micrometers, belonging to the colloidal domain and incorporating polymer solutions, foams, gels and emulsions. Here emulsified products are considered primarily because of their large use in the food, detergency and cosmetic industries.

Emulsified products can be described as a mixture of two normally immiscible liquids, representing the continuous and the dispersed phases, kinetically stabilized by so called "emulsifiers" which mainly lie on the surface between the two phases. Active ingredients and additives can be dissolved both in the continuous and in the dispersed phases. A systematic seven-step methodology for design of emulsion based chemical products has been recently proposed and it is summarized in Figure 1. In step 1, consumer assessments are converted into target properties to be used in following steps; from step 2 to step 6, ingredients are selected one-by-one to satisfy each class of needs; and finally in step 7 the composition of the formulated product is determined.

[1] Cussler E.L., Moggridge G.D.; Chemical Product Design. Cambridge University Press; 2011.
[2] Gani R.; Chem. Eng. Res. Des., 2004; 82(11): 1494-1504.
[3] Conte E., Gani R., Ng K.M.; AIChE J., 2011; 57(9): 2431-2449.

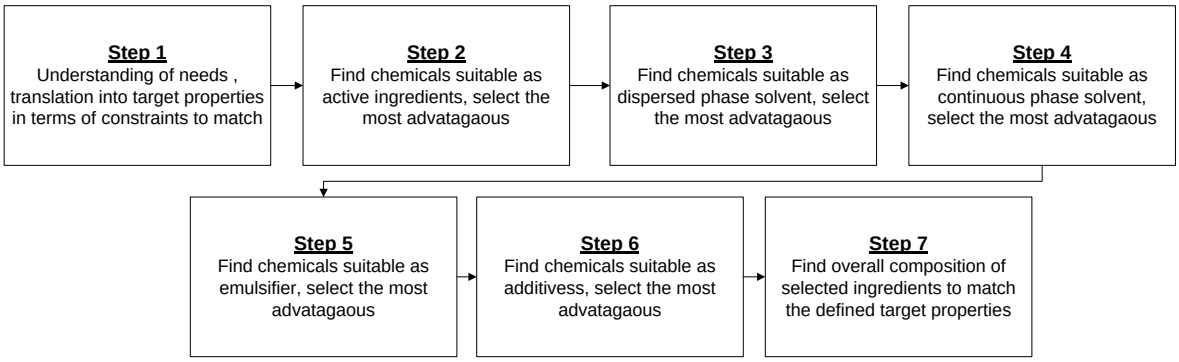

Figure 1: Step-by-step methodology (Stage-1)

One of the main issues to face when applying this methodology is the availability of the needed properties. Experimental data are often scarce and the development of models for pure component and mixture properties is then necessary[4]. Many predictive property models have already been developed and are now available in the open literature. However, when considering emulsion based chemical products, it is necessary to consider pure component properties relative to the emulsifier (most often a surfactant) as well as mixture properties relative to the emulsion, not strictly a mixture. These properties are often scarcely available in literature and reliable predictive models are also rare. Table 1 lists the main properties needed by the methodology of Figure 1, dividing them between pure component properties, relative to surfactants, and mixture properties, relative to the emulsion, highlighting also data availability. The objective, therefore, is to develop predictive models for use in product design.

Table 1: List of pure component properties, relative to surfactants, and mixture properties, relative to the emulsion, needed by the methodology of Figure 1, for which predictive models are needed

Pure Surfactant Property	Data Availability	Emulsion Property	Data Availability
Cloud Point	Large	Density	Large
Critical Micelle Concentration	Large	Viscosity	Sufficient
HLB or equivalent	Complete	Surface Tension	Scarce
Krafft Temperature	Sufficient	Interfacial Tension	Sufficient
Phase Inversion Temperature	Scarce		
Surface Tension	Sufficient		

Pure component properties, relative to surfactants, are intended to be modeled through group contribution methods, while emulsion properties are to be modeled with different models depending on the property involved. Once reliable predictive models for these properties are available, the computer-aided stage of the chemical product design systematic methodology will be performed independent of experimental data and databases. The paper will give illustrative examples of the developed models and methods.

[4] Kontogeorgis M.G., Gani R.; Computer Aided Property Estimation for Process and Product Design. Elsevier; 2004.