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Selection of the right ingredients including solvents and calculation of their amounts and composition in the final formulation, is a critical step in coating product design [1]. To perform this task efficiently, if the potential of the computer can be used, then the resource and time intensive procedures involved in formulating these coatings can be completed rather quickly. However, even-though the computer-aided procedures could theoretically design a complete product formulation, they would not suffice on their own. They are required to be supplemented with verification using experimental procedures. Hence, the computer-aided stage is used only to speed-up the design process and serve as a guidance for a formulation chemist.

It is known that solvents account for one third of the cost in coating formulations and are extremely important in order to deliver the active ingredient of the formulation and confer the final aesthetic and functional properties of the coating [2]. In the work by Conte et al. (2010) [3], a general Computer-aided Mixture/blend Design (CAM^{b}D) methodology for the design of solvent-based formulations from various industrial sectors is proposed. Here, as a first step, the demands of the consumer are translated into a set of target properties. Then, using the constraints on these target properties, property prediction models and mixing rules, the mixture properties are predicted using a generate and test approach. A stability analysis is also performed to determine the miscibility of the solvents. Finally, the product composition at which all target properties are satisfied to yield a stable formulation is selected for further evaluation using experiments.

The CAM^{b}D methodology has been tailored to specifically design coating formulations. The presentation will highlight the complete framework for the design of coatings that dry by solvent evaporation (without chemical reaction with atmosphere or other ingredients of the formulation). The developed methodology and associated tools will be described via a solved case study, wherein given the desired target properties of the coating, the ingredients and their composition that are required to be put together can be predicted.

References:

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[3] Conte, E., Abildskov, J. and Gani, R. (2010). Innovation in Integrated Chemical Product-Process Design: Development through a Model-based System Approach. PhD. Technical University of Denmark.

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