Book of Abstracts
European Congress of Chemical Engineering (ECCE-6)
Copenhagen, 16-20 September 2007

Solving Complex Problems in Formulation Processing by Building a Pragmatic Multi-Scale Model

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1. Summary

A methodology for building pragmatic multi-scale models to solve complex problems is presented. The methodology is exemplified using a manufacturing process for a lyotropic liquid crystal product. The methodology generated a model that could be validated using specifically designed experiments. As a result it was discovered that spontaneous emulsification occurs during the process (which was previously unknown); this could be a crucial design factor in implementation of a manufacturing system.

Keywords: multi-scale, model, structured fluids,

2. Introduction

Traditional modelling techniques tend to model processes using complex mathematical formulae and equations (Noro & Gelbart, 1999). However, it is often not practicable to employ such techniques when dealing with highly complex systems as it would be expensive, time consuming and most importantly for many such systems the underpinning physics and quantitative data required for the models to work are lacking (Prausnitz, 1998). Traditional modelling tends to concentrate on either the molecular level (performed by chemists) or the macroscopic level (performed by engineers) of the problem. There is often insufficient linkage between them which makes scale-up difficult.

The methodology adopted in this work is to build a pragmatic multi-scale model using the observed phenomena and known basic science of the system. The model will be used to drive the design of specific experiments to explore the system and could also be potentially used as a basis for a mathematical model.

The methodology is exemplified using a manufacturing process typical of personal care products and pharmaceuticals which involves a lyotropic liquid crystal (Holmberg, 2001). The use of this process is appropriate as there are multiple phenomena involved at different length scales which include soft solid phase formations, phase transformation, mixing and mass transfer among others. At a micro level, little is known about the kinetics of the process and the microstructure of the products. At a macro level, there is a lack of reliable scale up parameters and scaling up of such processes has been a long problem.

3. Methodology

The initial step of the methodology is to develop a starting model for the process using available scientific knowledge and information about the system. In the case of the lyotropic liquid crystal example it contains a high level process map of the process, which identify the key macroscopic variables of the system, and a transformation map, which tracks the microscopic transformations of the materials during the manufacturing process. Figure 1 and Figure 2 shows simplified version of the high level process map and transformation map respectively

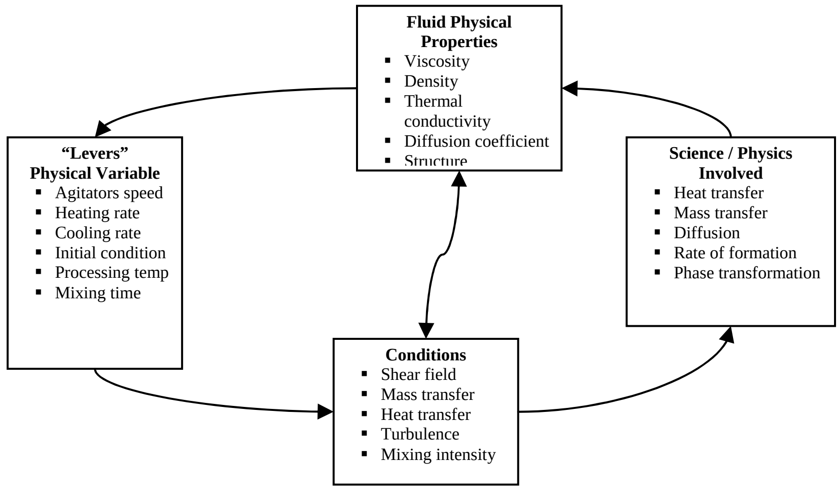

Figure 1 High level process map which shows how the different process-related entities are linked

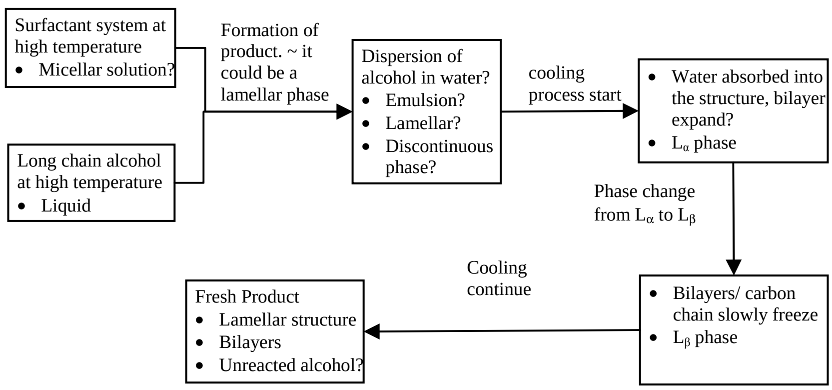

Figure 2 Initial version of the transformation map based on available information which identifies the key transformations which the materials experience and the states of the materials as well as information gaps

Another element of the methodology is to hold a structured discussion with knowledgeable stakeholders of the process, such as the scientists and the engineers. The model is tested against known behaviours and extended with models agreed during the discussion, thereby closing some knowledge gaps and identifying others.

The proposed models need to be validated with experiments. A contact experiment was designed to test the credibility of the model for the formation pathway of the liquid crystal phase. It was concluded from the experiments that the proposed formation pathway is credible and most importantly spontaneous emulsification was found to occur when the fatty alcohol comes into contact with the surfactant solution. This phenomenon is previously unknown in the system and this could imply that the ratio at which the surfactants solution and the fatty alcohol come into contact is a crucial design factor in determining the overall structure and stability of the product.

With the new information from the experiments the model is updated and will be presented to the panel of experts who would again suggest improvements to the model. The process is an iterative one whereby the model is tested and the model modified as new results are obtained.

4. Conclusion

The methodology enables the team to look into the complexity in processing problems and be able to gain a better understanding of the process. By employing the methodology for the lyotropic system we were able identified phenomenon previously unknown to the system which could have a serious impact on the product and scale-up. This potentially represents a significant improvement on the widely used approach in such system which is to use statistical design of experiments.

References

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