EMMC case study:

COSMOlogic and Bayer Technology Services

Identification of Solvents for Extractive Distillation

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1. Which are your objectives as an industrial consumer of modelling?

a. *Description of the industrial problem:* Extractive distillation is utilised as a means of separating mixtures having a low value of relative volatility or in case the mixture forms an azeotrope. Key to the

success and commercial viability of extractive distillation is the identification of a suitable additive component (solvent) which enables efficient separation. The solvent needs to have the right property profile: first and foremost it needs to selectively shift the phase equilibrium, have a boiling point which is 30-50K above that of the mixture, be thermally stable and not react with the compounds of the mixture. For commercially viable application, further properties such as corrosiveness, toxicity and of course cost are important too.

Finding suitable compounds is a considerable challenge. In the particular case example, no suitable additive compound for extractive distillation of the mixture was known and hence a slow and expensive additive crystallisation procedure had to be used.

b. *Classification of the project:*

   i. *Material:* Isomer mixture with nearly identical boiling points.
   ii. *Scale of the material phenomena to be described:* nanometre and sub nanometre scale, as well as macroscale
   iii. *Industrial application:* fluid state thermodynamic properties as well as compound separation subsystem model prior to implementation in an extractive distillation mini-plant.
   iv. *Industrial sector:* Basic and fine chemicals
   v. *Weakness of approach used up until now:* The traditional approaches involve trial and error based on chemical intuition as well as using thermodynamic models based on group contributions such as UNIFAC. Although the latter is very accurate in the case of well-known compounds, it is much less reliable in the case of complex, poly-functional molecules. It also requires experimental input data which can be expensive and time-consuming to obtain for new classes of materials.

c. *Requirements and expected results to understand the material behaviour.*

A method which provides accurate, validated thermodynamic properties such as fugacities.

2. How did materials modelling play a key role in problem solving?

It was possible to devise a combined modelling and experimental screening approach which provided valuable data early on in the development programme. Hence one of the key roles of modelling was to provide early indication of potential compounds which could then be evaluated in terms of commercial viability (stability, availability, cost, etc.). Hence modelling enabled the R&D programme to be more tightly integrated with business decisions. Furthermore, the materials modelling approach (COSMOtherm) made it possible to consider completely new classes of materials. A new separation agent was detected based on a computational pre-screening of thousands of molecules. The compound would never have been considered without the screening procedure where it showed up as one of the top ranked candidates.

3. What tools and methodologies have been applied?

The key tool used in this project is the thermodynamic modelling method COSMO-RS. The determination of thermodynamic properties is based on a model of atomistic interactions (molecular charge density surfaces). The charge density surfaces are themselves derived from an electronic model (Density Functional Theory).

The combination of COSMOtherm and a fast experimental method (the headspace method) enabled fast and cost-efficient initial screening. For lead candidates, the complete phase behaviour was determined experimentally which also provided input for process simulations using methods such as Aspen Plus before going to pilot plant trials.

4. What are the expected improvements of the material behaviour simulation?

Since the performance of the described industrial application at Bayer the accuracy of the COSMOtherm method for predicting free energies and activity coefficients of compounds in liquids has been further increased by several improvements of the interaction functional, especially for hydrogen bonding and dispersive interactions. The COSMObase database of pre-calculated compounds of common interest meanwhile provides more than 9000 small and medium sized solvents, additives, and other compounds, which form a large reservoir of compounds which can be easily used for such a solvent or entrainer screening project. Furthermore, COSMOtherm has been validated for screening of ionic liquids (ILs), so that this novel class of compounds can be included in a screening project. The COSMObaseIL provides COSMO files of roughly 400 cations and roughly 100 anions typically used in ionic liquids and thus represents a reservoir of almost 40000 real and virtual ILs.

The work on improvements of interaction descriptions and the extension of the databases is ongoing.

5. What investments were made during the project?

As is typical for successful integrated computational materials engineering, the project required investment in and synergy of a range of activities, including the identification of the solvent, which then was followed through to the technical process design, pilot and plant engineering. The materials modelling part was a key enabler, however, which required the relatively modest investment of roughly one person month by a scientist with experience in using modelling techniques at Bayer Technology Services, one month of an 8-CPU workstation, and software licence fees (which are typically in the range of a few ten thousand euros per year).

6. What technical and technological benefits resulted from the project?

The efficiency of the screening method enabled by materials modelling opens up the potential use of extractive distillation for separation in cases that were so far inaccessible and required much slower and more expensive methods. New separation agents can be proposed and tested in a fraction of the time, and new classes of materials (such as ionic liquids) can be assessed. With this method separations have been achieved that were once deemed impossible.

7. What was the business impact versus previous approach?

A screening methodology was established which enables a closer integration of scientific and business considerations with evident business benefits resulting from faster and better decisions. The specific project resulted in a successful pilot and implementation of extractive distillation using a compound proposed by materials modelling. The use of extractive distillation has led to savings of several million euros per year compared to the previous separation process based on solvent crystallisation.

Reference:

[1] G. Ruffert, G. Olf. CHEMIE TECHNIK 2004, 3, 86-88

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