CONCEPTUAL DESIGN OF PROCESSES FOR STRUCTURED PRODUCTS

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Abstract

Systematic approaches to the design of processes for structured products are still relatively underdeveloped, despite their gaining industrial importance. We propose a method for the conceptual design of processes for structured products, which is an expansion of Douglas’ hierarchical decomposition. The novelty of the method is threefold: firstly, the internal structure of the product is considered explicitly rather than only composition, secondly the method is applicable to multiple product plants, this is almost always a necessity for the type of products considered here, and thirdly, the batch/continuous choice does not have to be made beforehand for the entire process, which means that hybrid batch/continuous processes can easily be considered. The hierarchical approach proved its potential by finding feasible designs for the example considered; mayonnaise and dressings. Additional effort has to be spent on the generation of more knowledge-based rules for flowsheet synthesis and the selection of equipment.

Keywords

Conceptual design, Hierarchical decomposition, Structured products, Emulsions, Mayonnaise and Dressings

Introduction

The performance properties of certain polymers, but also of non-chemical products like paint, liquid detergents, ice cream and mayonnaise depend critically on the internal microstructure of such products. These so-called structured products have an internal spatial structure on a nano or a micro scale. Such structures can manifest themselves in different ways, e.g. on a molecular scale in polymers, or on a nano or micro scale as phase domains with distributed sizes, e.g. droplets, embedded in other thermodynamic phases, as in emulsions. These products therefore cannot be characterised only by a composition. Take for instance mayonnaise. It consists of 80 vol% small oil droplets, dispersed in an aqueous matrix, stabilised by a protein network. The quality of the product depends critically on the droplet size distribution of the oil droplets.

Despite the industrial relevance of structured products, chemical engineering has paid only limited attention to these products (Villadsen, 1997). Traditionally, conceptual design in the food and cosmetics industries takes place in an evolutionary way, the main focus being on equipment design, rather than on the systematic exploration of alternative processing configurations. The purpose of this paper is to propose a method for the conceptual design of processes for structured products, based on the method developed by Douglas (1988). A more recent description is given by Douglas and Stephanopoulos (1995). Since most
structured product plants must accommodate for multiple products, the method has to cover this. An optimisation-based method is not considered, since the required mathematical models are generally not available for this type of process.

**Approach.**

A level decomposition is proposed, based on the level decomposition presented by Douglas and Stephanopoulos (1995):

0. Input information
1. Processing structure
2. Plant I/O structure
3. Task structure
4. Unit operations
5. Equipment design

The batch/continuous choice does not have to be made beforehand. Parts of the process can be batch, whereas other parts can be continuous. The choice will be made in level 4, for each part of the process separately.

Level 0.

At this level the battery limits and conditions need to be defined. The input information to be given is divided into two classes: basis of design and physical properties. The basis of design consists of process targets and constraints, a description of the desired physical chemical transformations and cost data.

It is not necessary to specify all the input information in this level; input data related to a finer degree of detail can be given in the scope of design at subsequent levels.

Level 1.

At this level the processing structure is determined, resulting in transformation blocks. All physical chemical transformations which change the internal physical structure of the product and which occur under the same conditions are grouped in one block. This is similar to the multiple plant description.

So transformations, like crystallising, emulsification and reaction, are grouped in separate blocks. Transformations like feed heating, followed by reaction can be grouped in the same block.

Level 2.

Level 2 considers the input/output structure. First it is determined where each ingredient is added to the process. Therefore an Ingredients Table is created, describing the function and the place of each ingredient in the final structure of the product.

Overall mass balances are created for all products, resulting in capacity requirements for the different processing blocks determined in level 1. Furthermore, the split ratios of feed distributions over the blocks and of recycles are set and the processing capacities of the blocks are optimised.

Level 3.

At level 3 each block is decomposed into sub-systems. Each sub-system is associated with a certain functional task. For structured product processes the following general sub-systems are proposed:

- feed preparation, to change the state of the ingredients to the required state for the next sub-system (e.g. heating, cooling, dissolving)
- reaction (including fermentation), to change the chemical identity of the product.
- micro-scale phase assembly or transition, to change the internal structure of the product.
- separation, to change the composition of the phases of the product.
- preservation, to prolong the shelf life of the product.

There is no strict order for these sections; the ingredients can, for example, be sterilised before the phase assembly, or the product can be sterilised after the phase assembly. An optimal structure needs to be determined for every process.

Level 4.

At this level specific unit operations and main types of equipment for the tasks identified in level 3 are selected. Characteristic parameters that determine the performance of the unit operations, like shear rate and residence time, next to temperature and pressures, are determined.

Level 5.

At this level the equipment is further specified and auxiliary equipment like pumps are selected. The parameters like shear rate and residence time, determined in level 4, are targets for this level.

**Example: mayonnaise and dressings**

Mayonnaise and dressings are essentially oil in water emulsions, stabilised by a protein network. The oil fractions vary from about 20 % for low-fat dressings, to about 80 % for mayonnaise. Ingredients for mayonnaise and dressings include water, oil, egg yolk, vinegar, salt, sugar, spices and pieces vegetables. Fig 1 shows schematically the structure of mayonnaise.

This example considers only the design up till level 4. The heuristics presented are based on prior knowledge and simulation results.
An important quality specification of mayonnaise is the droplet size distribution. The oil droplets have to be small enough to get the correct consistency. A typical droplet size for the oil droplets is 2 – 8 µm (Ranken et al., 1997). This droplet size can be obtained by break-up of the oil droplets due to shear stresses in the production process. Walstra (1993) and Ottino et al. (1999) give extensive overviews of possible break-up mechanisms.

We assume the following product portfolio for 30 h production time: 150 ton 80% oil product X, 100 ton 40% oil product Y and 50 ton 20% oil product Z.

For products with an oil fraction below 80 % there are two processing options; first part of the continuous phase is added, resulting in a pre-emulsion with an internal phase fraction of 80 % which is subsequently diluted with additional continuous phase, or all continuous phase is added directly.

With the given product portfolio, the processing structure for this process consists of two blocks. In the emulsification block the emulsions are prepared. In the mixing block the emulsions can be diluted with additional continuous phase.

Table 1 shows an ingredients table for mayonnaise. On the basis of this table the following heuristics about where the ingredients have to enter the process become clear:

- **The egg yolk has to be added before emulsification starts.**
- **The vinegar has to be mixed with the water before emulsification starts.**
- **The salt and sugar has to be dissolved in the water before emulsification starts.**

Now mass balances can be generated. For products with a fraction dispersed phase smaller then 80%, it has to be determined which part of the water phase is fed to the emulsification block, and which part is added in the mixing block. The following heuristic was determined:

- **The minimum amount of water should be added to the emulsification block.**

Table 1. Mayonnaise ingredients table.

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Fraction</th>
<th>Function</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>oil</td>
<td>80%</td>
<td>disp. phase</td>
<td>interface</td>
</tr>
<tr>
<td>egg yolk</td>
<td>8%</td>
<td>increase stability</td>
<td>cont. phase</td>
</tr>
<tr>
<td>water</td>
<td>7%</td>
<td>taste, preservation</td>
<td>cont. phase</td>
</tr>
<tr>
<td>vinegar</td>
<td>3%</td>
<td>increase stability</td>
<td>cont. phase</td>
</tr>
<tr>
<td>salt</td>
<td>1%</td>
<td>taste, increase stability</td>
<td>cont. phase</td>
</tr>
<tr>
<td>sugar</td>
<td>1%</td>
<td>taste</td>
<td>cont. phase</td>
</tr>
</tbody>
</table>

Products with different oil fractions require different capacities of the blocks. The design capacity of the different blocks for the product portfolio given in level 0 is determined. The heuristic presented above will lead to the capacity requirements shown in Table 2.

Table 2. Required capacities.

<table>
<thead>
<tr>
<th>Product</th>
<th>Emulsification block [ton]</th>
<th>By-pass [ton]</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>150</td>
<td>0</td>
</tr>
<tr>
<td>Y</td>
<td>52</td>
<td>48</td>
</tr>
<tr>
<td>Z</td>
<td>14</td>
<td>36</td>
</tr>
<tr>
<td>total</td>
<td>216</td>
<td>84</td>
</tr>
</tbody>
</table>

Therefore the minimum capacity of the emulsification block should be 216 ton / 30 hr = 7.2 ton/hr. The following heuristic is proposed:

- **The design capacity of the emulsification block should be 130 % of the minimum capacity.**

So the design capacity of the emulsification block is 9.4 ton/hr, and this will result in a production time for product X of 16.0 hr. To calculate the by-pass capacity the following heuristic is proposed:

- **The by-pass capacity should be the same for all products.**

The resulting by-pass capacity is 84 ton / (30 -16) hr = 6 ton/hr. This leads to the results shown in Table 3.

Table 3. Results capacity calculations.

<table>
<thead>
<tr>
<th>Product</th>
<th>Production [ton]</th>
<th>Production time [hr]</th>
<th>Production rate [ton/hr]</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>150</td>
<td>16.0</td>
<td>9.4</td>
</tr>
<tr>
<td>Y</td>
<td>100</td>
<td>8.0</td>
<td>12.5</td>
</tr>
<tr>
<td>Z</td>
<td>50</td>
<td>6.0</td>
<td>8.3</td>
</tr>
<tr>
<td>total</td>
<td>300</td>
<td>30.0</td>
<td></td>
</tr>
</tbody>
</table>

Level 3

Here each block determined in level 2 is decomposed in subsystems. Since a preservation step is not considered,
only a feed preparation step and an assembly step are present. This leads to the structure shown in Fig 2. Only the emulsification block will be discussed here.

Figure 2. Structure of the mayonnaise/dressings process

The tasks that have to be fulfilled in the feed preparation system of the emulsification block are to:

- dissolve salt and sugar in the water
- mix vinegar and egg yolk in the water

The targets that should be met are a 100% dissolution of the salt and the sugar and complete mixing with the vinegar and the egg yolk.

The tasks that have to be done in the assembly system of the emulsification block are to:

- disperse the oil in the water
- reduce the oil droplet size to the specification

The target that should be met is the specified droplet size distribution

<table>
<thead>
<tr>
<th>Criterion</th>
<th>Stirred vessel</th>
<th>Colloid mill</th>
<th>Static mixer</th>
</tr>
</thead>
<tbody>
<tr>
<td>droplet size range (µm)</td>
<td>5 – 100</td>
<td>1 – 20</td>
<td>10 – 100</td>
</tr>
<tr>
<td>high internal phase emulsions</td>
<td>±</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>cont. processing</td>
<td>±</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>batch processing</td>
<td>+</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>residence time</td>
<td>long</td>
<td>very short</td>
<td>short</td>
</tr>
</tbody>
</table>

The alternative designs of colloid mills have been evaluated numerically. A short-cut model was developed, based on a rigorous population balance based model by Wieringa et al. (1996).

Up till now, no choice batch/continuous has been made. We selected continuous operation, however heuristics for this choice are currently lacking.

The process thus designed is rather similar to processes for mayonnaise and dressings production which are nowadays common in industry (Lopez, 1987). The method results in a plant that is less overdesigned than a traditional designed plant.

Conclusions

It can be concluded that the use of hierarchical decomposition can certainly be extended to structured product processes. The method has the following main features: the internal structure of the product can be considered explicitly, the method is applicable to multiple product plants, and the batch/continuous choice does not have to be made beforehand for the entire process which means that hybrid batch/continuous processes can easily be considered.

Additional effort has to be put into generating more knowledge-based rules for flowsheet synthesis and the selection of equipment, for the products discussed in this paper, as well as for different types of products which are not yet considered.

References