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Modular dynamic simulation for integrated particulate processes by means of tool integration

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Abstract

In this contribution a sequential modular strategy for the dynamic simulation of particulate process flowsheets is presented and the efficiency of the approach is demonstrated by means of an example process for the crystallization of pentaerythritol. The flowsheet of the process consists of a number of different unit operations, e.g. evaporator, crystallizer, hydrocyclone, and mixer, which are described by mathematical models of largely varying complexity and structure. A key advantage of the presented sequential modular strategy is that specialized tools can be selected for the modelling and solution of each unit operation in the flowsheet. The tools are then coupled together by means of the tool integration framework CHEOPS in order to capture the overall structure of the flowsheet. In a case study, a startup of a crystallization flowsheet is carried out. As a result, detailed information about the dynamic plantwide process behavior is obtained. The practical relevance of the approach is demonstrated by means of a scenario where potential blocking of the filters following the crystallizer has been analyzed.

Keywords: Crystallization; Sequential modular approach; Dynamic simulation; Tool integration; Modular algorithm; Population balance

1. Introduction

Over the past decades process simulation has become an established tool in industrial applications and academic research. However, the tools available for process simulation still show certain limitations. Especially the dynamic simulation of complete process flowsheets of particulate processes is far from being a resolved issue.

Dynamic modelling of any fluid phase unit operation usually leads to the same type of equations: the material and energy balances are augmented by constitutive equations and closing conditions which results in a system of differential and algebraic equations (DAE). When these units are integrated into a process flowsheet the system size obviously increases but the type of equations remains unchanged. For the solution of the arising possibly large DAE system several powerful algorithms have been developed (e.g. Brenan et al., 1989) which have been implemented in stand-alone solvers like e.g. DASSL (Petzold, 1983) and LIMEX (Deufhardt et al., 1987) as well as integrated into commercial tools (e.g. Pantelides, 1996). This availability of easy-to-use software strongly promoted the widespread use of dynamic process simulation in industrial practice in the last decade.

Considering the simulation of processes involving particulate matter, the situation is quite different. The current lack of a versatile flowsheeting tool dealing with particulate matter has several reasons.

On the one hand one has to admit that, due to the higher complexity of the processes involved, the knowledge of particulate processes is not as advanced as for fluid phase processes where standard model libraries are already available. For particulate processes these libraries are not yet at hand,

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although research efforts are undertaken to set up such a library at least for steady-state models.[1]

On the other hand the mathematical structure of particulate process models is often not of DAE type. Particulate products are often characterized by distributed properties (e.g. particle size). Therefore, the population balance concept (Hulburt and Katz, 1964; Randolph and Larson, 1988) is often employed to model particulate processes, which results in partial integro-differential-algebraic equation (PIDAE) systems.

The numerical solution of PIDAE systems is by far more complicated than that of DAE systems. Appropriate numerical schemes often depend on the particular problems to be solved. Therefore, current simulation tools mainly deal with specific problem classes and unit operations. Typically, a single unit or a single flowsheet of a fixed structure is considered. Such tools, however, exploit the available process knowledge and often use tailored numerics for an efficient solution.

In this contribution we suggest to realize the dynamic simulation of particulate process flowsheets by means of existing specialized software tools, instead of trying to build a new simulation tool from scratch. The models as well as the solution algorithms encoded in the simulation software for individual process units are reused in an a posteriori fashion by means of a modular dynamic simulation strategy (Marquardt, 1991) and a component-based software platform. The concept of dynamic modular simulation has again been in focus of a number of works done in recent years (Abdel-Jabbar et al., 1999; Grund et al., 2003; Garcia-Osorio and Ydstie, 2004). However, these efforts were predominantly concentrated on the development of the modular dynamic simulation algorithms from scratch and their usage for the simulation of general models.

The focus of this contribution is on the application of dynamic simulation algorithms for the software integration of different, existing process simulation tools. A clear benefit of such an approach is that if a certain process unit model is used within a mixed fluid-particulate process flowsheet, the unit model already implemented in some tool does not have to be reimplemented but can be reused directly. Also, the development of complex process models can be shared between different process specialists who use their preferred modelling and simulation tool, avoiding the usage of some general purpose tool which can hardly be found for all problem classes. Finally, the integration approach can take advantage of well-developed and highly specialized numerics in the particular software packages to increase solution robustness and efficiency.

In Section 2 an example crystallization flowsheet is presented. Section 3 describes the software solution for the tool integration, and the simulation algorithm used. The simulation case study and the results are discussed in Section 4, and general conclusions are presented in Section 5. The models used for the simulation can be found in the appendices.

[1] http://www.vt1.tu-harburg.de/vt1/toebermann/solidsim.htm (Accessed 05.03.2004).

2. Case study: crystallization of pentaerythritol

Crystallization from solution is one of the most important operations used in industry. The driving force for particle formation is the supersaturation in the liquid phase, which is depleted by nucleation and crystal growth. The supersaturation can be generated by cooling of the solution, by evaporation of the solvent, or by reactive generation of the solute. The crystal product is usually characterized by the *crystal size distribution* (CSD) (Randolph and Larson, 1988) represented by the population density function $n(l,t)$ of particle size l and time t.

In our case study, a process flowsheet for the evaporative crystallization of pentaerythritol from an aqueous solution is investigated. Pentaerythritol is commonly used in the production of high-quality alkyd resins, lacquers and lubricant additives, and its physico-chemical properties are well-studied and available in many databases. Also studies on the crystallization kinetics of pentaerythritol in have been carried out (O'Meadhra et al., 1996; Plácido et al., 2002).

The investigated process flowsheet shown in Fig. 1 does not claim to represent a real industrial process. Nevertheless, it comprises the most important steps of a typical crystallization process: (i) preparation of the concentrated solution; (ii) crystallization; (iii) separation of the product. Here, like in many other industrial processes the partial recycle of the product stream is used to minimize the loss of valuable materials. The flowsheet consists of four units—a mixer (4), an evaporator (1), a crystallizer (2) and a hydrocyclone (3), and shows one recycle stream.

In the evaporator, the solution is heated to 102 °C and partially evaporated in order to increase the concentration of pentaerythritol in the stream entering the crystallizer and to assist the generation of the necessary supersaturation. The concentrated solution is fed to the crystallizer where the supersaturation is generated by vapor withdrawal from the top of the unit. Thus the required level of supersaturation is generated and crystallization occurs. The crystal slurry leaving the crystallizer is passed to the hydrocyclone, where the larger crystals are separated from the smaller ones. The larger crystals in the bottom stream are the desired product whereas the overflow stream is recycled and mixed with the fresh feed. The fine particles contained in the recycle are dissolved during mixing, thus increasing the concentration of pentaerythritol in the solution.

The flow rate in the recycle can be controlled by the recycle ratio $\alpha = V_t^{hc}/V_f^{hc}$, and it is assumed that there is no purge in the recycle. The other process inputs are the feed flow rate V_{feed}, the feed composition w_{feed}, the heat supplied to the evaporator Q_{evap}, and vapor withdrawn from the crystallizer V_v^{cr}.