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Flowsheet simulation of solids processes: Current status and future trends

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Abstract

Complex manufacturing processes are nowadays applied for production of various solid products. It is very common that for production of particles with desired properties several transformation steps like drying, milling, classification, granulation, etc. should be involved. This leads to the process structures consisting of different apparatuses or transformation substeps connected with material and energy balances. Consequently, development of new processes or optimization of already existing, as well as an optimal control, is a very challenging task, which can be partially solved using numerical modelling.

For the simulation of modern production processes, the flowsheet calculations can be effectively used. Starting from the 80s a lot of work focused on the flowsheet simulation of liquid-vapor systems has been done and as result various well-established systems exist today. With respect to the solid processes the intensive research has been started much later. In this contribution we present our view about a current role of flowsheet simulation for modeling of particulate materials and specify the open fields which can be covered in future research.

Keywords

Flowsheet Simulation, Solids Processes, Process Modelling, Simulation Frameworks

1. Why flowsheet simulation?

Most of industrial processes which are used to manufacture products in form of particulate materials involve many transformation steps occurring in different equipment. In Fig. 1 the structures for such processes such as cement manufacturing [1], continuous fluidized bed granulation [2, 3], concentrator plant [4] as well as continuous tablet manufacturing [5] are illustrated. Nowadays, the major part of manufacturing processes is operated in the continuous mode. Even in the relatively conservative areas, such as pharmaceutical industry, the migration from batch-wise to continuous operation mode can be observed [6-8].

Fig. 1. Different solids manufacturing processes with complex process structures.

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The modeling of the behavior of integrated production processes cannot be done based only on the information of single process units. Due to the existence of recycle streams and application of strategies for process control and plant wide optimisation, the behavior of each single unit can have a strong influence not only on the downstream processes but on the entire process. Therefore, it is necessary to treat the integrated system as a whole. For this purpose, flowsheet simulation can be effectively applied. Alternative approaches, such as a manual subsequent calculation of units, is very inefficient and can be applied only for very simple structures.

Generally, flowsheet simulation can be performed in steady-state or in dynamic mode. From the computational point of view, the simulation, as well as the development of models, is simpler for the steady-state analysis. However, despite the fact that the dynamic modeling is a more challenging task, process behavior during start-up or shut-down phases, transient process behavior, development of dynamic control strategies, etc. can be investigated only in this mode. In the ideal case, the advanced simulation framework should provide a possibility to combine steady-state and dynamic analysis modes [9].

Not all unit operations in solids process engineering show transient behavior that have a noticeable influence on the dynamics of the whole process. Many unit operations with relatively small holdup mass such as screens, some types of mills or mixers can be efficiently treated as steady-state models during dynamic simulation [2, 3]. However, in some cases, dynamics of the same classification or solid-fluid separation units cannot be neglected and play an important role [10, 11].

The flowsheet calculations can be used for four main purposes: modeling of process behavior, sensitivity analysis, process optimization and process control. In most cases, empirical or semi-empirical models are used for the simulations [2, 3, 12, 13]. Therefore, only macroscopic states like mass flows, particle size distributions, temperatures, etc. can be predicted. At the same time, numerous product properties which play important role for comprehensive material characterization are not considered. Many such properties like an internal granule microstructure, mechanical properties like stiffness or strength, spatial distribution of components, etc. are neglected or estimated only partially. From the computational point of view there already exist methods to treat such information such as multidimensional population balance models or transformation matrices [14]. The main challenge is in the derivation of mechanistic or first-principles models, where knowledge of microscale processes like a formation of nuclei, their further agglomeration, densification [15], etc. is properly considered in a macroscale model.

Important benefit which can be gained from the use of flowsheet simulation is to answer the question “what if?”. Modelling the variation of process parameters or even process structures can be effectively used for a wide range of tasks, starting with personnel training [16] ending with process optimization. Using flowsheet-based sensitivity [17] or bifurcation [18] analysis, the influence of process parameters can be investigated and, for example, stable steady-state regions identified. Furthermore, flowsheet simulation plays an important role in the development of control strategies [19-22].

Nowadays, there are several robust software systems which can be applied for the flowsheet simulation of solids processes. Most of them such as Aspen Plus (Aspen Technology Inc.), gPROMS Formulated Products (Process Systems Enterprise Ltd.), JKSimMet (JKTech Pty Ltd.), CHEMCAD (Chemstations Inc.) are commercial products. In contrast, the Dyssol framework which was especially developed for solids processes is an open-source system [23]. All of these systems contain library of units that allow the users to get an access to the up-to-date knowledge database.

2. Complexity of solids

The first flowsheet simulation methods and frameworks were developed for modeling of liquid-vapor systems [24, 25]. The necessity to distinguish between processes for manufacturing of products in fluid or solid form has been pointed out by different authors [2, 23, 26-28]. One of the most decisive differences is the characterization of the material. In case of vapor-liquid systems, the material can be completely described by a set of bulk parameters, typically thermodynamic properties. In contrast, a comprehensive description of particulate materials requires the use of multidimensional distributed parameters. When one property changes, other secondary attributes also change. For example, during an agglomeration process not only particle enlargement takes place, but also the distribution of particles over other property coordinates such as porosity, form factor or chemical composition are simultaneously changed (Fig. 2). Therefore, solids processes require more complex models for different process units. As a consequence, more recently new calculation approaches and models have been developed especially for treatment of solids.

Fig. 2. Two-dimensional particle distribution after agglomeration process [14].

For the correct processing of multidimensional distributed parameters during steady-state and dynamic calculations transformation matrices have been effectively applied [2, 23, 29]. Instead of explicit calculation of all output variables, the transformation laws are formulated for each

model and a transformation matrix is generated. This matrix is afterwards applied to transform holdup and input streams implicitly. Such implicit calculation makes it possible to extend applicability of model significantly. In this case the models developed for strictly limited dimensions of parameters space can be used for a larger number of dimensions [14].

From the computational point of view, there exist equation-oriented (simultaneous) and sequential-modular (modular) approaches [9]. For an application of the equation-oriented approach, open-form models are needed [30], whereby in the case of modular approach “black box” type of models can be modeled [31]. This advantage can play an important role for the simulation of solids processes, where mathematical models of single process units are often of heterogeneous nature and contain discontinuities. Equation-oriented approaches are standard in commercial software platforms such a gProms. They provide fast and robust solutions and are amenable to optimization and global sensitivity analysis. Flowsheeting packages designed for solids processing can easily handle distributions of one internal ordinate and solution techniques are suitable for one dimensional population balances [31]. However, some processes like crystallization, granulation, drying etc. may be described by multi-dimensional population balance equations which are partial integro-differential equations [32]. As a result, the combining of all models into a single equation set and application of equation-oriented approach is a rather challenging task. Thus, some of the flowsheet frameworks such as Dyssol [23] are based on the sequential-modular approach.

For the modular dynamic flowsheet simulation of solids, a waveform relaxation (Picard-Lindelöf iteration) approach [33] has been proposed [2]. Using waveform relaxation, the whole simulation time is divided into smaller time windows. Afterwards all models are iteratively solved on this window and the convergence is analyzed. If the convergence is reached the calculations are started from a new window. This method can be effectively applied to perform simulation on several abstraction levels:

- to couple different simulation frameworks [34];
- to perform the process simulation within one framework [2];

- for component-based simulation on the scale of a single process unit [35].

3. Models of single process units

The models of single process units play the crucial role in the flowsheet simulations. The models can be generally distinguished by detailing levels and application purposes. Werther et al. [36] have proposed three main levels:

- level 1: short-cut models, where no knowledge of specific apparatus is required. This type of models can be used for rough estimation at an early stage process or product development;
- level 2: semi-empirical and physical models, which can be applied for process optimization, de-bottlenecking or unit design;
- level 3: comprehensive physical models. These models are based on microscale simulation approaches like CFD, DEM, MD, etc. and allow to perform detailed unit design or optimization.

Only the models of the first and second level can be directly solved with a flowsheet simulator. For more sophisticated models of the third level the incorporation of other type of simulators is needed.

Compared to the models developed for liquid-vapor systems, the major part of models for solids processes have more complex behavior and reveals heterogeneous nature. This is caused due to the fact, that:

- many models for particulate processes are based on various empirical correlations which have been obtained for a strictly limited parameter space. As a result, combination of two or more correlations into one model can lead to large discontinuities;
- even small deviations in process conditions can cause the transition between rate processes occurring in a unit operation. For example, increased flow rate of suspension

mass flow injected into fluidized bed granulator, can change particle growing mechanism from coating to aggregation. Often, these transitions can be linked to different transformation regimes that are expressed by dimensionless regime maps or design spaces [37].

4. Future directions

4.1 Multiscale simulations

One of the most promising future directions is the multiscale process treatment, where submodels from different time and length scales are linked together to obtain detailed process description [36, 38]. Most of currently available unit operation models are empirical or semi-empirical nature. In order to improve these models and to estimate unknown model parameters [39], microscale simulation techniques like DEM, CFD, SPH etc. can be applied to describe processes occurring within single process unit with a higher detailing grade. The central role here plays model decomposition and inter-scale relations [40]. Depending on the way how the models are linked, Ingram et al. [41] have proposed to distinguish five main categories: multidomain, embedded, parallel, serial and simultaneous. These linking strategies have been used for investigations of different processes like granulation or classification [10, 42-45].

Nowadays, there are two main limitation factors which hinder the further industrial usage of multiscale simulations:

- large computational effort caused due to the usage of the microscale models;
- simultaneous usage of various simulation approaches and automatic inter-scale data transfer.

The first problem can be partially solved using the modern computer architectures, such as GPUs and applying coarse-graining methods, such as the multiphase particle in cell MPPiC [46] method. To solve the second challenge, different numerical methods such as MD, CFD,

DEM, PBM, etc. should be directly integrated into one general software framework and the whole calculation procedure consisting of model decomposition, inter-scale data transfer, analysis of the inter-scale convergence should be automated. Brief overview about some of proposed frameworks and interfaces can be found in Groen et al. [47]. Such frameworks are beginning to become available even in commercial software platforms [48].

4.2 Incorporation of experimental data

The incorporation of the available off-line and on-line measured process data into the mathematical models of integrated process or into single process steps is one of key directions in the improvement of future models. The measurements may be done to characterize raw materials, products, intermediates and especially key process parameters which influence the efficiency [49]. The straightforward strategy to use experimental data is the estimation of unknown model parameters, where adjusted parameters are varied with a goal to minimize discrepancy between numerical and experimental results [50-51]. In most cases a raw experimental data should be pre-processed to reduce volume and dimensionality of data and to treat problems caused by measurement error [52].

While few models are fully predictive, robust, mechanistically based models exist for most unit operations and flowsheeting tools are now mature enough for a move to Model Driven Design (MoDD) for many particulate processes and products. Here the simulation drives the design and experiments are used primarily to refine and validate the model. Robust, general workflows for MoDD are still being developed. These workflows should minimize the number of model parameters that needed to be backfitted from pilot or full-scale experiments. Sensitivity analysis using the flowsheet simulation is a powerful tool for choosing key parameters and designing appropriate experiments [48, 53].

Other strategies to use experimental data are based on the generation of semi-parametric or nonparametric models. They can be generally classified into three main groups, depending on the type of knowledge which models are based on [54]:

- parametric: “conventional” type of models which formulated a priori based on knowledge about process;
- nonparametric: formulated exclusively from data;
- hybrid (semi-parametric): combines parametric and nonparametric in the parallel or in serial arrangement [55].

For the generation of a nonparametric model different types of artificial neural networks (ANNs), such as radial basis function network and multilayer perceptron can be used. These types of models have been applied for different apparatuses from solids process engineering like crystallizer [56], mills [57], granulators [58] etc. For training of ANN’s not only real experimental data can be used, but also the data generated from the microscale simulations, like for example, from DEM calculations [58].

Finally, the structured gathering of the process data and incorporation of this data into virtual image (flowsheet model) of physical process allows to build digital twins. Such coupling between real process and its digital representation can be realized in both directions. On the one hand, the data flow is going from a physical object to digital model through sensor updates to mirror behavior of a corresponding twin [59]. On the other hand, the flow in reverse direction allows to use a twin as a controlling instance. For example, the digital twin can be used for in silico experiments for tuning sophisticated control strategies such as model predictive control without need for expensive and material intensive experiments on the real plant (see Fig. 3).

Fig 3. Using a process simulation digital twin for twin screw granulation of pharmaceuticals to tune a model predictive controller [60]. Integration of gPROMS and PharmaMV.
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4.3 Simulation frameworks

In the next decade we expect further intensive developments focused on multiscale process treatment. Thus, the interoperability between different simulation frameworks and the data exchange between them will be critical. In recent years, attempts have been made on the

integration of different tools. For example, Shopfer et al. [30] have proposed a component-based platform for integration of modeling tools. Especially for the chemical process engineering, the CAPE-OPEN standard has been developed and integrated into several simulation frameworks [61]. For the multidisciplinary data exchange, Fillinger et al., [62] have proposed to use functional mock-up interface.

With respect to further development and implementation of simulation frameworks we expect increased research in the following fields:

- intensified usage of modern computer architectures like graphic processor units to improve calculation performance for solution of complex multidimensional problems;
- migration from desktop simulator to the cloud-based solutions. The cloud computing and development of Web-based user interfaces can significantly simplify usage of flowsheeting tools.

4.4 Linking process and product models

The currently available unit operation models and process substeps do not allow to describe multidimensional properties of granular materials. In many cases, distribution of particles over only one property coordinate, namely size, is predicted with a high accuracy. Meanwhile, many properties such as particle porosity, internal structure, surface properties, etc. are being left behind. However, this information is of major importance for many applications of granular product design, such as the development of pharmaceutical products where information of internal structure allows estimation of a-priori dissolution time [63]. Furthermore, incorporating additional information about solid product into flowsheet simulation is a necessary step to solve inverse problems: find optimal process configuration and parameters for a given product specification (see figure 4).

With respect to the detailed characterization of a final solid product, the further research should be performed in three main areas:

- extension of mathematical models for single process units, where such effects like influence of the thermal conditions onto granule morphology will be considered [64];
- development of numerical methods for proper treatment of multidimensional distributed parameters. This can include solvers of multidimensional PBM, like finite volume method [65], calculation approaches like transformation matrices [14] or alternative methods like Monte Carlo approach [66];
- development of a much better library of product performance models to link with the process simulations.

Fig. 4. Combining product and process engineering
for particulate product design and manufacture [67].

5. Concluding remarks

In the recent years increased interest to the flowsheet simulation of solids processes can be observed. The fact that particulate materials should be treated differently compared to the liquid-vapor systems lead to the development of new models, calculation approaches and implementation of simulation frameworks. As a result, there exist different systems which already allow to simulate and to optimize different production processes with a relatively high detailing grade. Simulation of solids flowsheets have now matured to the point where they can be used as powerful tools for design, optimization and control in industry.

In the near future we expect intensification of research in the four main fields:

- multiscale process treatment direct inclusion of microscale simulation methods (DEM, CFD, SPH, etc.) to macroscale flowsheet model;
- incorporation of experimental data to generate nonparametric or hybrid models and to build digital twins;
- more sophisticated product models that make use of more detailed structural characterization of the product, and more sophisticated process models to provide this structural information;

- further development of simulation software into directions of unified multiscale frameworks, cloud computing and Web-based user interfaces.

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Fig. 1.

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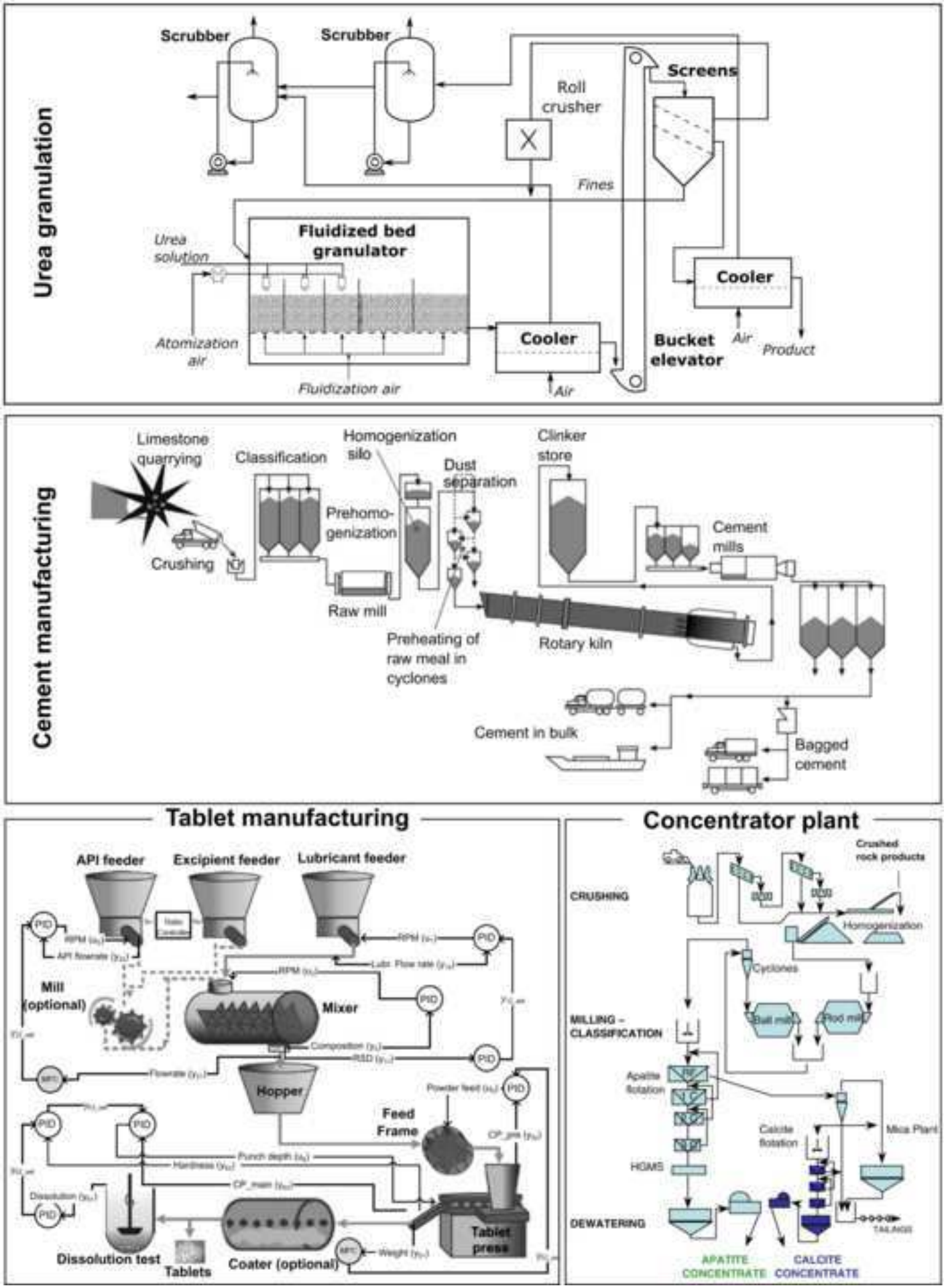


Fig. 2.

Click here to access/download;Figure;Figure2.tif

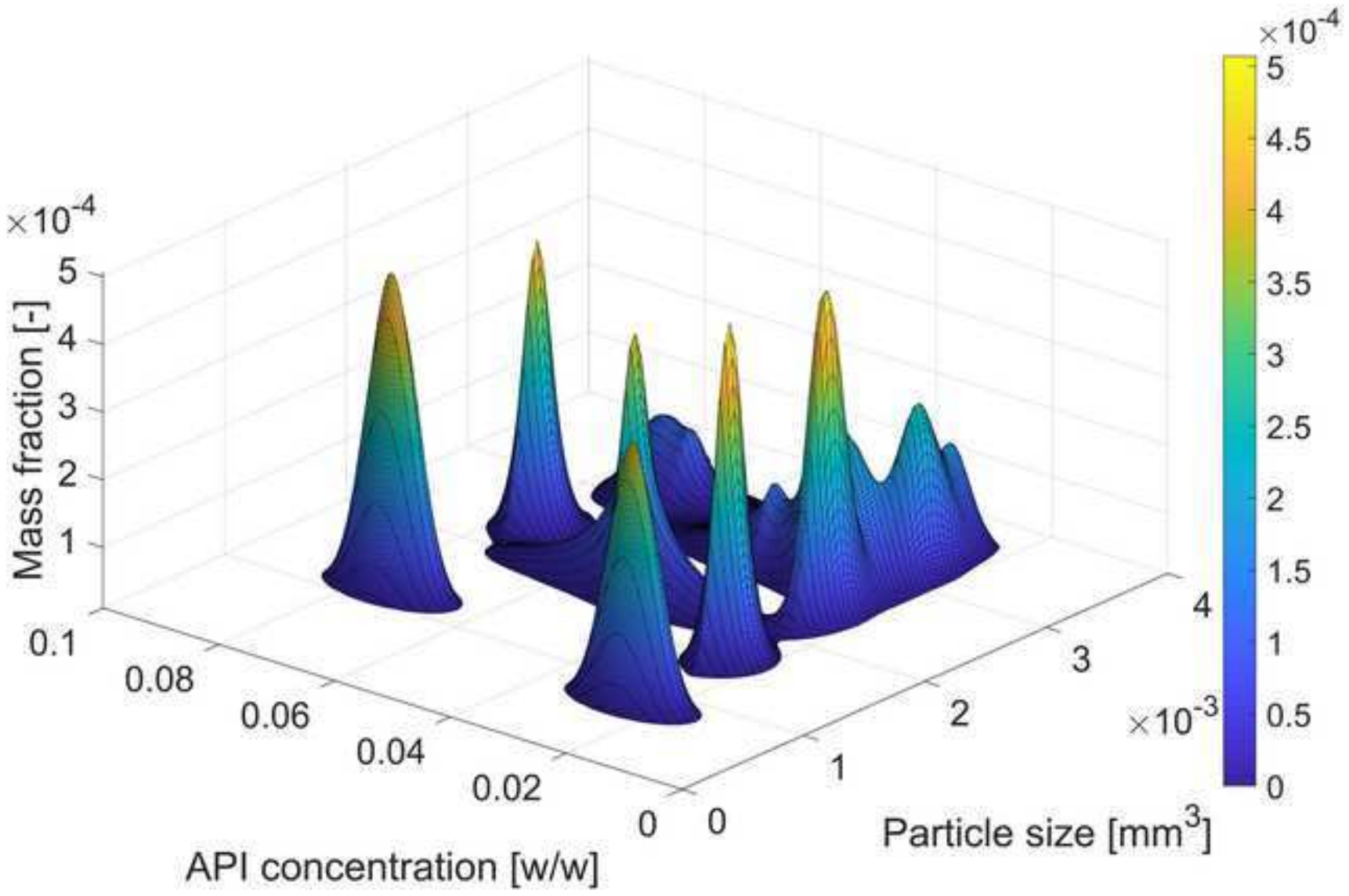


Fig. 3.

Click here to access/download;Figure;Figure3.tif

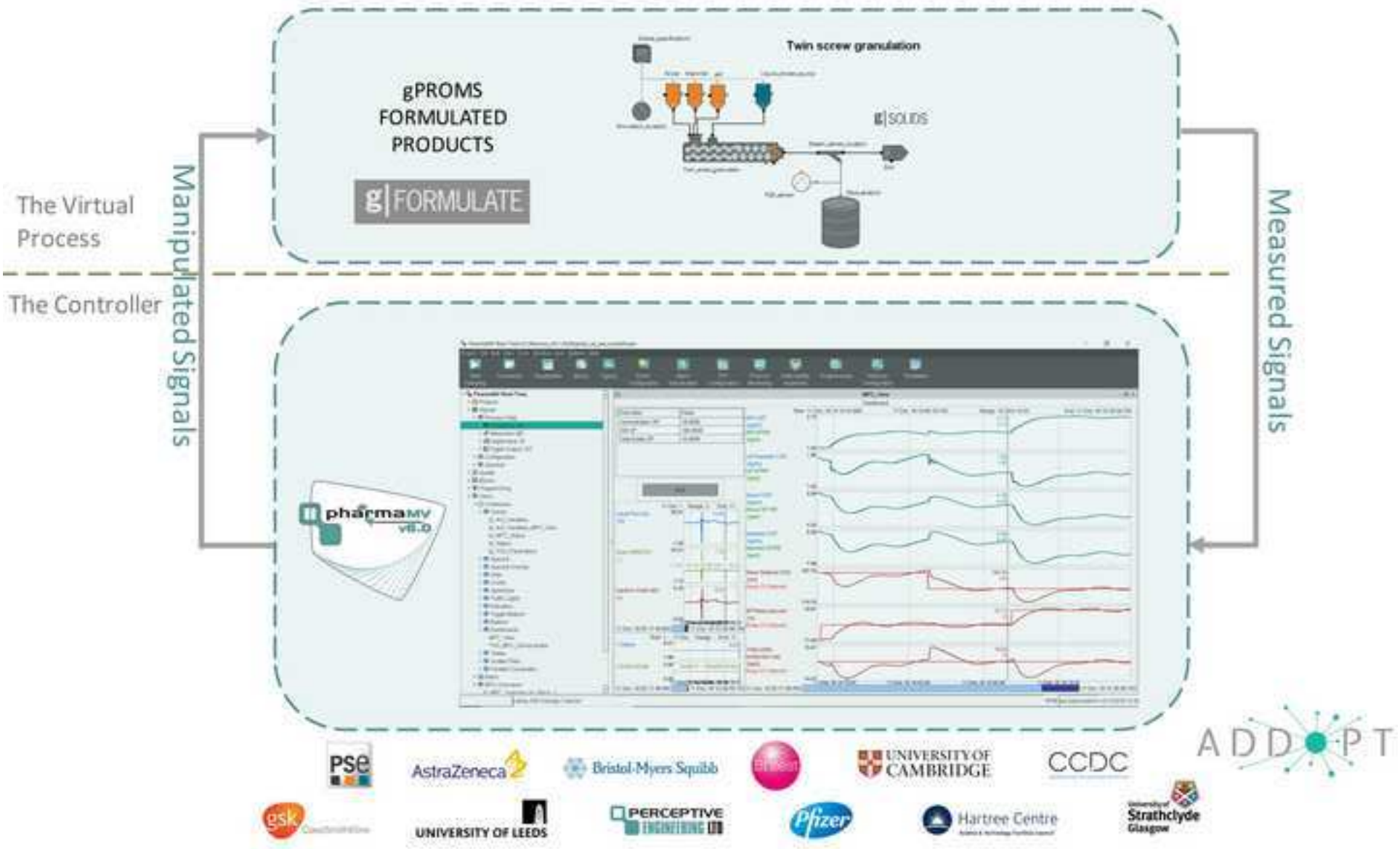
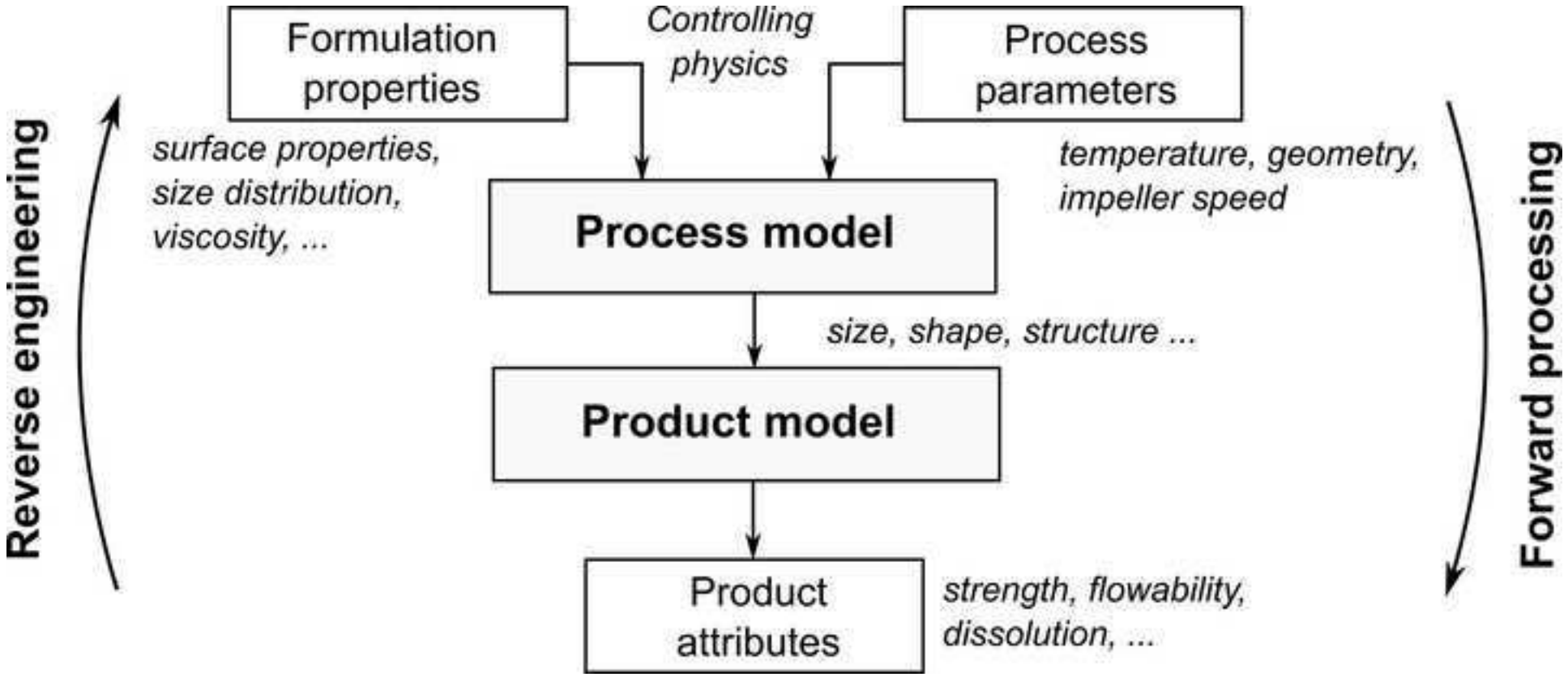


Fig. 4.



Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: