Powder Technology 314 (2017) 665–679

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Novel system for dynamic flowsheet simulation of solids processes

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ARTICLE INFO

Article history:
Received 18 August 2016
Received in revised form 16 January 2017
Accepted 25 January 2017
Available online 27 January 2017

Keywords:
Flowsheet simulation framework
Dynamic modelling
Solids processes
Distributed parameters
Transformation matrix

ABSTRACT

The dynamic flowsheet simulation of solids processes is an area of increasing interest in recent years. Compared to the well-established flowsheet modelling of liquid-gas systems, the modelling of granular materials requires different approaches, strategies and algorithms. Therefore the new dynamic flowsheet simulation framework Dyssol has been developed within the Priority Program SPP 1679 "Dynamic simulation of interconnected solids processes (DYNSIM-FP)" of the German Research Foundation (DFG).
In this contribution the architecture of the novel simulation framework and computational methods employed in it are presented. The system is based on the sequential-modular approach supplemented with partitioning and tearing methods. Waveform relaxation method, as well as several convergence methods and data extrapolation algorithms have been implemented to improve system performance and to increase convergence rate. To perform a correct calculation of multidimensional distributed parameters an approach with transformation matrices is used in the Dyssol system. Simulation case studies calculated with new system have shown good stability, convergence rate and agreement of simulation results with test systems and experimental results.

1. Introduction

The development of new or optimization of existing solids production processes is a very challenging and expensive procedure, due to a huge number of parameters which must be taken into account. Therefore, the investigation of stability and dynamic behavior of these systems is an important task at the stage of design. Moreover, such solids processes usually have a complex structure and consist of numerous separate modules, connected to each other with the energy and mass streams. As examples can be named: dewatering and separation process for contaminated dredged sludge [1] (Fig. 1), which involves several screens, hydro-cyclones, an elutriator, a screen belt press and some other units; granulation process [2], consisting of fluidized bed reactors, screens and a mill; or chemical looping combustion process [3], which includes fuel and air reactors, a cyclone and siphons.

Complex interconnection between different apparatuses and sub-processes in such flowsheets complicates process modelling because it is necessary to investigate the whole process at once, rather than its individual entities. Dynamic flowsheet simulation is a powerful approach for calculation of time-dependent behavior of such complex processes.

The dynamic flowsheet simulation implies numerical modelling of transient behavior that occurs in apparatuses and sub-processes of the flowsheet in order to obtain values of all process variables. By using this approach the process is represented using models of individual units connected with material or energy flows. Each unit can describe:

- one part of an apparatus (filter in fluidized bed, one section of zig-zag classifier, etc.);
- a particular industrial apparatus (screen, mill, etc.);
- an entire sub-process or connection of several apparatuses (circulated fluidized bed, screen-mill shortcut, etc.).

This methodology allows the designing and exploring of a large number of different processes (e.g. particle formulation, milling, separation) by combining units in arbitrary configurations. Thus, flowsheet simulation is not only concentrated on individual units, but gives the possibility to investigate the entire process chain and mutual influence of its components.

One can distinguish between steady-state and dynamic modelling [5]. The first one implies that the system state is calculated at steady operation conditions, so that process variables are constant with respect to the time. The mass and energy balance is always fulfilled, as no accumulation in the system occurs. Contrariwise, the dynamic simulation reflects the time-dependent behavior of the investigated process and takes accumulation of mass and energy into account. This allows to investigate a wide range of problems like oscillating, batch or semi-batch processes, load changes, start-up and shut-down stages, etc. Thus, a dynamic simulation system covers a much larger number of theoretical and practical problems and, despite the larger computational costs, it is more widely applicable.

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http://dx.doi.org/10.1016/j.powtec.2017.01.061
0032-5910/

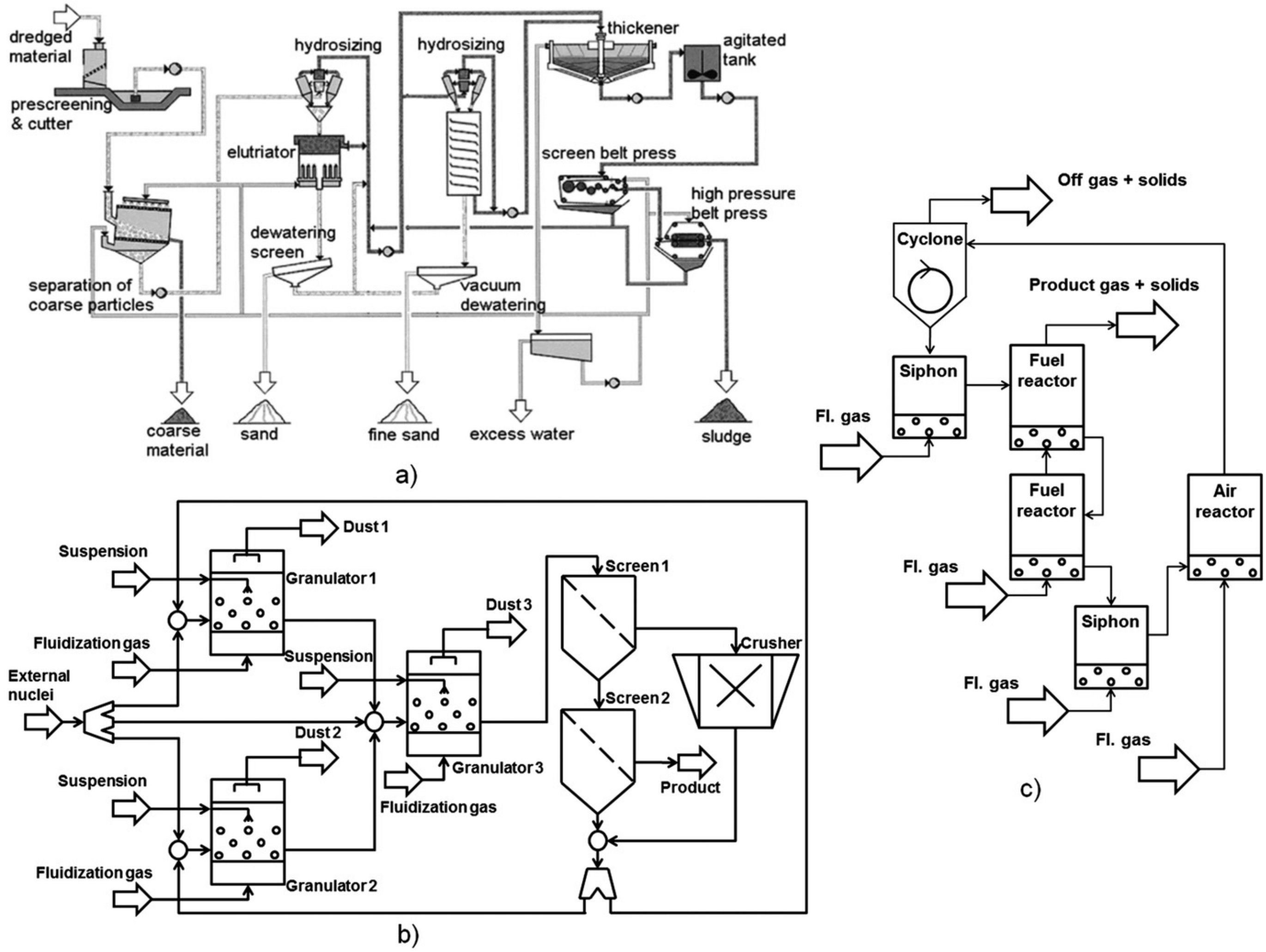

Fig. 1. Examples of solids production processes: soil dewatering and separation [4] (a); granulation (b); chemical looping combustion (c).

It should be noted, that units described by models with different time scales and different dynamics can be present on the flowsheet at the same time. Thus, the simulation system must also provide a way to calculate such processes without affecting the simulation efficiency and accuracy.

The need to distinguish simulators of solids processes also arises from the complexity of the solid phase [4]. The most significant difference between solids and fluids is the way of treating material parameters: liquid-gas systems are described by concentrated parameters, whereby solid materials are characterized by a set of distributed parameters, which describe different properties, such as particle size, shape, moisture content, density, etc. Moreover, they can be dependent on each other, forming an interdependent multidimensional distributed set of parameters [6]. Each operation on material flow, such as separation, mixing, agglomeration or splitting, results in change of one or more parameters of the multidimensional distribution. Thus, if distributed parameters are interdependent, it may be necessary to recalculate all dimensions of the multidimensional set, even if the value of a single parameter only has been changed. Hence, the correct handling of the solid phase is more challenging as the calculation of fluids and requires special technics and algorithms.

Using multidimensional distributed parameters to describe characteristics of a material flow causes another important issue – the methods of storing and processing of such data in the simulation environment. The usual approach for their representation involves discretization of the entire interval, where parameters are introduced, with a set of shorter intervals, called classes. For the description of the distribution each of such a class is put in line with fraction of material, which falls within this interval. The discretization scheme must be sufficiently precise to omit significant numerical error. In the case of dynamic simulation these issues get even more important, because a lot of data is being generated, which can influence the computational rate and require additional efforts for the organization of data storage.

There are also difficulties in terms of addition of new unit models to the simulation system. Most of the developed models in solids processing are complex and involve the use of various numerical methods and different types of solvers [7]. And the simulation system must provide a possibility to solve all possible models, regardless of the type of equations used.

Due to these complications modern tools for dynamic simulation are mostly developed for fluid processes, sometimes with limited consideration of the solid phase. Some of them are limited to particular process types or process structures (e.g. [8]).

Especially for the steady-state modelling a generally applicable simulation system SolidSim has been developed [9] in recent years. It implements an idea of representation of the solid phase as a set of multidimensional distributed parameters and offers an approach with transformation matrices for their correct handling. To extend the scope of this system a module SolidSim-Dynamics for dynamic simulation of flowsheets, as well as several dynamic units have been developed [2,10].