MODELING OF CONTINUOUS FERTILIZER GRANULATION-DRYING CIRCUIT FOR COMPUTER SIMULATION AND CONTROL PURPOSES

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Keywords: Granulation, Modeling, Simulation, Control.

Abstract: The paper presents the model-based approach to process simulation and advanced control in the industrial granulation circuit of fertilizer production. Different knowledge sources, such as physical phenomena, statistical analysis of process parameters, expert information cover different cognition domains of the process. The mechanistic growth model developed is based on particle coating phenomena, mass and energy transfer. The model partially takes into account the main process parameters, features and the equipment used. Simulation has been executed to test the model performance. The model built can be used for the evaluation of plant control methods and staff training.

1 INTRODUCTION

Drum granulation is a commonly used process in a commercial fertilizer production. Many continuous granulation plants operate well below design capacity, suffering from high recycle rates and even periodic instabilities (Wang and Cameron, 2002). The main reasons are related to raw material properties, process equipment and control problems.

The process control still depends on the experience and skills of process operators, namely experts. Diagnostic systems show potential to apply systems engineering approaches to complex operational problems such that operators are well informed, are able to quickly diagnose abnormal conditions, test quickly possible solutions via detailed simulations and then proceed to apply corrective actions (Salmon et al., 2007). However, a number of interacting process variables (some of them are stochastic in nature) lead to a complex dynamic system that might be hard to predict and optimize just by intuition, especially for unskilled operators. Fortunately, it is possible to use granulation process simulations provided by PC for the investigation of such complex problems.

The aim of this paper is to propose the process simulator based on an extended modeling approach for continuous drum granulation-drying processes, focused on simulation and control. This approach involves the dynamic process model built from heterogeneous knowledge sources such as physical principles, empirical (measured) data and expert information.

The mechanistic part incorporates the understanding of physics and underlying mechanisms (e.g. mass and energy balances, growth kinetics).

The empirical part uses raw and/or filtered process sensors' data, their storage, retrieval and parameter identification techniques in addition to the mechanistic (white box) model.

The expert component involves the process experts' recommendations, which are of great value due to the lack of other knowledge mentioned above.

2 MAIN PROCESS DETAILS

Drum granulation is a particle size enlargement process often obtained by spraying a liquid binder or slurry onto fine particles as they are agitated in a rotary drum (Wang and Cameron, 2002). The particle circulation is achieved mechanically (by the action of the rotating drum and lifters). Granules are cycled many times through the spray zone and the liquid layer attached is pre-dried before the particle returns to the spray zone again (Figure 1).
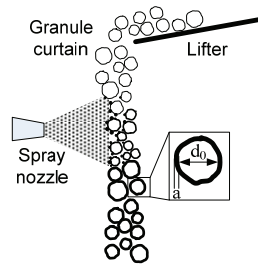
Figure 1: View of the coating phenomenon.

The desired mode of granule growth is layering (coating), resulting in very tight granule size distributions.

A commercial continuous granulation circuit for granulated diammonium phosphate fertilizer (formed by the reaction of phosphoric acid and ammonia) production consists of the following major parts: a pipe reactor, spray nozzle system, drum granulator-dryer, granule classifier (screens), crusher and nuclei feed system (Figure 2).
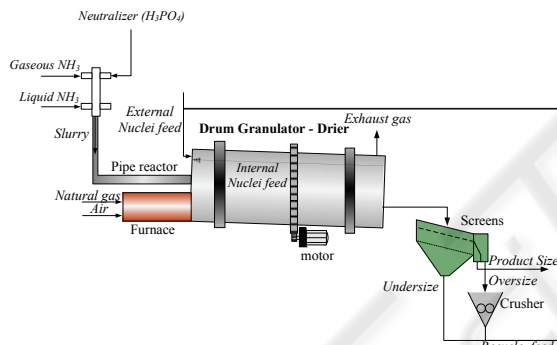

Figure 2: Typical drum granulation-drying circuit utilized in the diammonium phosphate (DAP) production industry.

A granulation drum is made of an inclined cylinder with simultaneous drying (there is no separate drying device). Drying is performed by the heat of burned natural gas and/or reaction heat of phosphoric acid and ammonia. Liquid DAP feed (slurry) is sprayed onto the tumbling bed of seeds via spraying nozzles. The drum is tilted lengthwise a few degrees to provide the flow of granules through the drum length. The backward screw sends a part of granules (internal nuclei) back to the spraying zone. Granules from the granulator-drier are transmitted to the classifier and split into three fractions: undersize, oversize, and marketable product size. The oversize fraction is crushed and sent back to the granulator together with undersize granules.

Fortunately, nowadays some important granule size distribution variables can be measured on-line using advanced particle size analysis systems.

Detailed and more accurate information provides the producers of granulated materials with more data to improve product quality and to control production processes. Size Guide Number (SGN), related to the median of granule population, and Uniformity Index (UI), which shows the dispersion of population, can be evaluated. A part of important granule size distribution intervals can be also provided.

However, some process variables connected with material and equipment properties can not be evaluated and controlled directly. In such a situation the process model can provide information about important process states, such as recycle size flow rate and distribution, drum system jamming factor, granule moisture content, size evolution of single granule inside the granulator-dryer. This information can help to predict future process states and prevent abnormal situations, which can initiate process stoppage and loss of productivity.

3 MODELING

The model presented here is essentially based on fundamental conservation principles, with partial consideration of equipment properties and the stochastic nature of the process. For modeling purposes, it is necessary to divide the granulation circuit into several balance areas with the central component of the model – the drum granulator-drier. There are two main processes inside the granulator-drier: the growth of particles and moisture evaporation (drying).

Basic modeling assumptions are:
- granule shape is spherical;
- each granule in the granulation circuit is analyzed;
- stochastic nature of the process is estimated;
- preferred growth is by layering;
- granule agglomeration is an unacceptable mode of operation;
- growth rate is a function of initial granule size, slurry flow rate, temperature inside the granulator, granule position in the drum, number of particles in the granule bed;
- mechanical attrition of granules inside the granulator-drier is defined by attrition function;
- presumable nucleation (formation of new seeds) occurs during slurry spraying;
- external classification of granules into three fractions (undersize, marketable and oversize) is defined by classification function;

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- external crushing of oversize granules is characterized by grinding function;
- residence and transportation delays in the plant are considered;
- internal and external seeds serve as nuclei for new granules.

3.1 White Box Modeling

There are two basic granule growth mechanisms that act independently or in combination (Findlay et al., 2005). A successive layering of binding material on an initial nucleus is termed layering, coating or ''onion-skin'' growth mechanism. Another mechanism is an agglomeration or coalescence process that occurs upon particle collision. Whereas growth by agglomeration mostly occurs when a binder is added, layered growth is the result of particle coating by the feed material, followed by solidification of the material on the particle surface (Degreve et al., 2006).

The granulation regime depends on some factors such as slurry viscosity and purity, N:P mole ratio, granule curtain density, temperature of slurry and seed to be coated, granule density, air temperature inside the granulator-dryer, etc. Some of these parameters can be observed and controlled, some of them are not.

The design and control scheme of the drum granulator-dryer normally force layered growth or coating and block coalescence or agglomeration. Sometimes the formation of undesirable agglomerates indicates a shift of granulation regime from layering to coalescence, which is not a normal case of operation and must be avoided.

Granule growth by spraying the slurry onto the previously formed seed is shown in Figure 3.

Initial seed   *dispersed slurry*   *granule with added layer*
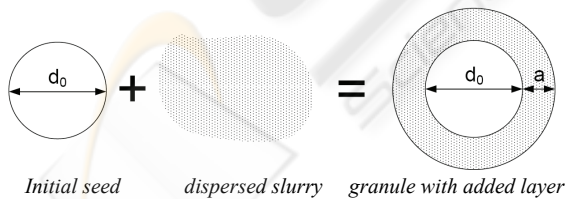
Figure 3: Granule growth by layering.

To model the layering phenomenon, the thickness of a new layer applied is determined by the diameter of the initial particle and the volume of the slurry applied. Assuming a spherical primary particle and a uniform distribution of all sprayed slurry applied onto the particle, the volume of the added layer V_l is calculated from the difference in the volumes of the layered particle and the initial one:

The thickness of the applied layer:

$$a = \frac{1}{2\pi} \sqrt[3]{\pi^2 (\pi d_0^3 + 6V_l)} - \frac{1}{2} d_0 \qquad (1)$$

here d_0 – initial width of granule (seed), a – thickness of the applied layer.

The explicit mass and energy balance model with its wide and quite complex mathematical and physical features is beyond the scope of this paper. Hence, the following is the simplified version of the model developed.

The overall mass balance inside the granulator in liquid phase:

$$\frac{dM_L}{dt} = F_{L,in} - F_{L,out} - F_e - \dot{m}_c \qquad (2)$$

here M_L – accumulated mass of liquid solution, $F_{L,in}$ – flow of liquid solution into the granulator, $F_{L,out}$ – flow of liquid solution out of the granulator, F_e – flow of evaporated liquid solution, m_c – mass of crystallized solution (solid material).

The overall mass balance inside the granulator in solid phase:

$$\frac{dM_S}{dt} = F_{S,in} - F_{S,out} + \dot{m}_c + \dot{m}_g - \dot{m}_{att} \qquad (3)$$

here M_S – accumulated mass of solid material, $F_{S,in}$ – flow of solids into the granulator, $F_{S,out}$ – flow of solids out of the granulator, m_g – mass due to growth, m_{att} – mass due to attrition.

The overall energy balance inside the granulator:

$$\frac{dE}{dt} = \dot{E}_{in} + \dot{E}_f + \dot{E}_r - \dot{E}_e - \dot{E}_l - \dot{E}_{out} \qquad (4)$$

here E – overall energy, E_{in} – energy provided into the granulator, E_{out} – energy removed from the granulator, E_f – energy due to gas furnace action, E_r – energy of reaction heat, E_e – energy for moisture evaporation, E_l – loss of energy from the granulator to environment.

The model presented is placed in stochastic background, which can better suit the growth kinetics, heat and mass transfer phenomena that actually happen in the real plant, with addition of uncertainty and plant equipment properties.

This section has presented only a part of the general model, which is in nature a grey box. Complementary models from measured process data

have been also built and expert information used to enrich the model presented.

3.2 Statistical Analysis for Modeling

Nowadays it is possible to measure, store and retrieve process sensors' data and afterwards perform statistical analysis to "mine" some knowledge. For this purpose, descriptive and inferential statistics need to be used.

Taking different combinations of data sets of the essential process variables, the following results have been obtained:

(1) Scatter plots of the parameters.

(2) Reduced linear correlation matrix with entries of defined correlation degree (used for fast determination of parameter combinations which have a strong linear correlation).

(3) Linear models of the first order polynomial (application of stepwise regression, which is a technique for choosing variables, i.e. terms, to include in a multiple regression model).

(4) Residuals, confidence intervals of parameters, t-statistic, p-value, R^2 calculated for the generated linear models.

(5) Plots of cross-correlation function for probable lead/lag determination.

Figure 4 presents the fragment correlation and regression analysis of two process parameters (*3* and *7*).
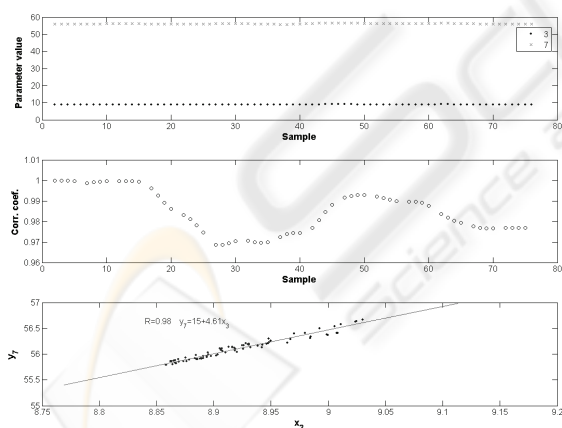

Figure 4: Results of the regression analysis of process parameters.

These findings are significant for determination of process parameters and their relationship. They can also provide additional knowledge for the plant diagnostics. A more detailed statistical analysis of granulation process can be found in (Valiulis and Simutis, 2007).

Mere statistical analysis is rarely helpful. Some heuristic knowledge should be also applied to make it work.

3.3 Knowledge-based Modeling

Complex multiscale process systems which are difficult to model properly (such as granulation) require a combination of various analytical and heuristic techniques. Effective solutions are often based on information from heterogeneous knowledge sources. One of them is knowledge-based systems built on the methods and techniques of Artificial Intelligence.

The expert knowledge of the process is an invaluable source of knowledge, especially, when there is a lack of reliable physical description and suitable measurement equipment. Rule-based expert systems use "if…then…" rules to represent human expert knowledge, which is often a mix of theoretical knowledge, heuristics derived from experience, and special-purpose rules for dealing with abnormal situations (Shang, 2004).

An example of the "if…then…" rule of new seed formation inside the drum granulator-dryer is presented as follows:

If *granule curtain in the spray zone is poor* and *gas temperature in the spray zone is high*, then *new small nuclei formation rate is high*.

In the proposed modeling approach, the expert knowledge is represented by the rule set. The rules involve variables such as "poor", "high", dealing with fuzziness, which is very common in real world problems. Unlike conventional expert systems, which are mainly symbolic reasoning engines, fuzzy expert systems are oriented toward numerical processing (Hemmer, 2008). These principles can be applied for the future development of the granulation process model and simulator for automated guidance and diagnostic purposes.

4 SIMULATOR

Increasing capabilities of computer hardware and software ensure the incorporation of complex knowledge (models) represented by differential and algebraic equations, measured process data, process experts' information, etc. But to be of use for the day-to-day work of the engineer these models have to become more user friendly, than the one that the scientist is dealing with (Ihlow et al., 2004). A new "GrowSim" simulation package for granulation process modeling and simulation is under
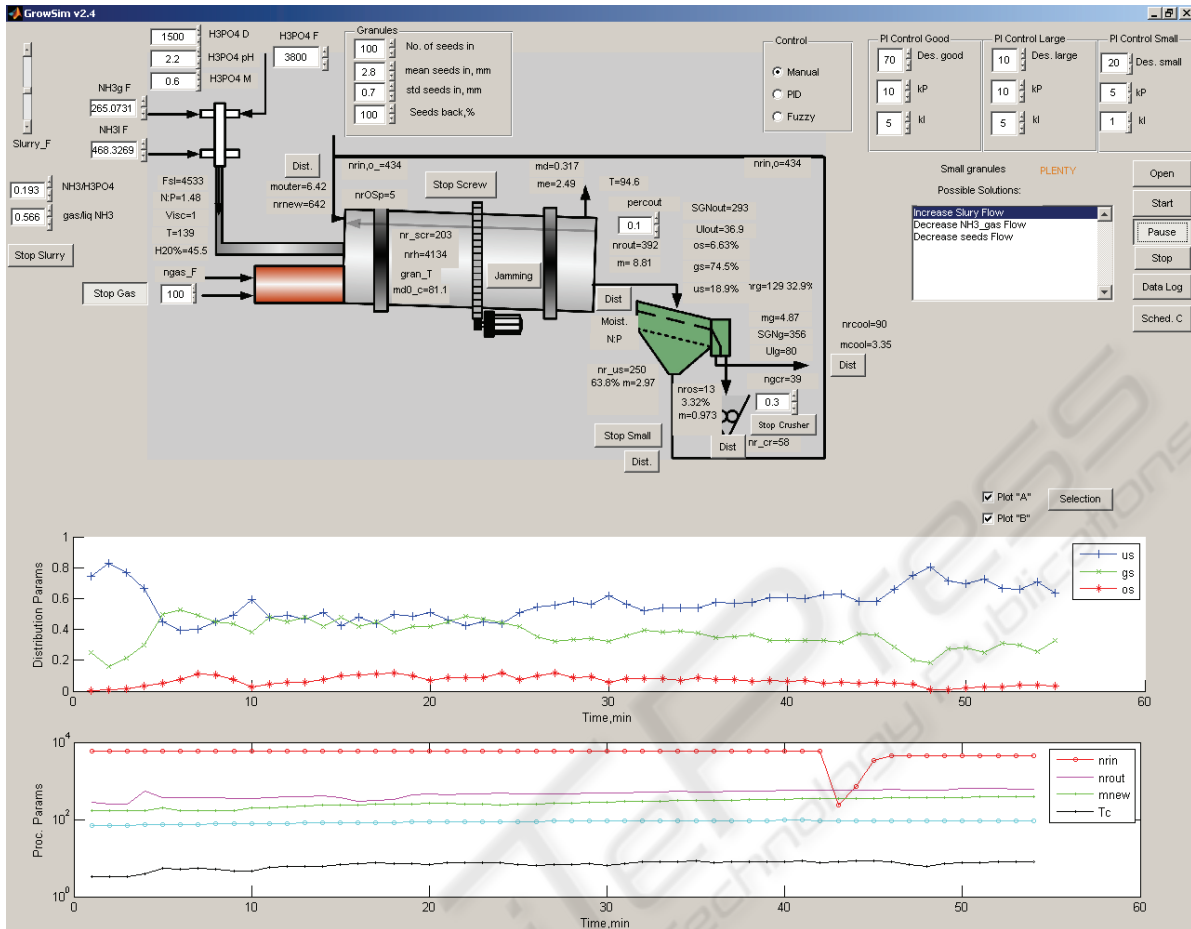
Figure 5: Graphical user interface of "GrowSim" simulator.

development to realize this concept. The simulator is intended to be used by novice process operators to improve their skills in process control and to acquire knowledge of underlying mechanisms. The graphical user interface (Figure 5) has been built to mimic the process control environment available to the process operator in the real plant, with important additional information provided.

The simulation environment is composed of sections where the operator can change the manipulative process parameters, observe the current or past output parameters, get some advice on how the process in the current state should be controlled by the skilled operator. The manual or automatic process control modes are available. The operator can take a challenge to manage the process by hand or leave all or part of the job to PID or Fuzzy controller. The simulation time is much shorter compared to the real process and can be easily adjusted if the computing resources are sufficient. It is important to note that simulation can be paused at any moment, to make it possible to

weigh one's decisions. The main process parameters are stored and can be observed during the simulation or even later. The simulator is provided with routine to compare the simulated and real measured process data.

5 VALIDATION EXAMPLES

Some experiments have been carried out to validate model performance against measured plant data in prediction of the granule size distribution. Experimental data have been obtained using particle image analysis system.

Figure 6 presents the impact of slurry feed rate on the cumulative granule size distribution.

In *phase A* the process is kept in some steady state, with the median granule size nearly 2.65 mm. In *case B* the slurry feed rate is increased approximately by 35 %. In this situation the granule median size is nearly 2.9 mm. Change in the slurry

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flow rate alters the granule growth rate. Increase in the slurry flow rate raises the granule growth rate and a shift of cumulative granule size distribution to the right is observed.
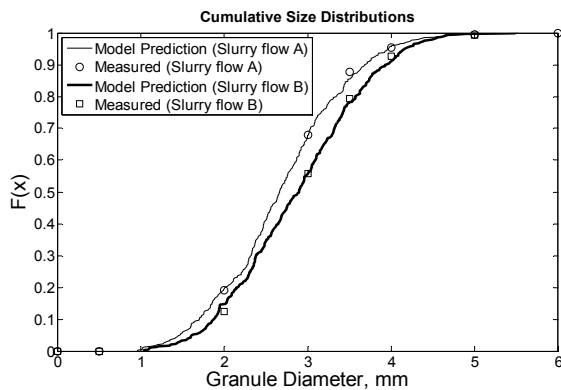

Figure 6: Impact of the change of the slurry flow rate on the cumulative granule size distribution.

Figure 7 presents the measured and simulated cumulative granule size distributions of initial seeds fed to the granulator (mean size is about 2.75 mm) and granules flowing out of the granulator (mean size is about 3.15 mm) in steady state.
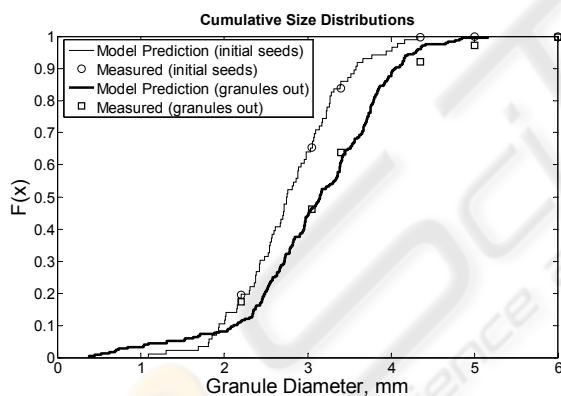

Figure 7: Cumulative size distributions of initial seed flow and granule flow out of the granulator.

6 CONCLUSIONS

An industrial DAP fertilizer granulation circuit, including drum, sieves, crusher, transportation system, has been modeled using basic physical principles such as growth kinetics, mass and heat transfer. Statistical analysis and system identification procedures have been performed for the estimation of unknown model parameters. As an extension to the model, additional information has been extracted from the process experts to define unmeasured parameters and assess some equipment properties. The whole model has been implemented and simulation executed using "GrowSim" simulator in the MATLAB environment.

Some model validation procedures have been performed and the results appear to be in fair accordance with the plant measured data. The findings, presented in Figures 6 and 7, show some kind of mismatch, but still can be treated satisfactory.

The current and future research is focused on further model development, implementation and testing of different plant control modes such as PID, Fuzzy and model predictive control. The primary results demonstrate the need of combination of the aforementioned control methods for a robust process control.

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