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MODELLING AND SIMULATION OF BATCH PROCESSES: A CASE STUDY

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Abstract: Modelling and simulation are inseparable procedures that include the complex activities associated with the construction of models representing real processes, and experimentation with the models to obtain data on the behaviour of the system being modelled. This paper shows how an objected-oriented modelling language can be used to build the dynamic simulation model of an industrial production process that contains both continuous and bath units. The selected case of study is an essential part of a sugar factory: the sugarhouse. *Copyright © 2002 IFAC*

Keywords: Batch modes, Dynamic Behaviour, Object-oriented modelling, Simulation

1. INTRODUCTION

In the process industry, the model libraries are thought as a set of modules, with a given syntax, that represent process units that can be interconnected to form a more complex system. In many equation oriented simulation languages, as ACSL (ACSL, 1995) or the block oriented ones as SIMULINK (Simulink, 1997), these modules encapsulate a set of fix ordinary differential equations (ODEs) and present an interface by means of a set of input and output variables. The blocks are connected, graphically or syntactically, linking the inputs of a block to the outputs of another ones until the whole system is complete. These inputs and outputs are given by the boundary variables of the mathematical model and, additionally, it is possible to define hierarchical structures of blocks providing modular descriptions.

Nevertheless, these tools have a limited usefulness because the blocks have fixed both the interface and the mathematical model, and they don't adapt the models to the context. When simple systems are modelled, for instance the control systems where the process are represented by transfer functions and the controllers by mathematical functions, not adapting the models is not a problem because neither the aims of the simulation changes nor any element changes its structure or function. However, when a real process is modelled using first principle models, neither the elements nor the connectors have fix descriptions and it is necessary to adapt to the context the mathematical descriptions that the blocks comprise.

For these reasons, some modelling tools that deal with model reusing and separate the simulation and the modelling problem have been developed. These tools can be considered simulation code generators. Normally, they use the object-oriented paradigms and are named Object Oriented Modelling Languages (OOML), defining classes of objects with attributes that characterise them (equations, data, parameters, variables...) and an interface (ports) to allow the connections of the class instances. The descriptions of the mathematical models of the objects use a predefined syntax, as a set of differential-algebraic equations (DAEs). A complex system is described by connecting the class instances that compounds it. Later, the equations, that the class instances contain, must be symbolically manipulated to generate the simulation code of the whole system and, finally, they are translated into a simulation language (Cellier, 1991). Modelica is an effort to standardise the description of the models in the OOMLs (Modelica, 1996).

The objective of this research is to build a dynamic model of the sugarhouse of a sugar factory to carry out operation studies and control system tests in simulation and to act as data server for a process-training simulator.

Some reports are published (Zsigmond and Hubay, 1995; Rádek, 1998) about sugarhouse simulation, but the development is in a stationary way and the model isn't an object-oriented one.

This industrial process is a large one that contains continuous, batch and semi-batch process units. The batch and semi-batch processes lead to the production of finite product quantities based on a quantity of input materials, using one or more parts of the equipment. These input materials are put through a series of processes in a finite period of time. The difference between batch and semi-batch processes depends on whether product input is maintained for

the entire batch. During semi-batch processes, product input is continuous, whereas during batch processing it is not. The modelling of batch and semi-bath process requires using ODEs and DAEs, state and time events and model discontinuities.

The paper is organized as it follows. First, a physical description of a sugarhouse of a beet sugar factory is shown. Second, the modelling of this process using an OOML named EL (Ecosim Language) is given. As an example of modelling of a batch process unit the model of a vacuum pan is developed and some simulation results are given using the simulation tool named EcosimPro (EA, 1999). Third, the paper finishes with some conclusions and the intended further research.

2. THE SUGAR HOUSE OF A BEET SUGAR FACTORY

The sugar crystallisation, whose process diagram is shown in Fig.1, is carried out in *the sugar house* comprising the 1st, 2nd and 3rd vacuum pans (known as A, B and C-vacuum pans), the tanks, the centrifugals, the crystallisers, the melter stations, the afination centrifugals and the necessary tanks and pipes.

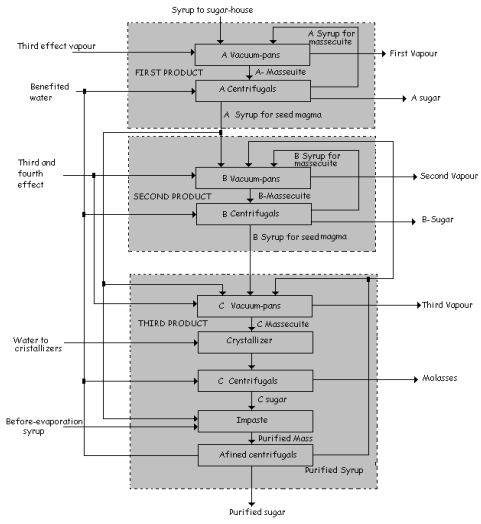

Fig. 1. Components of the sugar house and flow lines

The crystallisation process (McGinnis, 1971; Van der Poel *et al*, 1998) can be subdivided into the following stages:

a) Melting
The *syrup* resulting from the evaporation stage is passed on to the melting station where the *B-sugar* and the *purified sugar* are dissolved to produce *standard syrup*. The standard syrup is then filtered and pumped to the *A-vacuum pans*.

b) First Crystallisation Process
Crystallisation is carried out in order to obtain sugar crystals that are as pure as possible. The first crystallisation takes place in the vacuum pans, where part of the sucrose dissolved in the standard syrup crystallises as the water in the juice evaporates. The vacuum pan becomes full of what is known as the *A-massecuite*, which is formed by crystallised sucrose, sucrose and non-sugars dissolved in a solution known as *mother liquor*. All the pans operate in vacuum conditions, in order to lower the boiling point of the products being processed in them and thus prevent thermal decomposition of the sucrose (loss of sucrose).

c) A-Product Centrifugation
The A-massecuite is discharged to the centrifugals where the crystals are separated from the mother liquor. This operation is carried out in centrifugals where, during a second centrifugal stage, the sucrose crystals are washed with pressurised water and steam.

d) Drying and Conditioning of the Sugar
The sucrose crystals separated in the A centrifugals constitute what is known as white sugar. These crystals are then put through a drying, cooling and subsequent screening process before being packed.

Stages b) and c) are repeated in the B and C vacuum pans with the following modifications: The B vacuum pans receive syrup from the A product centrifugals and the resulting massecuite is known as B product massecuite. The B product massecuite is centrifuged to obtain B sugar and B syrup. This process is carried out in continuous centrifugals, the effect of which is analogous to that of the first product.

The C vacuum pans are fed first with syrup for seed magna to make up the vacuum pan level and then with B syrup and *purified syrup*. The product obtained is *C massecuite,* which after centrifugation, produces *C sugar* and *molasses*. The C sugar and the purified liquor are mixed during a crystal washing process in the purifier. The resulting mass is centrifuged and a purified sugar and the purified liquor are obtained.

Lastly, the molasses obtained is converted into alcohol in an annexed factory to the sugar factory.

So, this is a closed cycle process where the majority of the obtained products are reprocessed, with the exception of A sugar (the objective of the process) and the molasses (a by-product).

3. THE SUGAR HOUSE MODELLING

3.1.Modelling objectives

The initial aim of the simulation model is operators training, so, the dynamic model of the sugarhouse must be the most realistic one. Besides, the simulation model will be used to make global optimization of the production process and to test new control structures and strategies of production. Then, a first principles

model is needed, in which the models of two kinds of process units are especially important ones (the vacuum-pans and the centrifugals), because they must be modelled using discontinuities. To simulate malfunctions, it is necessary to include failure modes in the models and, it is not an easy task, because the model must be robust in hard situations. The introduction of failures can cause changes in the model structure, so, the modelling of failure is much more complex than changing the parameters values.

3.2.Modelling and Simulation tool

To make a first principles model, an equation oriented modelling language is required. By other hand, in the crystallization processes, as almost all industrial processes, the products pass through several process units that are interconnected. Then, it is logical to divide the model in parts that fit with the process unit and later to generate the model of a complex plant connecting process units.

So, to make a model library based in first principles models, the more proper modelling language is an OOML that solve, partially, the causality assignation problem and the simulation model generation.

EcosimPro was selected as simulation tool, because it disposes of an OOML named Ecosim Language to generate the simulation model, a graphical tool to build complex models by connecting components from predefined model libraries and a simulation tool named Ecomonitor to run the simulation programs. Besides, the simulation code is generated as a C++ class that can be included easily in any other program.

3.3 The model library of the sugarhouse components

All necessary components for the simulation of a crystallization section have been modelled making up an EcosimPro library (Garcia, 2001). The main ones are vacuum-pans, centrifugals, crystallizers, melter, horizontal tanks, sensors and controllers. In addition, it exists auxiliary libraries that include connection ports and a series of auxiliary functions.

3.4.Modelling a batch process unit: the vacuum-pan

a) Process and control structure description

Operating in semibatch mode, it is in the vacuum pans (Fig. 2) where the sugar is separated from the juice that is extracted from the sugar beets by means of a crystallisation method controlled by evaporation in a vacuum environment.

Initially, a subsaturated sugar juice known as standard liquor, which is stored in standard liquor tanks, is pumped into the vacuum pan. This standard liquor is then heated in vacuum conditions in order to reduce the boiling point and prevent thermal decomposition of the sucrose. When it becomes supersaturated, it is seeded into small crystals and grown by adding more liquor and maintaining the supersaturated conditions. When the maximum level is reached in the vacuum pan, the contents are discharged and the pan is cleaned, ready for a new cycle.

To heat the juice and evaporate part of the water, the vacuum pans are equipped with a heating element known as the *calandria*. Steam flows through the calandria at a pressure above that of atmospheric pressure and as it condenses, it releases heat to the massecuite in the vacuum pan. The steam is supplied to the vacuum pans through steam supply pipes that form a closed circuit that runs around the complete industrial plant.

To maintain a partial vacuum (0.2-0.3 bar) in the vacuum pan in order to evaporate the water at low temperature (65-70°C), the vacuum pan must be connected to a *barometric condenser*. This condenser maintains a determined vacuum as it absorbs the steam coming from the vacuum pans and condenses it by means of cooling. The cooling effect is obtained by the entry of water that is carried via pipes from the outside. The vacuum produced in the condenser depends on the outside temperature, which means it works better in winter.

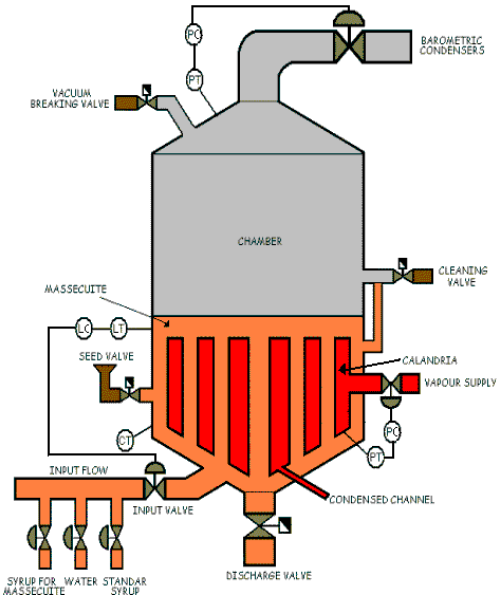

Fig 2. Sketch of a Vacuum Pan

Then, the operation of a vacuum pan has several stages, and in each one some valves are open and others remain close. The change of stage is driven by state events in some process variables and time events. Fig. 3 shows the time consumed by each one.

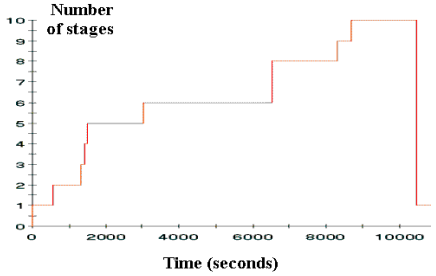

Fig 3. Stages of a semibatch vacuum pan

b) Mathematical model

The massecuite (characterised by the total mass, m_T) consists of two phases, the crystals and the liquor (characterised by the crystal mass, m_C, and the liquor mass, m_J). The liquor consists of water, sucrose and dissolved impurities.

Balance of sucrose

The sucrose mass receives its part of the inlet flow, and is transformed into crystallised sucrose during the crystallisation process:

$$\frac{dm_S}{dt} = q_e^S - \frac{dm_C}{dt} \quad (1)$$

Balance of impurities

The inlet flow is the only source of impurities, and there is no process, which eliminates them (apart from an insignificant fraction which evaporates in the form of incondensable elements).

$$\frac{dm_I}{dt} = q_e^I \quad (2)$$

Balance of water

The mass of water receives its portion of the inlet flow and is eliminated through evaporation due to the heat emitted by the calandria.

$$\frac{dm_A}{dt} = q_e^A - F_{ev} \quad (3)$$

Growth of crystals

The eq. 4. models the mass variation of a crystal:

$$\frac{dm_{cris}}{dt} = f_T(T) \cdot f_y(y) \cdot f_{px}(px) \cdot f_{ag}(rpm) \cdot A_{cris} \quad (4)$$

The following explains the main factors that affect the speed of crystal growth:

- Dependency on the temperature. For their incorporation into the crystal surface, the sucrose molecules must overcome an energy barrier because of the need to break the links of the crystal cell:

$$f_T(T) = Ae^{-\frac{E^*}{R(T+273.15)}} \quad (5)$$

- Dependency on supersaturation. Crystallisation is the transformation of sucrose from the liquid phase to the solid phase.

  Crystal growing is a process of diffusion modified by the effect that the solid surfaces have on the surfaces where the crystals are grown. The molecules of ions of the solute reach the growing surfaces of a crystal by means of diffusion during the liquid phase. At this stage, the usual coefficient for mass transfer is applied K_y. Once the molecules or ions reach the surface, they have to be accepted by the crystal and organised within the network. The reaction takes place on the surface at a finite speed and the overall process consists of two stages in series. Neither of the two stages -diffusion nor interface- is carried out if the solution is not supersaturated.

  Both processes help to determine the speed of growth of the crystal, but as long as resistance to molecular transformation is predominant with 'normal' supersaturation and high temperatures (higher than 50°C), the resistance to molecular incorporation will have an effect at low temperatures and supersaturation. We can therefore use the ranges of the above equations and write an overall equation as follows:

$$f_y(y) = \begin{cases} -K_{dis}|y-1|^{K_{ydis}} & y<1 \\ K_{red}(y-1)^{K_{yred}} & T<50℃ \ \& \ 1<y<1.1 \\ K_{nor}(y-1)^{K_{ynor}} & T>50℃ \ \& \ 1.1<y<1.4 \\ K_{nuc}(y-1)^{k_{nuc}} & y>1.4 \end{cases} \quad (6)$$

- Dependence on the shaking of the medium. Shaking the medium reduces the energy need for the incorporation of the crystal molecules and also diminishes the resistance to transformation and consequently accelerates crystal growth. The eq. 7 is an empirical formula that models this effect:

$$f_a(rpm) = (1 + rpm)^{K_{rpm}} \quad (7)$$

- Dependence on the presence of impurities. Impurities have very different effects on the growth of crystals. In small quantities they favour crystallisation by acting as crystal formation nuclei and creating surface defects that promote the growth of the facets of the crystals. In significant quantities, however, they generally have an inhibiting effect. The following equation expresses the inhibiting effect on growth due to diminishing purity:

$$f_{px}(px) = e^{-K_{px}(1-\frac{px}{100})} \quad (8)$$

Gathering together all the effects on crystal growth, we obtain an overall equation for mass growth of a crystal. Such growth will depend mainly on the surface that the crystal presents for the incorporation of new molecules, and the excess sucrose in the medium, quantified as a measurement of supersaturation. The equation is designed for standard working conditions, that is, supersaturation is in the metastable area but may take into account the growth of crystals in the nucleation area and even in the solution area (in the event that y is less than the unit), accordingly adjusting the constants K_Y and the overall constant K.

$$\frac{dm_{cris}}{dt} = K(1 + rpm)^{K_{rpm}} e^{-K_{px}(1-\frac{px}{100})} e^{-\frac{E^*}{(T+273.15)}} (y-1)^{K_y} A_{cris} \quad (9)$$

The bibliography usually defines a function denominated G, which covers the rate of linear growth of the crystals:

$$G(y, T, px, rpm) = \frac{KK_s}{3\rho_c k_v}(1 + rpm)^{K_{rpm}} e^{-K_{px}(1-\frac{px}{100})} e^{-\frac{E^*}{(T+273.15)}} (y-1)^{K_y} \quad (10)$$

And expressing the growth in mass of each crystal as a function of G(10), we obtain the following equation:

$$\frac{dm_{cris}}{dt} = \frac{3\rho_c K_v}{K_s} G A_{cris} = R_G A_{cris} \qquad (11)$$

Balance of liquor

$$\frac{dm_J}{dt} = q_e - F_{ev} - \frac{dm_C}{dt} \qquad (12)$$

Balance of total mass

$$\frac{dm_T}{dt} = q_e - F_{ev} \qquad (13)$$

Next, the energy balance is developed. Since the dynamics of steam flows in the chamber are much faster than the temperature variation, we will assume that the flow of steam is determined by the dynamic equations of the chambers and that the temperature variable used by the equations is constant in any significant variation in steam flow.

Heat transfer in the vacuum pan

From the energy point of view, generally the process consists in the evaporation of water, first to reach certain supersaturation conditions and then to maintain them. Because sucrose is lost during the crystallisation process, the corresponding amount of water has to be evaporated to maintain the concentration of the juice. The heat needed to produce the evaporation of water is supplied by the calandria that exchanges heat with the system by condensing steam at temperatures and pressures greater than those in the vacuum pan. Fig. 4 shows the main heat flows in the vacuum pan.

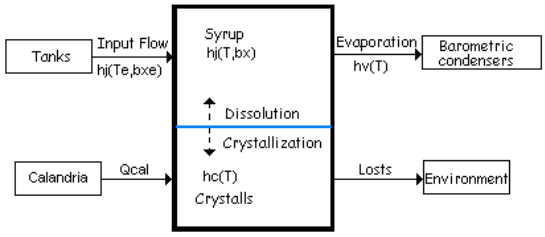

Fig. 4. Heat flows in the vacuum pan

This is shown mathematically in eq. 14.:

$$\frac{d(m_T h_T)}{dt} = Q_{cal} - K_p A(T - T_{ext}) - F_{ev} H_v + q_e h_J(T_e, bx_e) + Q_c(Te, bxe, pxe) \qquad (14)$$

Calandria dynamics

Next, The equations that govern the calandria performance are developed.

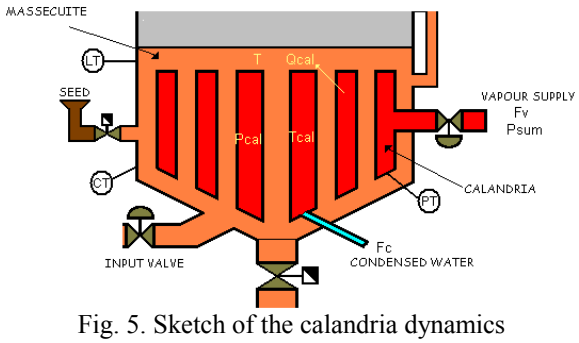

Fig. 5. Sketch of the calandria dynamics

Flow of heat towards the vacuum pan:

$$Q_{cal} = A_{cal} U_{cal} (T_{cal} - T) \qquad (15)$$

To calculate the heating steam flow, it must be had to bear in mind that the heat provided by the calandria comes from the condensation of that steam.

$$Q_{cal} = F_v \lambda(T_{cal}) \qquad (16)$$

Chamber dynamics

Chamber is the name given to the top part of the vacuum pan limited by the juice level, full of steam. The chamber dynamics have similar characteristics to those of the calandria, but with the following differences. Unlike that of the calandria, the volume of the chamber V_{cam}, is not constant but, rather, varies with the vacuum pan level. However, compared with the chamber processes this variation is very slow and its derivative with respect to time can therefore be considered as negligible. The direct contact of the chamber with the massecuite gives rise to appropriate conditions that create a thermal balance between the two. It can therefore be assumed that the temperature of the chamber is equal to that of the massecuite. In addition, given the chamber dynamics, we can assume that the outlet flow of steam towards the condenser, F_{vc}, will be equal to the flow of evaporated steam, F_{ev}, with the exception of transient periods lasting just seconds during which the pressures will be re-established. Then. eq. 17. is assumed for the chamber pressure in the overall process:

$$P_{cam}(T, bx) = \begin{cases} P_{eq}(T, bx) & \text{if } P_{eq} \geq P_{con} \\ P_{con} & \text{if } P_{eq} < P_{con} \end{cases} \qquad (17)$$

Stages modelling

To model the different stages in a vacuum pan, state and time events are used. The modelling language allows including them using the sentence WHEN. A suitable use of it allows describing cycles, which makes it an indispensable statement in the modelling of batch processes, and model hybrid system whose model equations change during the execution of the model.

An example of the use of this sentence is:

```
WHEN (Ma>=0.00050 AND stage==7) THEN
  M_tc=M_t ; M_solc=M_sol ; M_cc=M_c
  etapa=8
END WHEN
```

c) Simulation results

The simulation was run for the maximum length of time so that we could observe the cyclic nature of the process. Some of the graphical results are shown in the following Figures.

Fig. 6 shows the evolution of the mass of products in A-sugar vacuum pans during two cycles. It can clearly be seen where the filling stage ends and where the crystal growth and the discharge stages begin.

Fig. 7 shows the performance of the brix and the total brix in the A-sugar vacuum pans during two cycles.

The total brix is greater than the brix from the concentration stage, because the formation of crystals is taken into account.

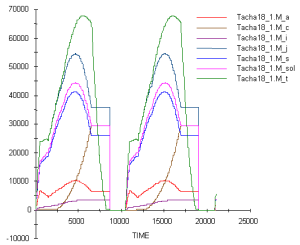

Fig. 6. Mass in Vacuum-pans A

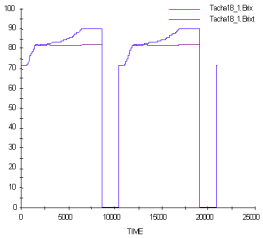

Fig. 7. Brix in Vacuum-pans A

3.5.The Model of the complete section

EcosimPro has an interface that allows the graphical modelling of complex systems by dragging and dropping components and making connections. Later, the EcosimPro model is automatically generated from the scheme, the computational causality is solved, the mathematical model is manipulated and the simulation model is generated. So, using the corresponding libraries the simulation model of the crystallization was generated from the process scheme (Fig. 8 shows a part of the sugar house of a reference factory in Spain). Also, it is possible to simulate the model from a graphical interface of EcosimPro named Ecomonitor. The resulting simulation model is quite complex (5762 equations, 7161 real variables, 418 state variables) and, it runs twice faster than real time(PENTIUM III to 500MHz and 256Mbytes of RAM).

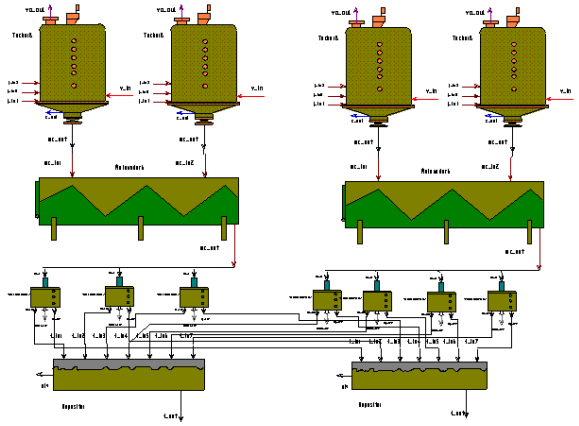

Fig. 8. Smart-Skech connection

4. CONCLUSIONS AND FURTHER RESEARCH

This paper shows a dynamic model library, developed using an OOML, for a sugarhouse of a beet sugar factory. It must be taken into account that according to the author's knowledge there doesn´t exist a similar one. Besides, as an example of modelling of complex batch processes the model of vacuum pan has been described, showing that EcosimPro, as an example of OOML, is a suitable language to model them.

The dynamic model of the sugarhouse is really complex and the execution of the resulting simulation model spends a lot of time (in some cases it is performed in a greater time than real time). One aim of the simulation is to act as data sever for a process-training simulator and the real time requirements are hard ones. Then, to manage the real time requirements, the model must be simplified or the simulation must be distributed in several computers.

As further research, as, the OOMLs have some difficulties, and, in some cases, the generated model is not the more optimum one. So, the intended further research is to implement the library of the sugarhouse in other modelling tool named SIMPD (Acebes, 1996). SIMPD is a modelling tool that using graphical and artificial intelligence techniques emulates the way of reasoning of an expert when he/she builds a dynamic model. SIMPD doesn´t uses an equation oriented approach but it uses a physical description oriented one. Nowadays, SIMPD is able to model continuous process but not the batch and semibatch ones. So, it is an open field of research.

Another open problem is the modelling of the crystal size distribution. It's a complex task that requires the use of probabilistic models.

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