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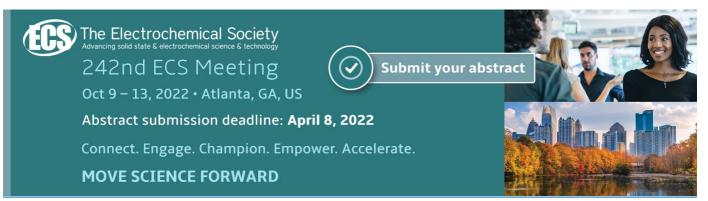
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Granulation machines with highly turbulized flows: creation of software complex for technological design

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Abstract. The article deals with author's software products review to calculate devices with highly turbulized flows as a part of granulation units. Principal scheme and model of the granulation unit, algorithm of the granulation technical calculation are represented in the work. The complex automated calculation technique of the granulation units is proposed. The proprietary software for calculation of main stages in the granulation process is observed in the research. Short description and functions of main software products to implement basic algorithm are given: Vortex Flow[©], Conical Channel[©], Conical Granulator[©], Multistage Heat Treatment[©], Vortex Tray[©]. As a result of the optimization calculation, the user of programs will get the following information: optimal construction of the vortex granulator's workspace, necessary number of stages in the multistage shelf drier for granules' final drying, number and construction of the vortex tray with heat and mass transfer-separation elements for exhaust gases cleaning. All software products enable to export the received data and to exchange these data between each other. The complex algorithm and software products, proposed in the article, let to carry out optimization calculation of the main technological equipment in the granulation unit at its designing stage without expensive multifactorial experiment. The presented granulation units' calculation algorithm and software products for its realization enable to carry out equipment changeover if raw material characteristics and the productivity of the unit are changed. The automated calculations results give a base to design industrial granulation unit for porous ammonium nitrate production.

1. Introduction

Nowadays automatization of main processes calculations, carried out in the chemical production, is an essential part of the enterprise's successful operation. Implementation of the informational systems to calculate and to design main equipment of products production units lets to:

- minimize cost for experiments on natural samples of the main equipment in the unit;
- carry out the optimization calculation of device by the optimization criterion, fixed by user;
- provide "flexibility" of calculation if basic data for technological calculation or optimization criterion are changed.

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In this research the object is a granulation unit to obtain granulated porous ammonium nitrate (PAN) through humidification and heat treatment of the ammonium nitrate granules. In order to carry out the target and secondary processes, one proposes to use devices with highly turbulized flows as the main equipment, working in the hydrodynamic regime. They are vortex granulator, multistage shelf drier, absorber with vortex mass transfer separation contact elements.

Formation of the complex automated calculation technique of the granulation units will enable simultaneously to carry out constructive and technological calculations of the main equipment.

Aim of the research is to create technique of the granulation units' complex automated calculation using author's applied programs pack.

The author's applied programs pack to calculate some stages of PAN obtaining process is proposed in the article. Their work is based on the author's mathematic models of the hydrodynamics and heat and mass transfer in the vortex highly turbulized flows.

Main programs, included to the optimization calculation complex pack of the granulation unit main equipment to obtain PAN, are described.

The software realization of the author's mathematic models to calculate hydrodynamic and thermodynamic models for hydromechanical, heat and mass transfer processes in the devices with vortex highly turbulized flows, is first proposed.

The presented results of the research enable to carry out optimization calculation of the granulation unit's main technological equipment at its designing stage without expensive multifactorial experiment. Besides, granulation units' calculation algorithm and software products to implement the algorithm, observed in the article, let to fulfill changeover if raw material characteristics and unit's productivity are changed.

2. Literature review

Review of the software products modern base (simulation modeling systems) to calculate units of the chemical industries (Aspen HYSYS®, PRO/II, GasCondOil, ChemCAD, DESIGN II, SIGMAFINE, gPROMS ModelBuilder, GIBBS etc) [1–8] shows that such software products can be mainly used for technological calculation of the equipment with set construction and with concrete technological parameters of the chemical units operation. In order to perform technological calculation, it is necessary to use multiple input of the basic data; there is a large number of such inputs in the optimization calculation. The software products to calculate hydrodynamic and heat and mass transfer processes in the equipment of chemical industry (ANSYS Fluent, COSMOS FlowWorks, FlowVision, Flow-3D CFD, Ansys CFX, COMSOL Multiphysics etc) [9–14] enable to find only one constructive variant of the device on the set solid model that reduces optimization calculation velocity. It should be mentioned that simulation modeling systems and software products for calculation of hydrodynamic and heat and mass transfer processes in the equipment of chemical industry are effective to estimate units with fixed technological parameters and equipment of the set construction. An additional difficulty in implementation of the above products for granulation unit, which is observed in this article, consists in the fact that there are no models to calculate the equipment, suggested by authors as a result of novelty in organization of flows motion, confirmed by a number of protection documents [15–19]. Authors have achieved success in the software realization of the author's mathematic models for calculation of the hydrodynamic and thermodynamic conditions of the vortex granulators' work [20-22], though, the created software products do not fully comprise the whole operation cycle of the main equipment in the granulation unit.

3. Description of the unit and basic algorithm of its calculation

Principal scheme of the PAN obtaining unit with the use of equipment with highly turbulized flows is demonstrated in the figure 1. The target technological processes in PAN production are heat treatment of the ordinary ammonium nitrate after humidification and the PAN final drying, significant secondary process – cleaning of the waste drying agent before its release into the atmosphere or utilization. Given this, basic algorithm of the granulation unit's calculation (technological scheme of the unit is

demonstrated in the figure 2) will be based on the defining of technological operation conditions and constructive characteristics of the vortex granulator (VG), gravitational shelf dryer (GSD) and absorber (A) with vortex mass transfer-separation contact elements.

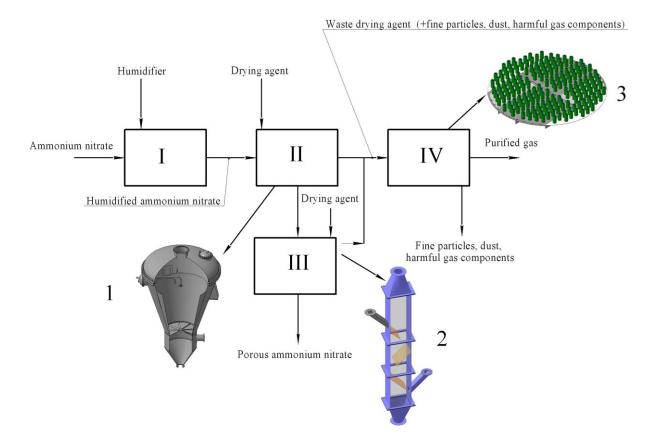


Figure 1. Diagram of porous ammonium nitrate production according to the method [15–18]. I - humidification of ordinary ammonium nitrate; II - heat treatment and drying of ordinary ammonium nitrate after humidification; III - final drying ig PAN; IV - cleaning of exhaust gases; 1 - vortex granulator; 2 - multistage gravitational shelf dryer; 3 - contact tray with heat and mass transfer-separation elements.

In general, the algorithm to calculate the main technological equipment of the granulation unit to obtain PAN, can be presented as a scheme, shown in the figure 3. One or several software products, which together constitute automated complex of the granulation unit calculation, correspond each block of the scheme.

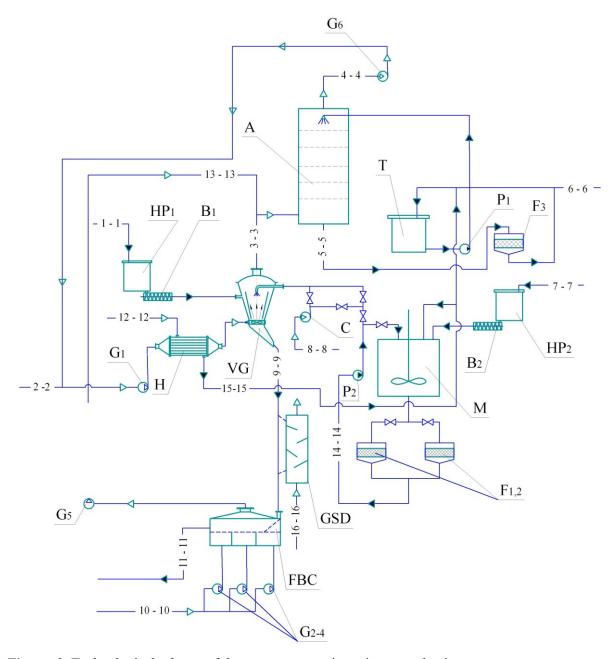


Figure. 2. Technological scheme of the porous ammonium nitrate production. Elements of the installation: VG - vortex granulator; H - heater; GHD - gravitational shelf dryer; FBC - fluidized bed cooler; A - absorber; F - filter; M - mixer; B - batcher; HP - hopper; G - gas blower; P - pump; T - tank; C - compressor. The main flows: 1-1 seeding agent; 2-2 manufacturing air; 3-3 polluted air; 4-4 purified air; 5-5 polluted water; 6-6 water; 7-7 substandard granules; 8-8 air for spraying of liquid material (solution, melt); 9-9 product; 10-10 air for cooling of granules; 11-11 granules for packaging; 12-12 steam; 13-13 dusty gas; 14-14 liquid material (solution, melt); 15-15 water condensate; 16-16 drying agent.

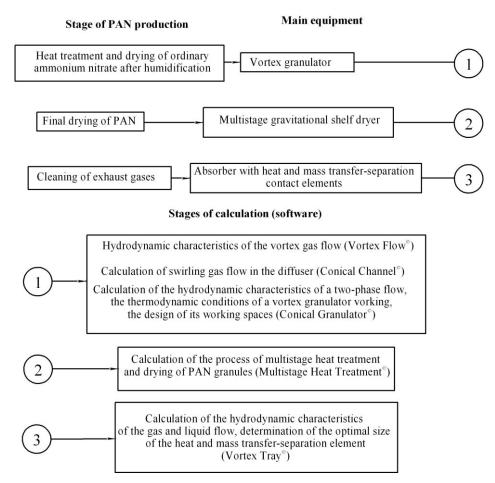


Figure 3. Algorithm of the main technological calculation of the PAN obtaining granulation unit.

Short description of the software products, which form automated complex of the granulation unit's calculation, is represented below.

3.1 Vortex Flow[©]

The program Vortex $Flow^{\circ}$ [23] (mathematic model, which is a basis of the software product, is shown in [24–26]) is for calculation of the hydrodynamic parameters of the twisted gas flow and particles, moving in it. It may be implemented in the hydrodynamic calculation of streams in the vortex heat and mass transfer (granulators, driers) and hydromechanical (classifiers, cyclones) equipment with variable cross sectional area of the workspace. The result of the calculation includes values of velocity's components of the gas flow and particles in the workspace of the device.

Having started the work with the program, one can see the dialog box on the screen of the computer. User inserts data for calculation into the corresponding fields in the dialog box. While setting basic data, user chooses the way to subdivide the workspace of the vortex device in the vertical and horizontal directions.

The next step is to output calculation results on the screen. The received data set is proposed to the user at the first stage (figure 4). Having carried out calculation, values set of the definite parameter in every computation grid cell appears on the screen according to their number in the basic data. Graphical dependences appear on the screen with right input of the basic data – figure 5.

3.2 Conical Channel^{\circ}

The program Conical Channel^{\circ} [27] (mathematic model, which is a basis of the software product, is shown in [28]) is for calculation of the axisymmetrical gas flows in channels, including twisted flows in diffusors.

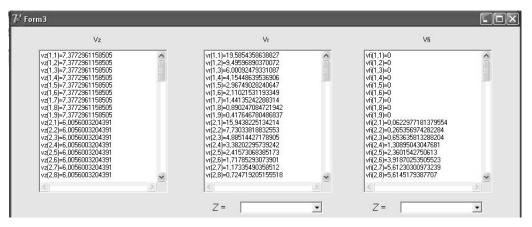


Figure 4. Computation data set (on the example of gas flow velocity calculation).

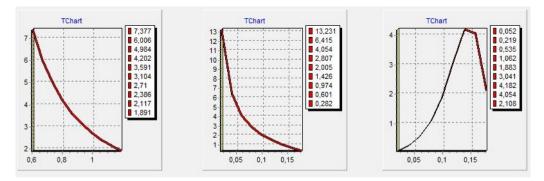


Figure 5. Output of graphical dependences (on the example of gas flow velocity calculation).

Mathematic model, which is a base of the investigated software product, includes so called generalized Prandtl equations (in Western terminology – Reduced Navier-Stokes Equations). Implementation of this mathematic model, realized in the curvelinear orthogonal coordinate system, enables rapidly and effectively to calculate streams per one pass from the inlet to the outlet cross-section of the calculation area.

The basic data for calculation include: geometric configuration of the channel, gas properties and parameters of the flow in the inlet cross-section. The task of calculation is to define velocity's fields and pressures in the whole calculation area and, consequently, to find size of energy loss between inlet and outlet cross-sections of the channel.

Having started the program, the dialog box is opened. The program starts its work from opening or creating of the new file of calculation area configuration. Example of the calculation area configuration is given in the figure 6.

After that, parameters, which have to be calculated (velocity components U, V, W or pressure P), are selected in the corresponding window. Having selected the necessary calculated parameter, the program forms computation grid (figure 7). Results of calculation are presented through graphic, which is shown in the figure 8.

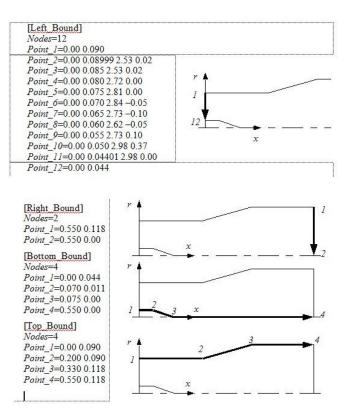


Figure 6. Example of calculation area configuration.

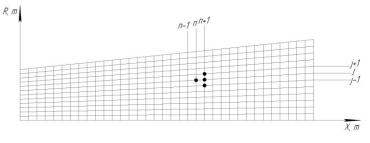


Figure 7. Formation of the computation grid.

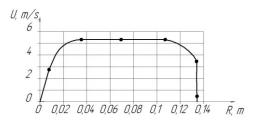


Figure 8. Results of calculation.

3.3 Conical Granulator[©]

The program Conical Granulator[©] [29] (mathematic model, which is a basis of the software product, is shown in [30–34]) is to calculate sizes of the variable cross sectional area of the vortex granulator's workspace. The result of calculation is velocity of the granule's levitation with definite physical and chemical properties, the way, which granule overcomes in the workspace of the vortex granulator and updated values of the main geometric sizes of the vortex granulator's workspace by requirement of

providing the granule's levitation. The calculation is carried out for cylinder areas, into which granulator's conic space is divided, and calculations results at one area are basic data to calculate on th next stage on the granule's motion way.

Having seen the dialog box on the screen (figure 9) user inserts data into the proper fields for calculation. While inserting basic data, user selects individually the way to divide residence time of the particle in the granulator's workspace. The program outputs data of calculation as a list of results – figure 10.

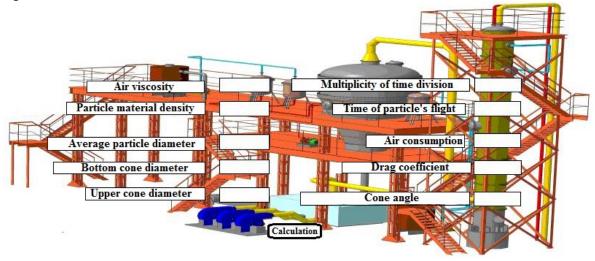


Figure 9. Dialog box of the program.

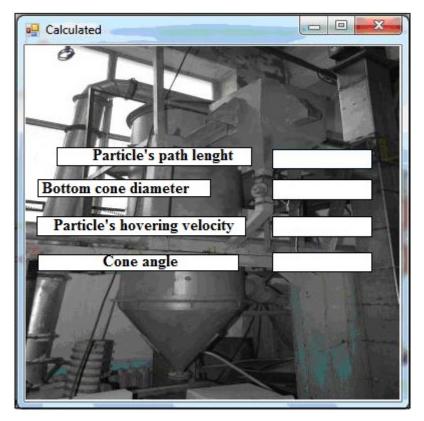


Figure 10. Results of calculation.

3.4 Multistage Heat Treatment[©]

The program Multistage Heat Treatment[©] [35] (mathematic model, which is a basis of the software product, is shown in [32, 36]) is to calculate the heat treatment processes and the dehydration processes (if it is necessary) in the multistage drying, granulation and cooling devices of the weighted layer. The result of calculation consists in value of temperature and humidity of the dispersed material and gas flow (drying and cooling agent) before and after every stage of the multistage device. The heat treatment process is calculated in the direction of gas flow (from lower to upper section of the device). Having started the work with the program, the system of mathematic model equations appears on the screen, figure 11. User fills basic data in the proper cells – figure 12. Work field of the program after the basic data input is shown in the figure 13. The next step is to carry out calculation – figure 14. This appropriate command enables to calculate required values.

```
k1:=(t1k1-t2k1)/(t1H1-t2H1)=E11;
k2:=(x2k1-x1k1)/(x2H1-x1H1)=E21;
k3:=G2*CM*(t2k1-t2H1)+GM*CB*(x2k1*t2k1-x2H1*t2H1)=G1*Cc*(t1H1-t1k1)+Gc*CB*
(x1H1*t1H1-x1k1*t1k1);
k4:=GM*(x2H1-x2k1)=Gc*(x1k1-x1H1);
```

Figure 11. Window with mathematical model for calculation.

tlml:=__;t2k1:=__;x1m1:=__;x2k1:=__;
G2:= ;G1:= ;Cm:= ;CB:= ;Cc:= ;E11:= ;E21:= ;

Figure 12. Input of the basic data.

$$kl := \frac{tlkl - t2kl}{tlHl - t2Hl} = Ell$$

$$k2 := \frac{x2kl - xlkl}{x2Hl - xlHl} = E2l$$

k3 := G2 CM (t2kl - t2kl) + GM Cs (x2kl t2kl - x2kl t2kl) = Gl Cc (tlkl - tlkl) + Gc Cs (x1kl tlkl) - x1kl tlkl)

Figure 13. Work field of the program.

rez:=solve({k1,k2,k3,k4},{t1k1,t2H1,x2H1,x1k1});

Figure 14. Performing calculations.

Having carried out calculation of the first stage, user starts further computations. The mathematic model equations at the next stage are analogical to the previous ones. The peculiarity of calculation at every further stage is to use calculation results of the flows characteristics at previous stage which are basic data for computation.

3.5 Vortex Tray[©]

The program Vortex Tray[©] [37] (mathematic model, which is a basis of the software product, is shown in [38, 39]) is to calculate optimal sizes of heat and mass transfer separation element of the vortex tray to clean exhaust gases and gas separation processes within technological units of chemical and gas-oil refinery plants. It may be used in the constructive calculation of the waste gases cleaner units of the weighted layer (granulators, dryers, coolers), and vortex trays as a part of column devices' mass transfer (absorption and rectification processes). The result of the calculation includes values of the vortex tray's heat and mass transfer-separation element's constructive parameters (diameter and height of fitting pipe) with variable hydrodynamic characteristics of liquid motion and its physical and chemical properties.

Having started the work with the program, start screen appears on the display (figure 15). In order to perform calculation, the user is provided with a list of boxes (figure 16), from which he selects necessary information for the research.

Having chosen the necessary box, user inserts data for calculation into the proper fields and displays the calculation results. While inserting the basic data, user chooses the way how to change parameter, which is varying.

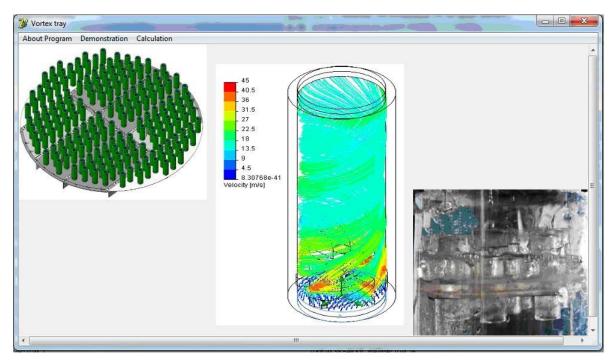


Figure 15. Start screen of the program.

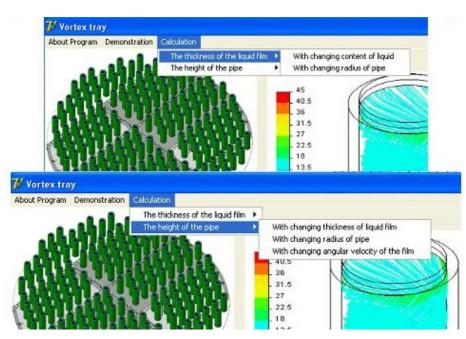


Figure 16. List of boxes for user's choice.

4. Conclusions and recommendations

The complex algorithm and software products, proposed in the article, enable to carry out optimization calculation of the main technological equipment in the granulation unit at its designing stage without an expensive multifactorial experiment. Besides, the granulation units' calculation algorithm and software products for algorithm implementation, observed in the article, let to changeover equipment if raw material characteristics and unit's productivity are changed.

The aim of further studies is to create exporting algorithm of constructive calculations results of the granulation unit's main technological equipment into the solid modeling programs with purpose to create device's models, and constructive and technological documentary for their production.

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