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Complex designing of granulation units with application of computer and software modeling: case "Vortex granulator"

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Abstract. The article is devoted to the description of the complex method to design granulation unit, which is based on the joint use of the computer modeling results on the simulation models and software modeling based on author's software products. The description of the software package Granulation Unit© to carrying out the structural and technological calculations for the granulation unit is given. The role of computer and software modeling in the general design algorithm of the granulation unit is shown. The optimization criteria are selected and an algorithm of design optimization for granulation unit is described using the example of the "Vortex Granulator" case. A general method of granulation unit designing "turnkey" with the use of automated design elements is presented. The results of automated calculations form the base to design an industrial granulation unit for the porous ammonium nitrate production. On the example of a specific product of the granulation unit (porous ammonium nitrate), the author's software product is presented to determine the quality of the porous surface in the granule. This approach in modeling allows to create the automated systems for the optimization calculation of granulation equipment.

1. Introduction

The optimal decision regarding the chemical apparatuses design of the chemical unit and technological principles of its operation can be made only on the basis of the complex design using modern means of the automated calculation [1, 2]. Under conditions of the multifactorial simulation experiment, such an approach lets to avoid systematical errors at the stage of the unit design. Therefore, combining various methods to carry out the simulation multifactorial experiment (computer simulation, use of the author's software packages) enables strictly to follow the optimization criterion, set by the designer thanks to the possibility for customer to take in excess the definite number of the initial parameters in the chemical and technological system, controlling actions and necessary final features of the unit (process, production) [3].

The project is based on the idea to investigate the small-sized granulation modules (units) using the equipment with active (intensive) hydrodynamic modes. Due to the turbulence of the flow, multistage

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phase contact implementation (and combination of such methods) and the specific power growth of the equipment, it is possible to increase the energy and ecological efficiency of the granulation processes and other secondary stages. The proposed Complex approach to creating small-sized granulation modules has to take into account the hazardous waste disposal processes (with the possibility of their repeated return to the process) and heat and moisture recovery with further use of this potential within the module. This thesis forms another idea of the project, which is to use separate waste heat and moisture recovery unit, and to use elements, built into the main equipment of elements for hazardous waste disposal, in the granulation module.

Conceptions and models, which are used in the project:

- conception regarding the ecological and economic objectivation of reasonability to implement changes in the organization of the flow motion forms in the granulation units applying devices with active hydrodynamic modes from the viewpoint of evaluation of specific emissions into the atmosphere (per unit of specific weight or per unit of the granulation unit productivity) and specific cost of the production unit;
- conception regarding the full disposal of material flows (dust, unconditioned granules, harmful components of the waste gases) owing to the disposal units implementation;
- the concept of energy (heat) resources recovery through the use of modern refrigeration compressor cycles;
- theoretical and computer models for the integrated assessment of the impact, made by hydro and thermodynamic factors of the granulation module equipment work, on the heat-mass transfer processes intensity.

In this paper, the object of the research is a granulation unit, in which the devices with intensive hydrodynamics (with active hydrodynamic modes) are used.

The aim of the study is to introduce a comprehensive algorithm to design granulation units based on the combined simulation modeling methods.

The project consists of the following interconnected structural elements:

- ecological and economic objectivation regarding the introduction of the devices with intensive hydrodynamics into the granulation unit;
- theoretical block – mathematic device and author's software package to calculate the hydrodynamic and heat-mass transfer indicators in the implementation of the target and related process in the granulation unit;
- experimental block – to check the adequacy of the created mathematic device using the software package: to study hydrodynamic and heat-mass transfer features of the processes, carried out in the granulation unit, to define the impact made by the constructive and technological parameters of the main equipment in the unit on the intensity and efficiency of the granulation process;
- block of analysis and comparison of the study results;
- block of evaluation of the energy efficiency and ecological safety of the stated technology and equipment for its implementation;
- block of investigation of the engineering calculation methods regarding the main technological equipment of the granulation unit.

The example of the case "Vortex granulator" shows the main stages of the industrial equipment sample creation with a description of all designing stages, based on the simulation modeling.

The complex approach to the simulation modeling, which combines author's theoretical models (software products) and multifactorial computer simulation models of the hydrodynamic and heat-mass transfer features with intensive hydrodynamics are represented for the first time.

The complex design instruments of the chemical industry units let to perform the optimization design of the unit at the pre-design preparation stage without using the expensive experimental base for physical modeling. Theoretical and experimental blocks of the project are described in more detail.

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2. Software Complex Granulation Unit© - Description and Principles of Work

The software complex Granulation Unit© is used for the complex design of the small-size granulation units, technological calculations of the granulation process and constructive calculations of the main equipment. The software complex is based on the software package, theoretical fundamentals of creation and detailed description of which are given in table 1. The cluster Granulation Unit© is designed for the technological and constructive calculation of the vortex granulator to produce granules from solutions or fusions and to form the porous structure on the granule surface and in the near-surface layers of the granule through humidification with further heat treatment. The user applies to the separate sub-programmes, implemented in the form of individual blocks of the general algorithm regarding engineering calculation of the vortex granulator. The consistent calculations determine the main technological parameters to carry out the granulation process, peculiarities of the constructive design and concrete sizes of the vortex granulator. Since it is necessary to investigate Rich Internet Application (RIA), the decision has been made to create a cluster and its components in the Java language. JavaFX, which lets to construct unified applications with the rich graphical interface of the user, was chosen as a platform for RIA development. JavaFX contains a set of utilities, with the help of which programmers can quickly create programs for desktops, mobile devices, etc.
Short description of every software product is shown in table 1.

Table 1. Short description of the software products in the software complex Granulation Unit©.

Theoretical fundamentals (references for a short description of the theoretical model)	Computed value	The software product
System of the Reynolds differential equations and flow continuity equations ([4, 5])	The average velocities field (vertical, circular, radial) of the gas flow in the workspace with the height-variable cross-sectional area.	Conical channel© [22]
System of the Navier-Stokes differential equations and flow continuity equations ([6])	The instant velocity field (vertical, circular, radial) of the gas flow in the workspace with the height-variable cross-sectional area.	Vortex Flow© [23]
System of the granule motion differential equations, kinetic equations of heating and drying of the capillary-porous body ([7–12])	- the instant velocity field (vertical, circular, radial) of granules in the workspace with the height-variable cross-sectional area; - trajectories of the granules motion; - “hydrodynamic” time the granule stays in the vortex granulator; - field of temperatures and humidities of the granule; - time for heating and drying of granules; - “thermodynamic” time the granule stays in the vortex granulator.	Vortex Granulator© [24]
Force analysis of the dispersed phase motion, the dispersed phase balance in the swirling gas flow ([13–15])	- distribution of granules of various size (mass) along the height of the vortex granulator’s workspace; - range of the vortex granulator’s stable operation; - separation of the small fraction granules and dust.	Classification in vortex flow© [25]
Force analysis of the dispersed phase motion ([16–19])	Time, the granule stays in the sectioned workspace of the device.	Multistage fluidizer© [26]
Force analysis of the solid and dispersed phase motion ([20, 21])	The trajectory of the gas flow and liquid film motion in the mass-transfer-separation element.	Vortex Tray© [27]

Java is a multiplatform programing language, and that is why it does not depend on the operational system, on which the program will run. The developers have created a special software JVM (Java Virtual Machine), which is downloaded to a computer, mobile phone or another electronic device. As soon as the program is written in Java language, it is compiled into byte-code, which is interpreted by the virtual machine for the concrete platform. Since the creation of Java, a number of libraries and add-ons have been developed, which extend the functionality of the programs, written in this language. One of such libraries, which was used, for example, during the investigation of the Vortex Granulator and Classification in vortex flow programs, is Apache POI library. Thanks to this library, the program has the opportunity to save the results in a spreadsheet format.

Operation of all the above software products is united in the cluster Granulation Unit© through separate structural blocks (figure 1).

Figure 1. The interface of the software complex Granulation Unit©.

3. Case "Vortex granulator"

The detailed analysis and patent review of the fluidized-bed granulation device show that the essence of most security documents comes down to the constructive improvement of the current equipment (in addition, in most cases without theoretical substantiation of the proposed constructive solution), and not to a new form of flow motion organization. All these tendencies prove the definite disadvantage of the reliable theoretical principles for calculating devices of such type. The proposed constructions of devices are definitely effective (in relation to the qualitative granulation production). The efficiency at this stage satisfies producers, but in future, they can lose competition due to the low energy efficiency and poor environmental safety. Besides, devices with classical fluidized bed (which do not have the regulated directional motion of the dispersed particles by installation of various guiding (accelerating) elements and inserts of various configuration; they make the main equipment park of the granulation unit), unlike the functional and multistage devices with directional fluidized bed (vortex, gravitational and others), have well-known calculation methods and due to constructive improvement, there is no need to observe such methods. In most cases, equipment, using the fluidized bed, has been patented by large industrial enterprises, which can carry out experimental research, because theoretical base to calculate such devices has not been highlighted in the scientific literature yet and is limited by basic knowledge of hydrodynamics and heat-mass transfer.

Additional interest in the project implementation is the study of the dispersed phase motion in the dense (constrained) flow mode, when it is necessary to take into account the mutual influence of the dispersed phase particles (particle ensembles) and granulator's elements on the particles motion velocity and on the time they stay in the device. Currently, scientists use probabilistic models to describe this process, which gives an approximate result. By providing directional motion of

the dispersed phase in various configurations of the fluidized bed and the mathematical description of this process, created in the framework of this project, it is possible to determine the properties of the motion of the particles in the fluidized bed with high accuracy.
The initial data for the engineering calculation of the vortex granulator are:

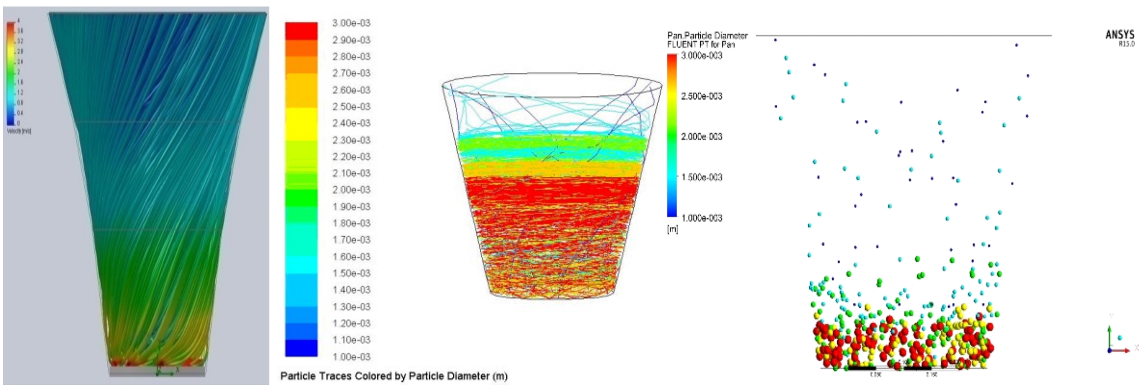
- granulator's production capacity;
- fractional composition of granules and/or average diameter of the seeding agent;
- the initial and necessary final humidity rate of the granule;
- the initial and necessary final humidity rate of the air;
- the initial temperature of granules and the temperature of the heat transfer agent.

One of the problems for scientists and industrial practitioners, who study theoretical principles of the granulation process in the vortex fluidized bed, is to calculate the hydrodynamic and heat-mass transfer conditions for the formation of granules.

The necessity to determine these properties is due to the fact that before designing an industrial model of the vortex granulator, it is necessary to define its optimal construction. The optimization criterion, in this case, is to ensure the minimum required time; the granule stays in the granulator workspace, which will let to form a complete crystal structure of the granule with certain hardness indicators and the monodispersity degree of the commodity fraction. It is especially important when designing the vortex granulators to obtain granules with special properties, particularly, porous ammonium nitrate. In addition to the above indicators of the final product quality, the porous ammonium nitrate granules must have regulatory specific indicators, for example, retentivity and absorptivity towards diesel fuel [28, 29]. In this case, it is important to follow the condition, when "hydrodynamic" time, the granule stays in the workspace of the device, should be no less than "thermodynamic" time (this parameter is defined by the kinetics of the dehydration process in the granule) [30, 31]. Therefore, in order to keep the core hardness of the granule, "hydrodynamic" time has not to exceed "thermodynamic" time more than by 5–10 %. Optimal design of the vortex granulator, which satisfies the requirements of the optimization criterion, is achieved through regulation of the hydrodynamic features of the flows motion.

The authors propose the following algorithm (case) to calculate the vortex granulator, based on the above structural elements.

1. Hydrodynamic calculation – computer simulation (figure 2).
2. Thermodynamic calculation – software modeling (figures 3 and 4).
3. Technological calculation – software modeling (figures 5 and 6).
4. Constructive calculation – software modeling, creation of the solid-state models granulator's units and its construction, based on the optimization calculation results, granulator's layout as a part of the granulation unit (figures 7–13).



a b c

Figure 2. Hydrodynamic calculation – stages of the computer simulation: a – a selection of the rational construction of the workspace and swirler; b – calculation of the granules classification process; c – calculation of the granules motion trajectory in the constrained mode.

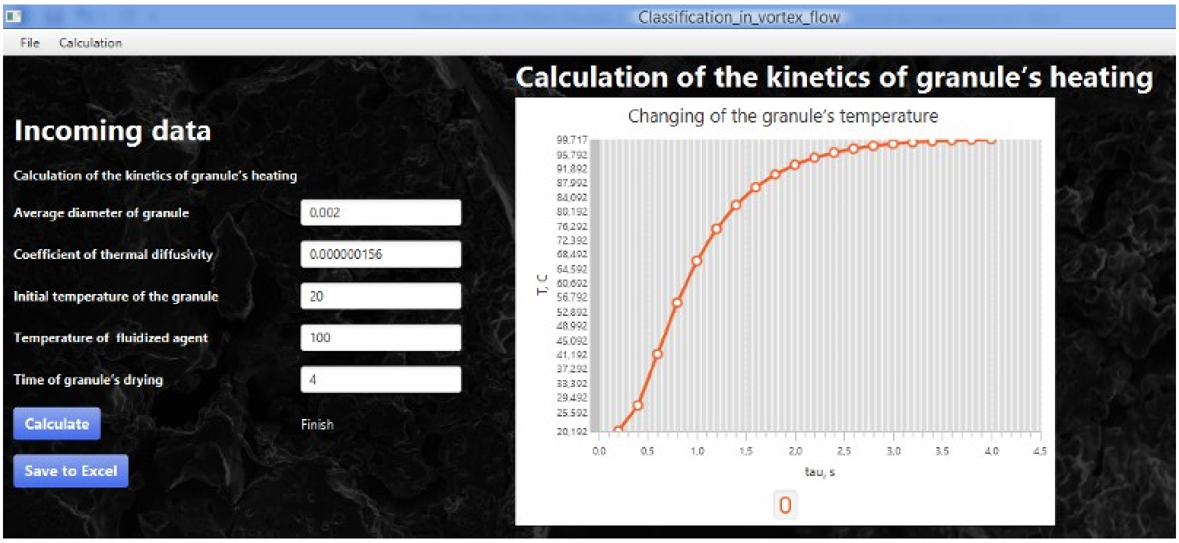


Figure 3. Thermodynamic calculation – stages of the software modeling: calculation of the granule heating process.

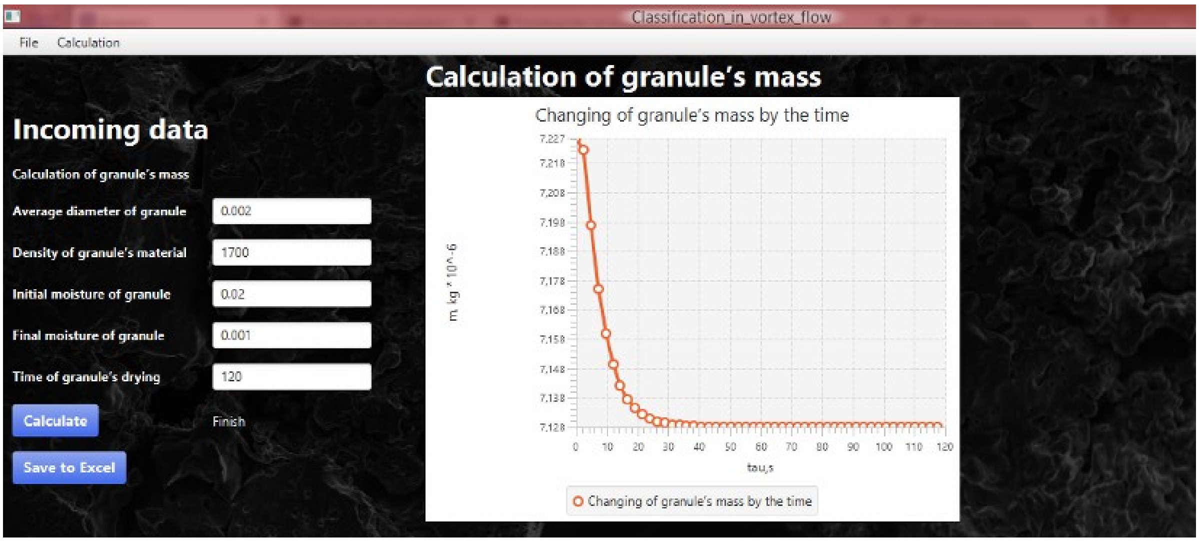
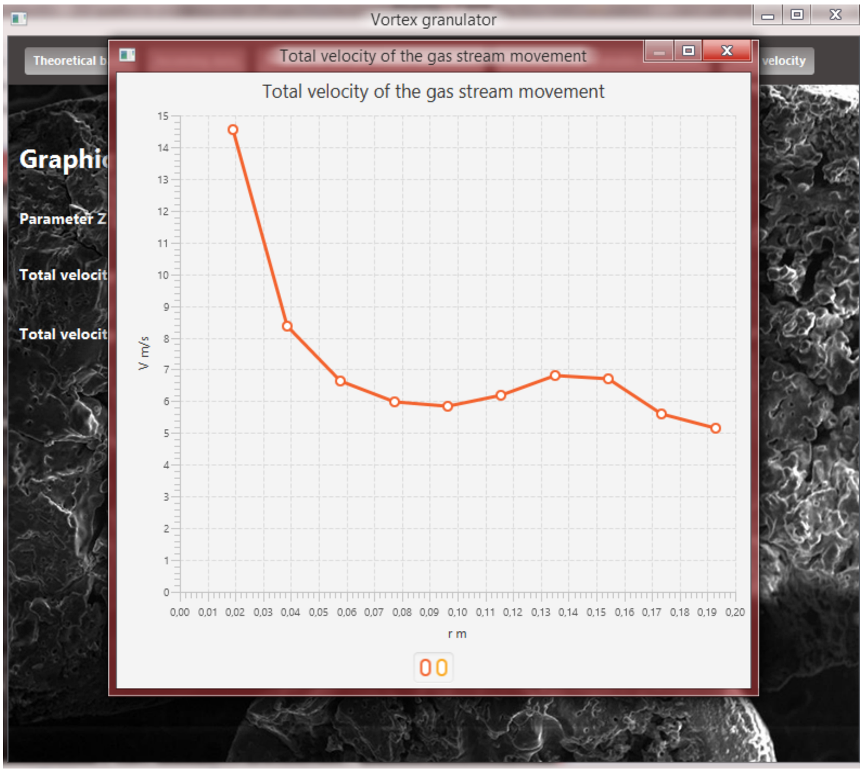
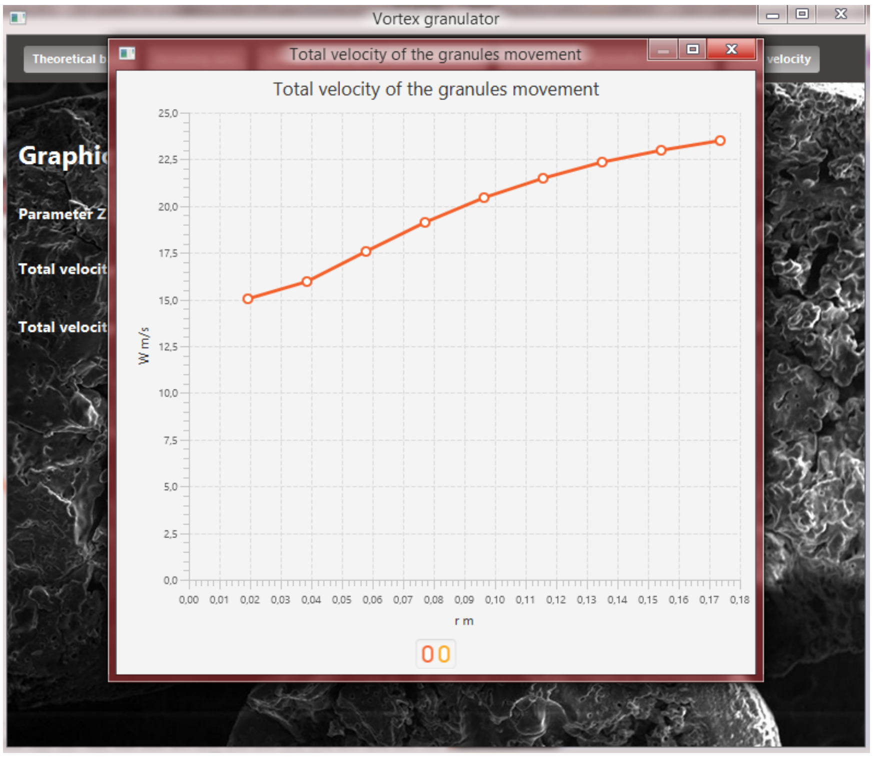


Figure 4. Thermodynamic calculation – stages of the software modeling: calculation of the granule mass changes.



a)



b)

Figure 5. Technological calculation – stages of the software modeling: a – determination of the gas flow velocity; b – determination of the granules velocity.

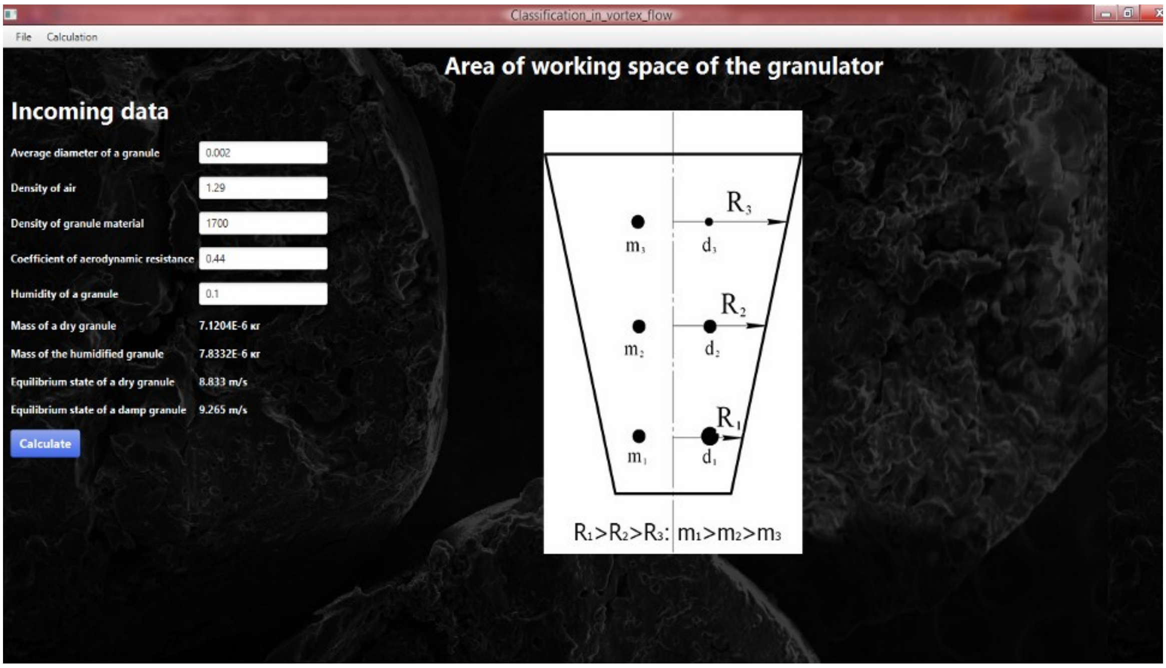


Figure 6. Technological calculation – stages of the software modelling: calculation of the classification process.

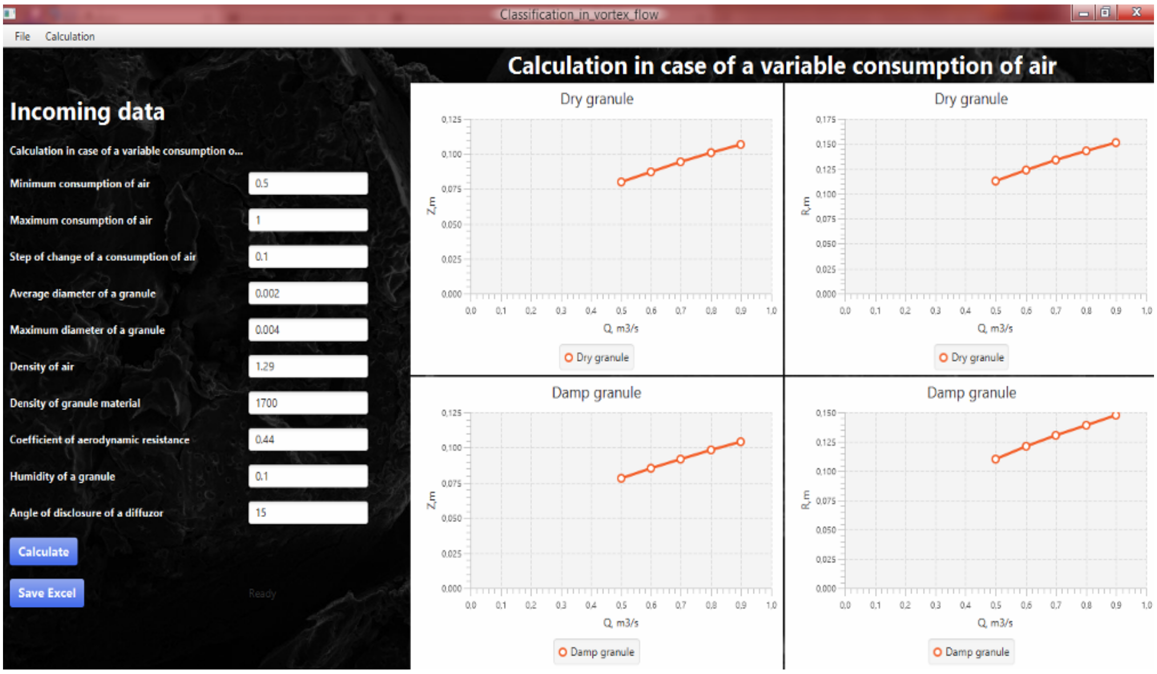


Figure 7. Constructive calculation – stages of the software modeling: calculation of the workspace size in the vortex granulator under various initial conditions.

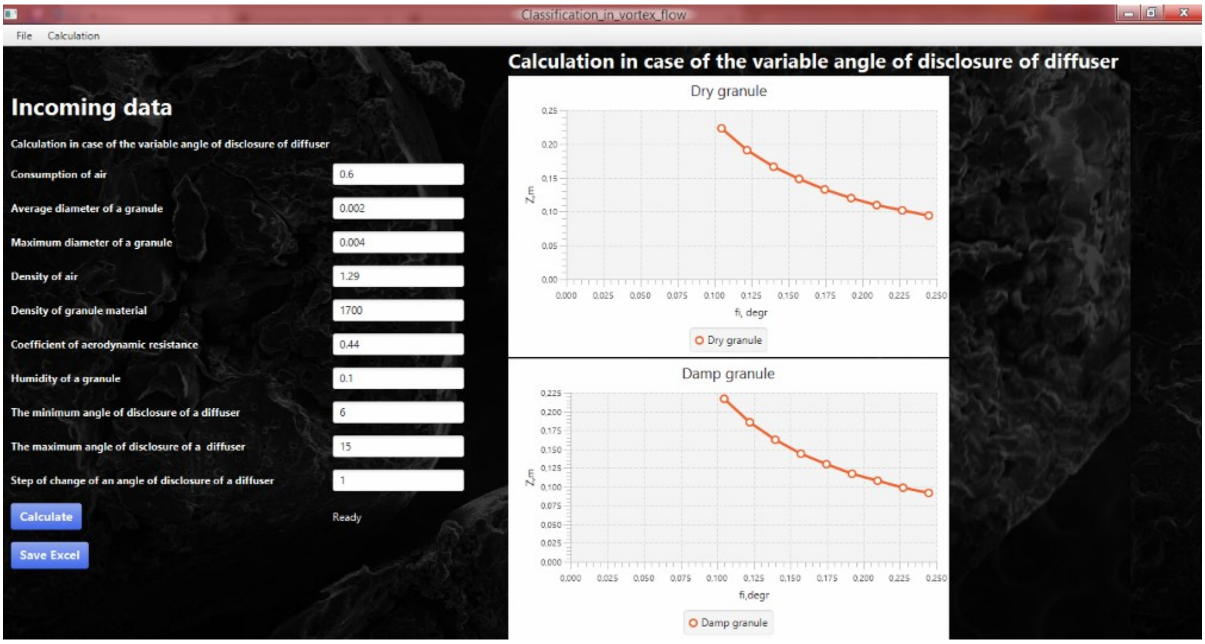


Figure 8. Constructive calculation – stages of the software modeling: calculation of the workspace size and classification processes and granule separation.

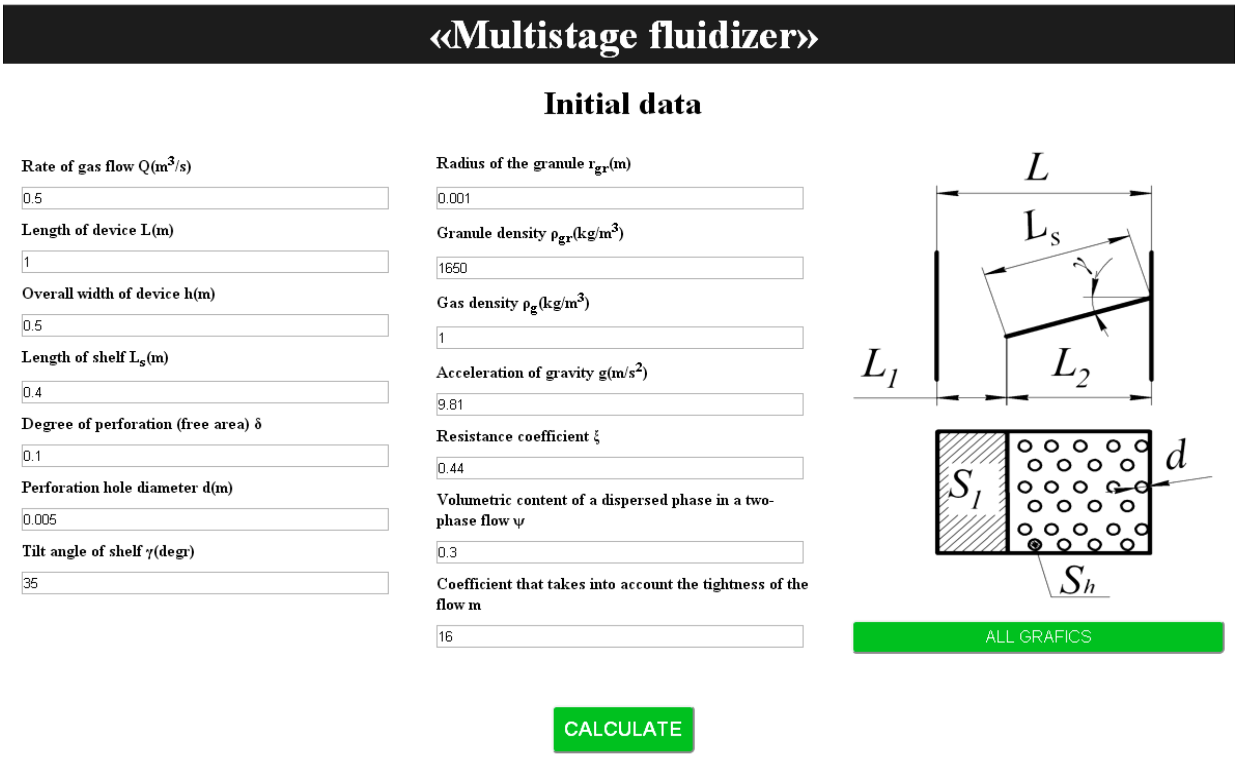


Figure 9. Constructive calculation – stages of the software modeling: calculation of the annular space in the vortex granulator.

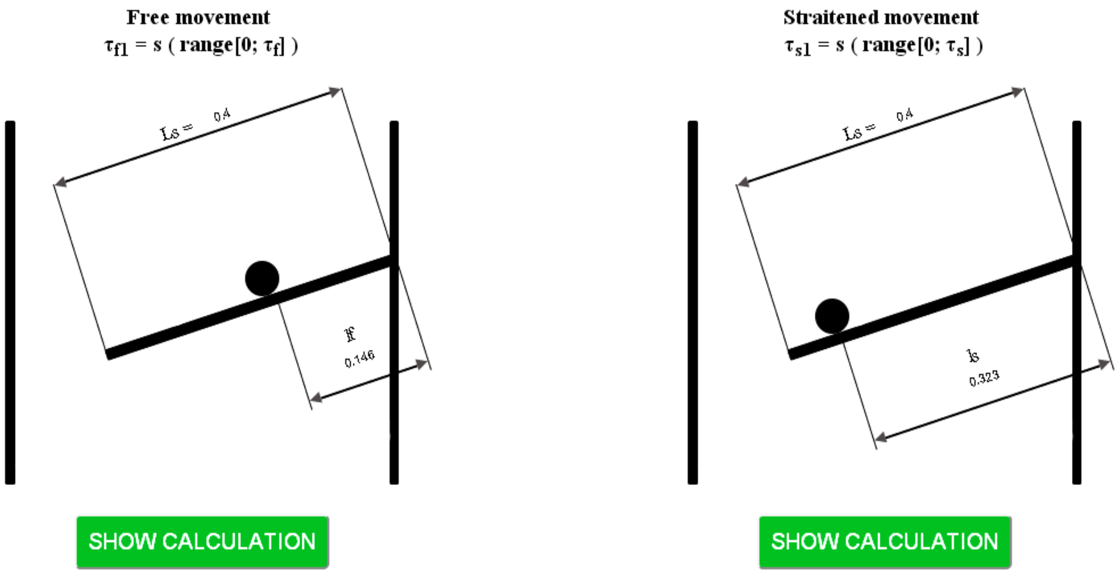


Figure 10. Constructive calculation – stages of the software modeling: calculation of the internal circulation of the seeding agent.

Calculation results are correlated with the data which is obtained by researchers of vortex flow. Comparing the results with the experimental data on the hydrodynamics of the motion of vortex flows in application to the processes of combustion [32], absorption and rectification [33], drying [34], in ejection devices [35], reactors [36, 37] and other processes [38] gives satisfactory convergence.

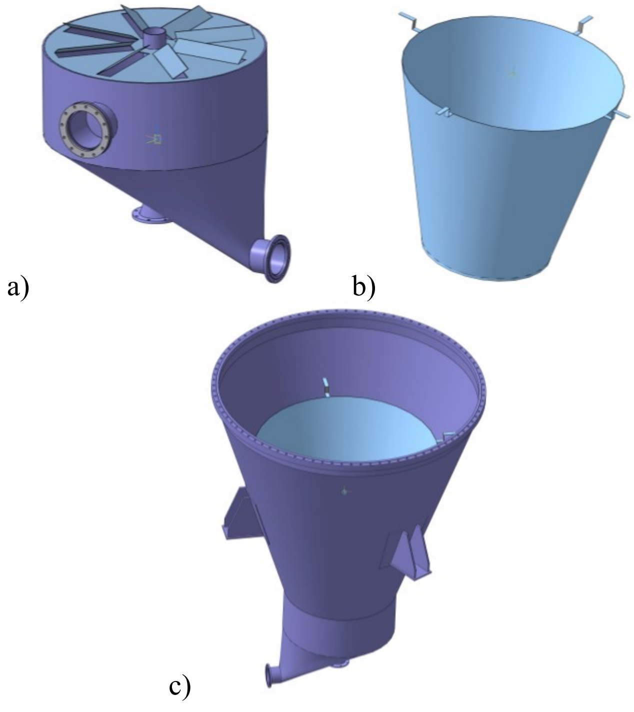


Figure 11. Constructive calculation – formation of the solid-state models of the granulator's units: a – gas-distributing device; b – internal cone; c – the body of the granulator.

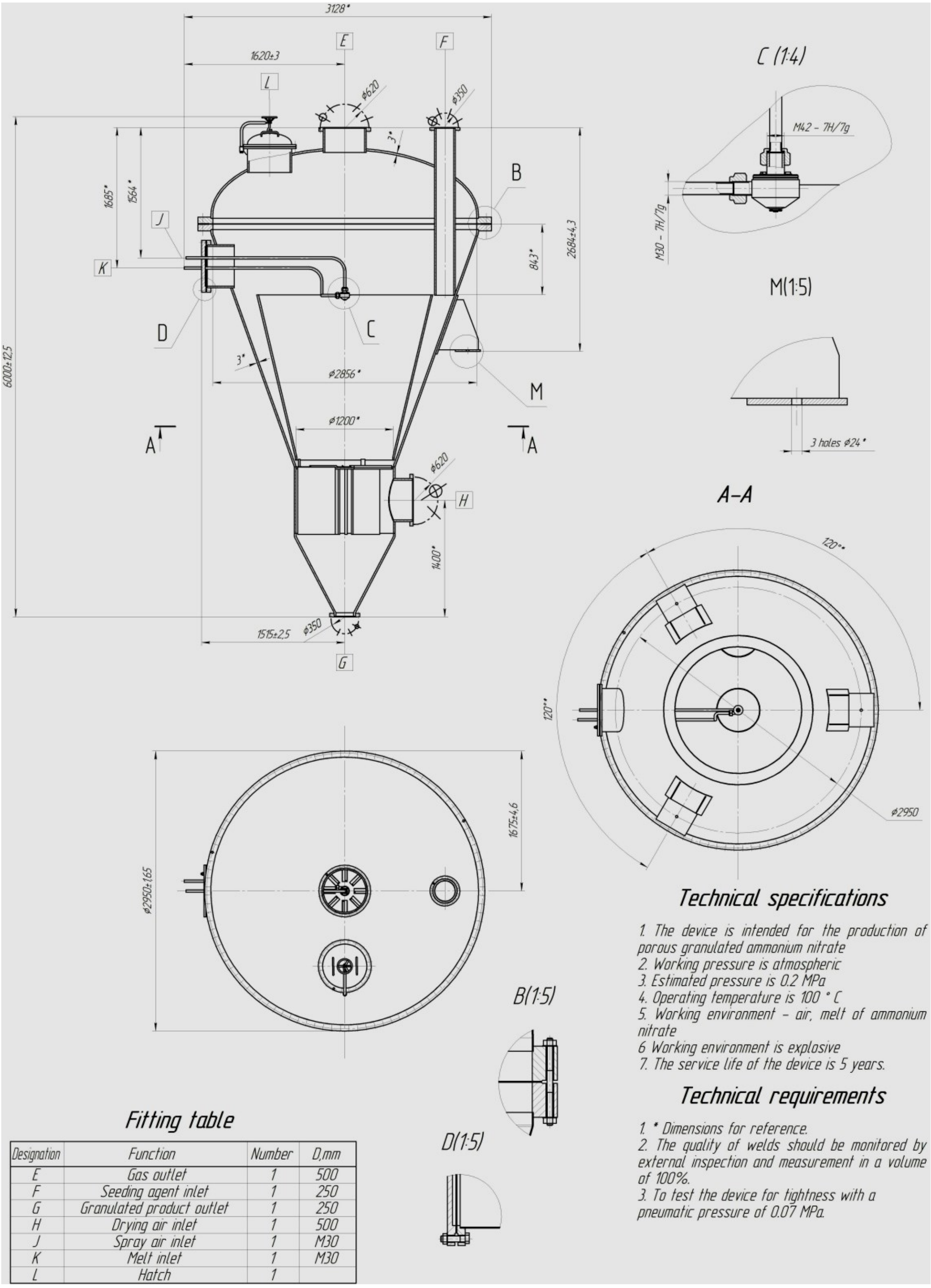
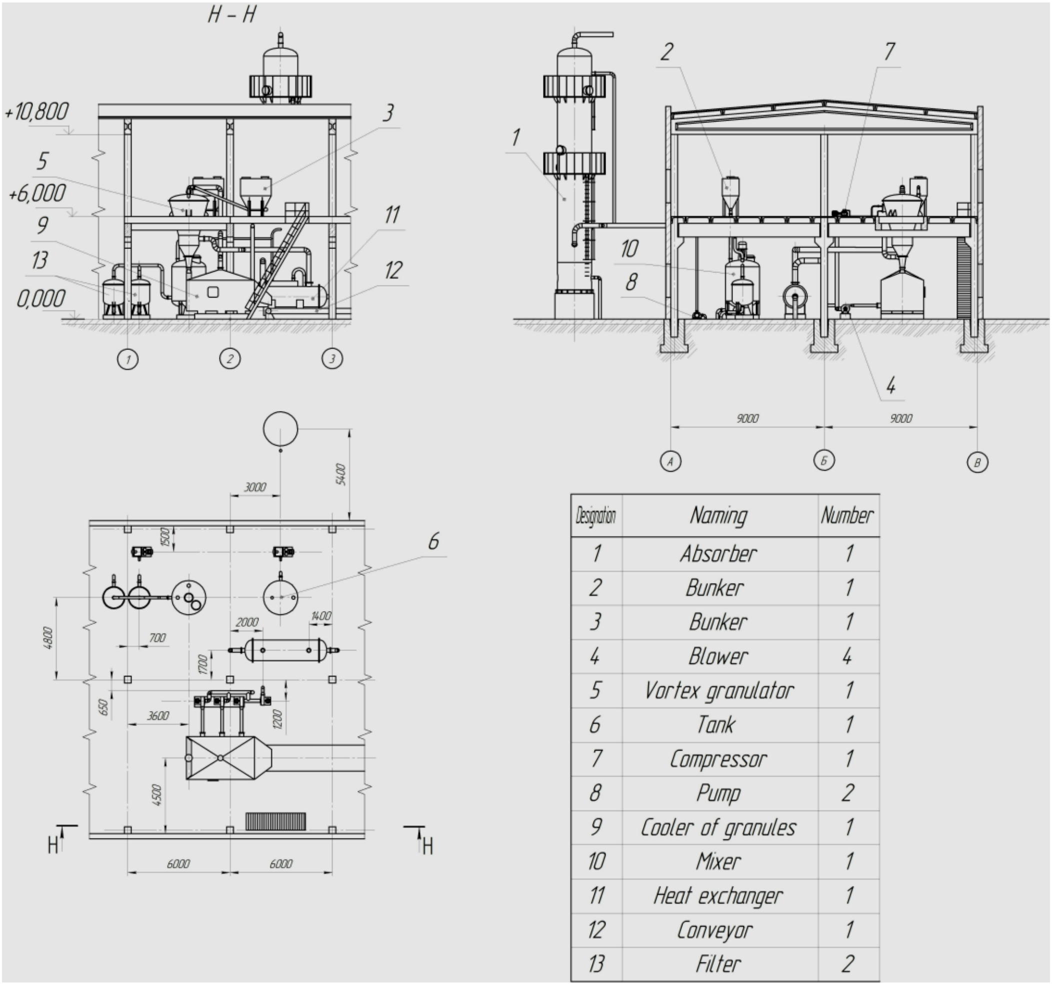


Figure 12. Constructive calculation – the creation of the granulator's solid-state model and obtaining of the working drawings.



Designation	Naming	Number
1	Absorber	1
2	Bunker	1
3	Bunker	1
4	Blower	4
5	Vortex granulator	1
6	Tank	1
7	Compressor	1
8	Pump	2
9	Cooler of granules	1
10	Mixer	1
11	Heat exchanger	1
12	Conveyor	1
13	Filter	2

Figure 13. Constructive calculation – the layout of granulator as a part of the granulation unit.

4. Conclusions and recommendations

For the first time, based on the ecological and economic justification (particularly, SWOT and PESTEL-analysis) of reasonability to introduce new types of the equipment to the granulation unit, the possibility to substitute or to modernize the current units under conditions of the industrial capacity and specific intensity (efficiency) increase at the industrial enterprises, was evaluated.

As a result of the original idea implementation to create compact and mobile granulation plants using technologies that reuse the drying agent potential, the ability to dispose harmful substances and heat and energy recovery, a scientific method has been developed for calculating small-sized and mobile energy-efficient and environmentally friendly modules based on the author's results of theoretical and experimental studies.

The obtained results of the project will enable to solve the following perspective tasks:

- to carry out further development of the convection drying conception in the multistage shelf dryers with heat and energy recovery within the drying unit;
- to study the influence of the shelf contacts construction and method to create various forms of the directional motion of the dispersed phase on the heat transfer processes intensity;
- to define the complex influence of hydro- and thermodynamic conditions to perform the convection drying process on the dehydration process from the dispersed particles with peculiar features (porous ammonium nitrate, capsulated by the organic fertilizer shell etc).

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