Computer Modeling of Hydrodynamic and Heat-Mass Transfer Processes in the Vortex Type Granulation Devices

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Abstract. The article is devoted to the development of software for calculating the hydrodynamic conditions and kinetic characteristics of granulation process in vortex devices. In the basis software Vortex Granulator© and Classification in vortex flow© original mathematical model for calculating the flow rate of gas and granules classification and separation processes of granules in a vortex granulator, kinetics of granules heating and removing moisture from the granules was put. The theoretical model, structure of software and algorithm of their work is shown. In the article an algorithm for calculation of the granulation process in the vortex granulator using the developed software is shown. Software designed in JavaFx platform. Vortex Granulator© and Classification in vortex flow© allow to conduct an optimization calculation of vortex granulator according the criteria of minimum required residence time of granules in device workspace.

Keywords: Software, modeling, vortex granulator, hydrodynamics, kinetics
Key Terms. Development, Software Engineering Process, Information Technology

1 Introduction

A large number of chemical industries use heterogeneous processes, that take place in «gas-liquid-solid» system and have a special place among other processes, because the speed of occurrence is determined by the laws of heat and mass transfer in phases that interact. These processes include various ways of granulation [1-8].

The theoretical basis for modeling of granulation process and development of methods engineering and optimization calculations of granulation equipment is theory and hydrodynamics of heat-mass transfer, that consider the relationship and interdependency between hydrodynamic and heat-mass transfer characteristics of phases in contact with each other.

Among the variety of ways of chemical technology processes intensification working environments flows twisting is one of the simplest and most common ways. This is caused by the fact, that the application of swirling flows leads to improving of heat-mass transfer efficiency and temperature irregularities equalization and flows stabilization [9-15].
Currently the software for the optimization calculation granulation process in vortex devices is not designed. This is explained by the fact that, due to insufficient knowledge of hydrodynamic view of traffic flows and kinetics of granulation in fluidized bed difficulties arise in design of vortex granulators. Vortex granulators in the most cases are patented by industrial enterprises which can conduct experimental research. The theoretical basis for calculation of such devices is limited by basic knowledge of fluid dynamics and heat and mass transfer in a classical fluid bed granulation. Calculation of vortex granulators is based on known algorithms of classical fluidized bed devices. Calculation by these techniques leads to significant error in results. A new software product that will be created is based on the original mathematical model for calculating exactly vortex granulators.
The purpose of the work is a creation of special software for calculating granulators of vortex type. One of the tasks of creating of software for system calculation of hydraulic and thermodynamic conditions for creating granules with porous structure, as well as the calculation of classification process and separation of granules in vortex granulator is to find the optimal programming language. It should allow to quickly calculate the values from the given formulas, it has a set of tools for developing client interface and visualization of values obtained in form of plots. It is also important to search for optimal programming language is the necessity to ensure application performance on different operating systems.

2 Theoretical Basics

Hydrodynamics of gas flow motion
We write the Navier-Stokes equation for the motion of the real gas flow in the diffuser (fig. 1), complementing it with flow continuity equations [16]

$$\left.\begin{aligned} & H_{V_r} - \frac{V_\varphi^2}{r} = F_r - \frac{1}{\rho}\frac{\partial p}{\partial r} + E\left(\Delta v_r - \frac{V_r}{r^2} - \frac{2}{r^2}\frac{\partial V_\varphi}{\partial \varphi}\right), \\ & H_{V_\varphi} + \frac{V_r V_\varphi}{r} = F_\varphi + E\left(\Delta V_\varphi - \frac{V_\varphi}{r^2} + \frac{2}{r^2}\frac{\partial V_r}{\partial \varphi}\right), \\ & H_{V_z} = F_z - \frac{1}{\rho}\frac{\partial p}{\partial z} + E\Delta V_z, \end{aligned}\right\} \tag{1}$$

$$\frac{\partial V_r}{\partial r} + \frac{1}{r}\frac{\partial V_\varphi}{\partial \varphi} + \frac{\partial V_z}{\partial z} + \frac{V_r}{r} = 0, \tag{2}$$

where E – a coefficient of turbulent viscosity according to the Boussinesq hypothesis [17]; H , Δ – differential operators, calculated by dependencies [17]:

$$H = \frac{\partial}{\partial t} + V_r \frac{\partial}{\partial r} + \frac{V_\varphi}{r}\frac{\partial}{\partial \varphi} + V_z \frac{\partial}{\partial z}, \quad (3)$$

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2}. \quad (4)$$

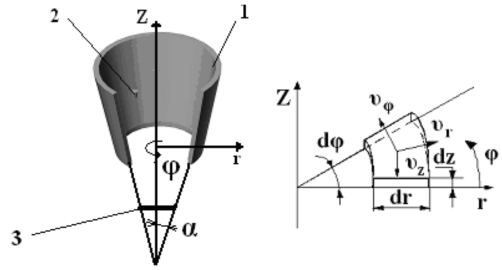

Fig. 1. Scheme of the elementary volume of the gas in the cylindrical coordinate system (r, φ, z): 1 – a workspace of the granulator; 2 – elementary volume of the gas; 3 – gas distribution unit; *dr, dφ, dz* – elementary growth for the corresponding coordinate axes; V_r, V_φ, V_z – radial, circumferential and axial/longitudinal/perpendicular components of the gas rate, respectively; α – half opening angle of the diffuser.

Decision of system (1) - (2) has allowed to determine gas flow velocity components at each point of height and radius of vortex granulator, depending on its workspace design and gas flow rate.

Hydrodynamics of granules motion

Theoretical calculations of components of the granule rate were based on mathematical instrument describing the hydrodynamic characteristics of the granules in the working space of the vortex granulator [18]:

$$\left.\begin{aligned} \frac{dW_r}{d\tau} &= \frac{W_\varphi^2}{r} + \psi \cdot \frac{\pi \cdot \mu_g \cdot d_{gr}}{8 \cdot m}\left(V_r - W_r\right), \\ \frac{dW_\varphi}{d\tau} &= -\frac{W_r W_\varphi}{r} + \psi \cdot \frac{\pi \cdot \mu_g \cdot d_{gr}}{8 \cdot m}\left(V_\varphi - W_\varphi\right), \\ \frac{dW_z}{d\tau} &= -g + \psi \cdot \frac{\pi \cdot \mu_{gs} \cdot d_{gr}}{8 \cdot m}\left(V_z - W_z\right), \end{aligned}\right\} \quad (5)$$

where m – mass of granules, τ – time; r – the current radius of the working space of the vortex granulator; W_r, W_φ, W_z – radial, circumferential and axial/longitudinal/perpendicular components of the velocity of the granules, respectively; g – acceleration of gravity; ψ – linear coefficient of the granule's resistance to the gas flow; μ_g – viscosity of the gas stream; d_{gr} – diameter of the granule.

To determine the granules trajectory in equations (5) we conduct the replacement given that during time τ granule passes a way in radial S_r, circular S_φ and vertical S_z directions

$$\frac{dW_r}{d\tau}=\frac{d^2S_r}{d\tau^2};\ \frac{dW_\varphi}{d\tau}=\frac{d^2S_\varphi}{d\tau^2};\ \frac{dW_z}{d\tau}=\frac{d^2S_z}{d\tau^2}. \qquad (6)$$

Solving system of equations (5) for the variable S in each direction occurs for some granules movement time inside the granulator.

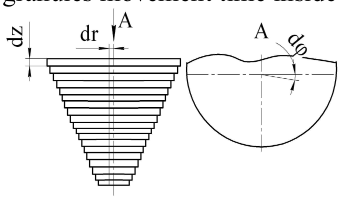

Fig. 2. Design scheme for numerical determination of the trajectory of the granules by the Runge-Kutta method.

With the use of the present system of differential equations of the granule rate in cylindrical coordinates and the numerical solution by the Runge-Kutta method (fig. 2) the trajectories were obtained according to the structure of the vortex granulator and properties of the granules

The solid phase flow, which is modeled with Navier-Stokes equations system (1) and flow continuity equation (2), gives part of amount of motion momentum to the granules. In the case of granules in device working volume appearing it is pulled into rotary motion by the energy of gas flow [19]. This is dispersed phase input to solid will lead to tangible change in value angular velocity component of gas flow. The gas flow circumferential velocity after the interaction with dispersed phase

$$V_\varphi^{'}=V_\varphi-\frac{\rho_{gr}}{\rho_g}\cdot\left(\frac{Q_{gr}}{Q_g}\right)W_\varphi, \qquad (7)$$

where ρ_{gr} – density of granule; ρ_g – density of gas flow; Q_{gr} – granules rate; Q_g – gas flow rate.

Classification and separation of granules

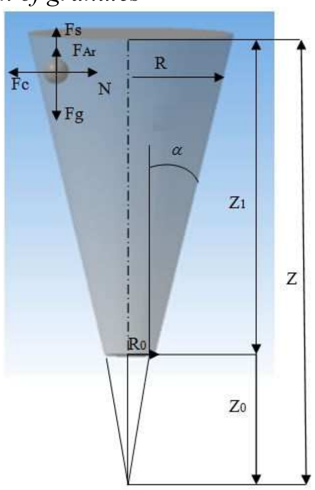

Fig.3. The calculated scheme of working space of the vortex granulator [20]: Z – general height of a cone; Z_0 – installation height of gas distribution device; Z_1 – height of working space of the granulator; R_0 – radius of gas distribution device; R – the radius of the current workspace; F_s – force of aerodynamic resistance; F_c – centrifugal force; F_{Ar} – buoyancy force; F_g – gravitational force; N – response of the wall.

Based on power analysis (fig.3) calculation formulas [20] for the determination of granules classification conditions in the working space of device with a variable cross-sectional area were obtained:

– gas flow velocity that meets the granules equilibrium conditions with size r_{gr} in gas flow

$$V_{op} = 1,63 \cdot \sqrt{\frac{\rho_{gr} \cdot g \cdot r_{gr}}{\psi \cdot \rho_g}}, \tag{8}$$

where r_{gr} - radius of granule.

– current location height of granule with size r_{gr}

$$Z = 1,584 \sqrt{\frac{Q_g}{tg\alpha^2 \cdot \sqrt{\frac{\rho_g \cdot g \cdot r_{gr}}{\psi \cdot \rho_g}}}}. \tag{9}$$

– current height of location of granule with size r_{gr} in case of mass changing (due to humidification and subsequent drying, for example in porous ammonium nitrate production):

$$Z = 1,584 \sqrt{\frac{Q_g}{tg\alpha^2 \cdot \sqrt{\frac{m \cdot (1+U) \cdot g}{\psi \cdot \rho_g \cdot r_{gr}}}}}, \tag{10}$$

where U – moisture content of granule.

– radius of lower cross-section of granulator workspace in condition of location on it granules with maximum size $r_{\max}$ in polydispersed system

$$R_0 = 0,442 \sqrt{\frac{Q_g}{\sqrt{\frac{\rho_{gr} \cdot g \cdot r_{\max}}{\psi \cdot \rho_g}}}}. \tag{11}$$

– heights according to fig. 3

$$Z_1 = Z - Z_0, \tag{12}$$

$$Z_0 = R_0 / tg\alpha. \tag{13}$$

Kinetics of granules heating and dehydration

Distribution of temperature in granule is described by the differential equation [21]:

$$\frac{d}{d\tau}(rT(r,\tau)) = a\left(\frac{d^2}{dr^2}(rT(r,\tau))\right), \tag{3}$$

where r – current value of radius, a – thermal diffusivity coefficient.

Given that U is a function of r and drying time τ, granules mass is determined by dependence

$$Mg_{n=\infty}(\tau)=\frac{4}{3}\rho_g \times$$
$$\times\left(1+\frac{\int_0^R U_{eq}+\left(U_0-U_{eq}\right)\left(\sum_{n=1}^{\infty}\left(\frac{2(\sin(n\pi)-n\pi\cos(n\pi))R\sin\left(\frac{n\pi r}{R}\right)e^{\left(-\frac{n\pi m\tau}{R}\right)}}{(n\pi-\sin(n\pi)\cos(n\pi))rn\pi}\right)\right)dr}{R}\right)\pi R^3 \tag{8}$$

where m – diffusion coefficient; U_0 – granules initial moisture content; U_{eq} – granules moisture content in kinetic equilibrium state.
The law of granules humidity changing in time

$$Us(\tau)=\frac{\int_0^R U_p+(U_0-U_p\left(\frac{2R\sin\left(\frac{\pi r}{R}\right)e^{\left(\frac{-\pi 2m\tau}{R2}\right)}}{\pi r}-\frac{R\sin\left(\frac{2\pi r}{R}\right)e^{\left(\frac{-4\pi 2m\tau}{R2}\right)}}{\pi r}\right))dr}{R} \tag{9}$$

3 Structure of the Software

Vortex Granulator©.
In the program Vortex Granulator© nine classes and one stylesheet were applied.
Program model is presented in form of UML diagrams (fig. 4).
Main.java class is responsible for displaying the main menu and connection to other program files.
Class ControllerInput.java provides input to calculate the gas flow velocity components and the total granules and the rates of these phases.
Class Theory.java presents theoretical information about Vortex granulators, its advantages and disadvantages.
SpeedGas.java and Granuly.java classes are displayed graphically based velocity components (vertical, radial and circumferential) of gas flow and granules.
Class Traektory.java displays the total rate of velocity.
Class Functional.java retains the input values of program and includes methods of forming solutions and data sets to display graphic dependencies.
Classification in vortex flow©.
Program Classification in vortex flow© has seven classes and one stylesheet were applied.
Program model is presented in form of UML diagrams (fig. 5).
Main.java class is responsible for displaying the main menu, and connects to other program files.

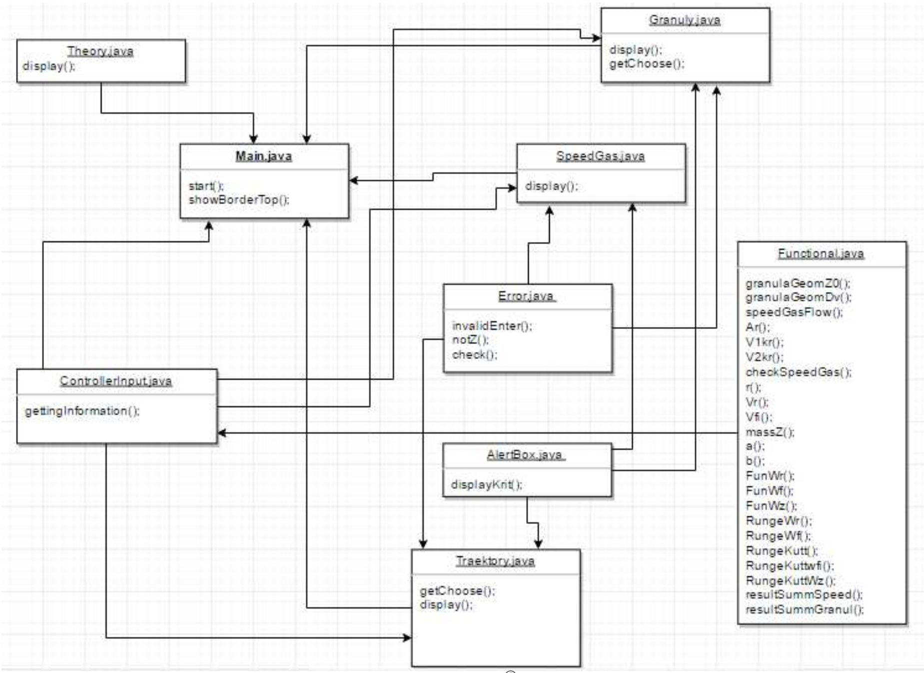

Fig. 4. Vortex Granulator© program model.

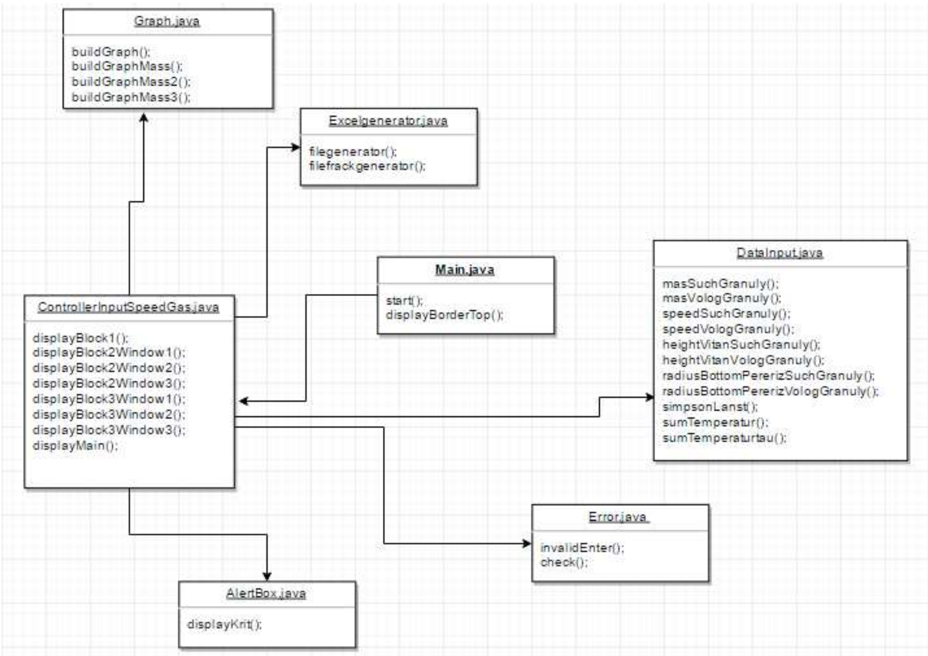

Fig.5. Classification in vortex flow© program model.

4 Software: Algorithm of Operation

Vortex Granulator©.

The main class of Vortex Granulator© program is Main.java which is responsible for displaying the main menu and connection to other classes. Default program after starting first connects class, which is responsible for data entry. After entering the input parameters (fig. 6), the program checks them for validity using Error.java class. If there is an input error, the program calls AlertBox.java class responsible for the output error information. Checked data Functional.java fall into a class that is responsible for the storage and calculation.

Program has three calculation areas: components of velocity of gas flow, components of granules velocity, total velocity of gas flow and granules. When activated menu items the program respectively calculates the radial, vertical, circumferential (circular) components of gas flow rates (fig. 7) and granules (fig. 8).

Class DataInput.java retains the input values, and the program includes methods of forming solutions and data sets to display graphic dependencies.

ControllerInputSpeedGas.java class contains the class for displaying the graphical interface.

Class Graph.java responsible for the output values obtained in the form of plots.

Class Excelgenerator.java generates a document electronically on the obtained values in the table format.

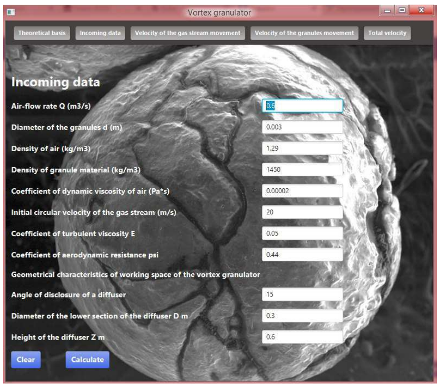

Fig. 6. Incoming data input unit.

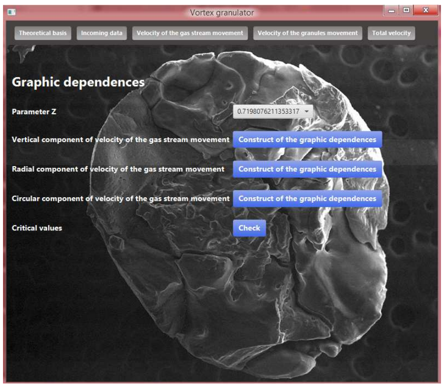

Fig. 7. Window of graphic dependences of gas stream velocity components.

Calculation results can be displayed in the form of graphic dependences.

The main methods of finding the components and the total gas flow velocity and granules are such methods:

• public speedGas - calculates the vertical component of the gas flow rate adjustment workspace of vortex granulator;

• public Vr - calculates the radial component of the gas flow velocity along the radius of vortex granulator ;

• public Vfi - calculates the circumferential component of velocity of gas flow along the radius of vortex granulator;

• public RungeKutt - implementing the Runge-Kutta algorithm for finding the value of the radial component of velocity of granules;

• public Wr - calculates the radial component of velocity of granules along the radius of vortex granulator;
• public RungeKuttWfi - implementing the Runge-Kutta algorithm for finding the value of the circumferential velocity component of granules;
• public Wfi - calculates the circumferential component of granules velocity along the radius of vortex granulator;
• public RungeKuttWz - implementing the Runge-Kutta algorithm for finding the value of the vertical component of velocity of granules;
• public Wz - calculates the vertical component of velocity of granules adjustment vortex granulator workspace;
• public resultSummSpeed - calculates the total gas flow velocity along the radius of vortex granulator;
• public resultSummGranul - calculates the total velocity of granules along the radius of vortex granulator.

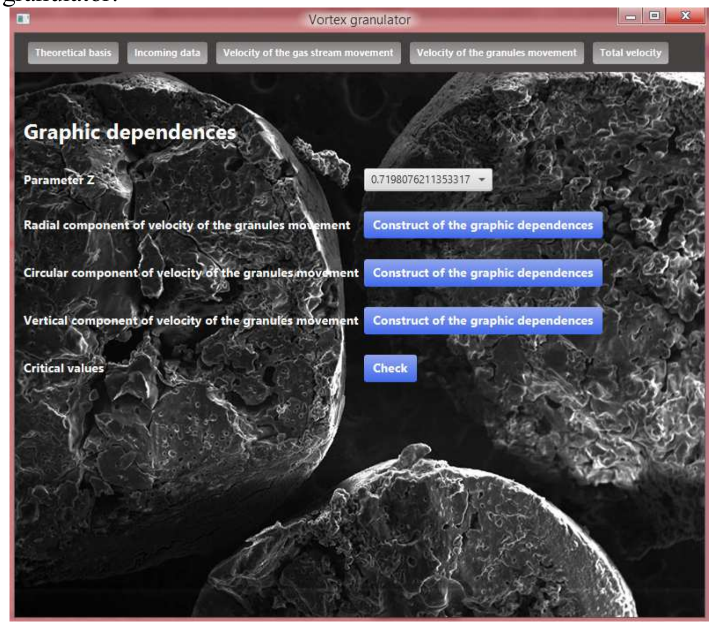

Fig. 8. Window of graphic dependences of granules velocity components.

Classification in vortex flow©

The main class of program Classification in vortex flow© Main.java is class that is responsible for displaying the main menu and connect to it other classes. After starting, the program displays the model and the general parameters of granulator.

The program has three calculation areas:

1. The gas flow speed (fig.9).
2. The geometry of workspace:

• calculation with a variable air flow - are displayed depending on the height of working space and the radius of cross section of air flow to dry and wet granules (fig.10);
• calculation at a variable angle diffuser disclosure - are displayed depending on height of working space from the diffuser opening angle for dry and wet granules (fig.11);

• calculation of the distribution of granules on fractions in working space of granulator - shows the distribution of granules of different diameters at the height of working space of vortex granulator (fig.12).

3. Calculation of mass and kinetics of granules heating:

• calculation of granules mass (fig.13);

• calculation of kinetics of granules heating (distribution of temperature according to granules radius);

• calculation of kinetics of granules heating (granule temperature change in time).

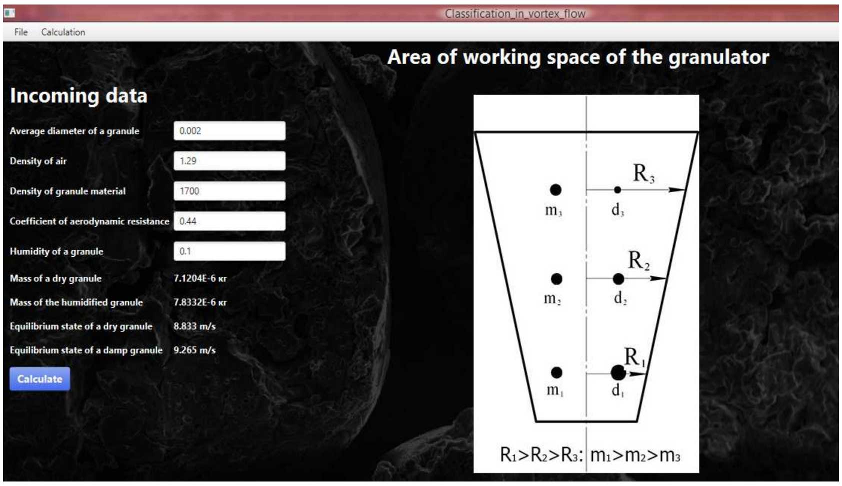

Fig. 9. Incoming data input window. Velocity of gas stream.

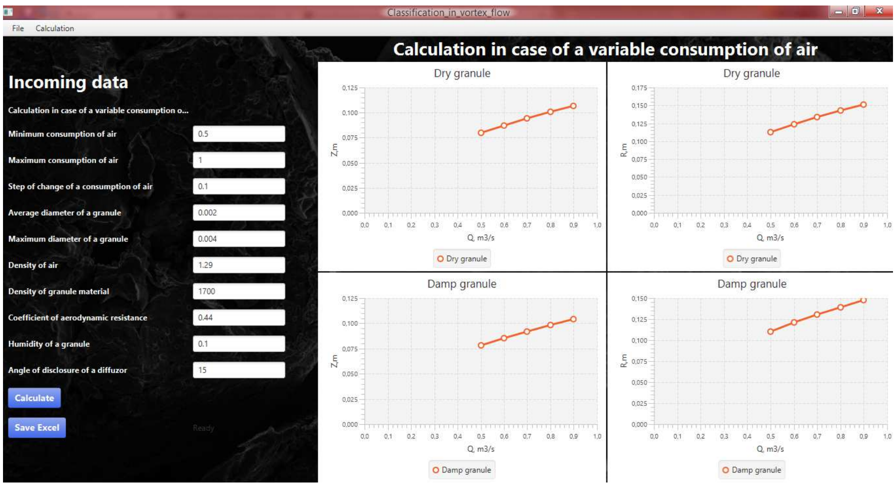

Fig.10. Calculation of geometry of working space of vortex granulator at a variable consumption of air.

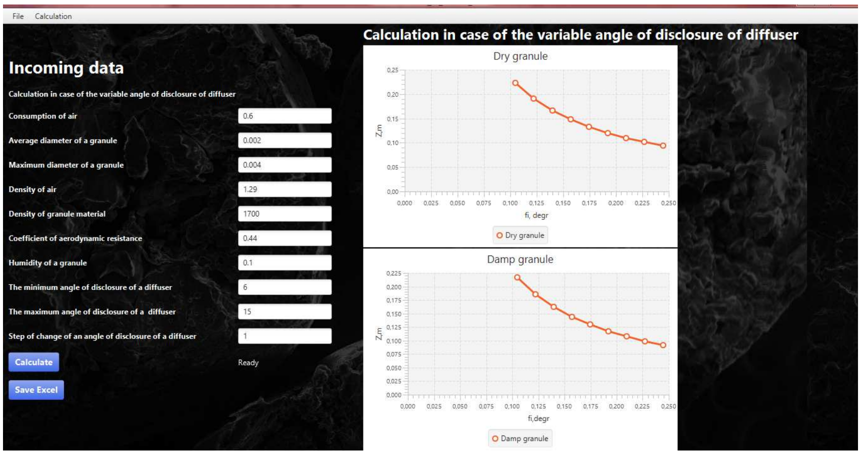

Fig.11. Calculation of geometry of working space of vortex granulator at a variable angle of disclosure of diffuser.

For calculation of the appropriate values, it is necessary to select a specific item, enter data and press the "Calculate" button. The program will check the correctness of the data, and then calculate the corresponding values and visualizes the values obtained in form of plots. The program Classification in vortex flow© has the ability to save the results in a spreadsheet format.

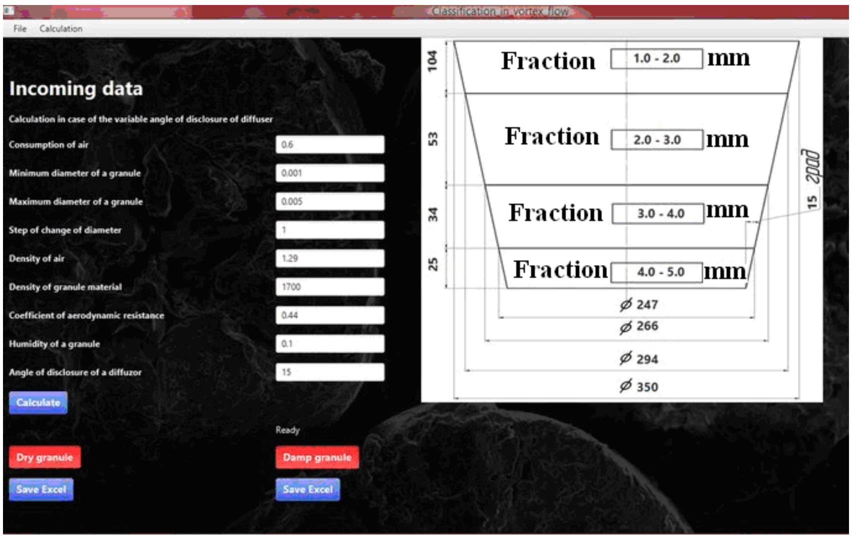

Fig.12. Calculation of distribution of granules on fractions in working space of granulator.

The main methods of calculation are follows:

- public double masSuchGranuly - calculates the weight of dry granules;
- public double masVologGranuly - calculates the weight of wet granules;
- public double speedSuchGranuly - calculates the speed of dry granules;
- public double speedVologGranuly - calculates the speed of wet granules;

• public double heightVitanSuchGranuly - calculates the height of the flight of dry granules;
• public double heightVitanVologGranuly - calculates the altitude moist granules;
• public double radiusBottomPererizSuchGranuly - calculates the radius of bottom section of granulator for dry granules;
• public double radiusBottomPererizVologGranuly - calculates the radius of lower section of granulator for wet granules;
• public double simpsonLanst - implements Simpson algorithm and is designed to calculate integrals;
• public double sumTemperatur - calculates the kinetics of granules heating (granules temperature distribution along the radius);
• public double sumTemperaturtau - calculates the kinetics of heating of granules (granules change over time temperature).

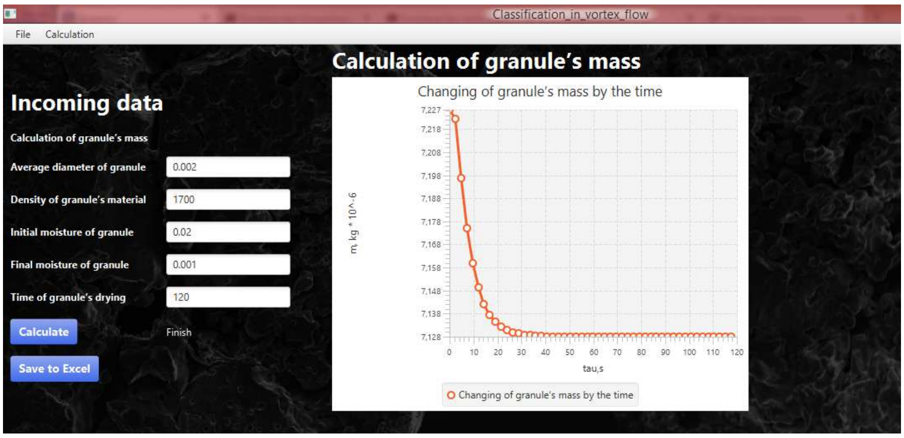

Fig.13. Calculation of granule's mass.

5 Conclusions

Creating of programs Vortex Granulator© and Classification in vortex flow© based on the author's mathematical model is a new stage in the construction of design algorithm of vortex granulator "theoretical calculation - industrial design".
The use of these programs allows for a rational choice configuration workspace vortex granulator. Automation of hydrodynamic and thermodynamic calculation of vortex granulator allows to conduct multivariate experiment without the use of experimental and industrial installations. Such an approach in modeling the vortex granulator is cost-effective since equipment design optimization calculation is carried out on the stage before the stage of pilot implementation in production. Thus, proposed software allows to quickly calculate the hydro- and thermodynamic conditions for creating granules of porous structure, as well as the calculation of classification and separation process of granules in a vortex granulator with results visualization.

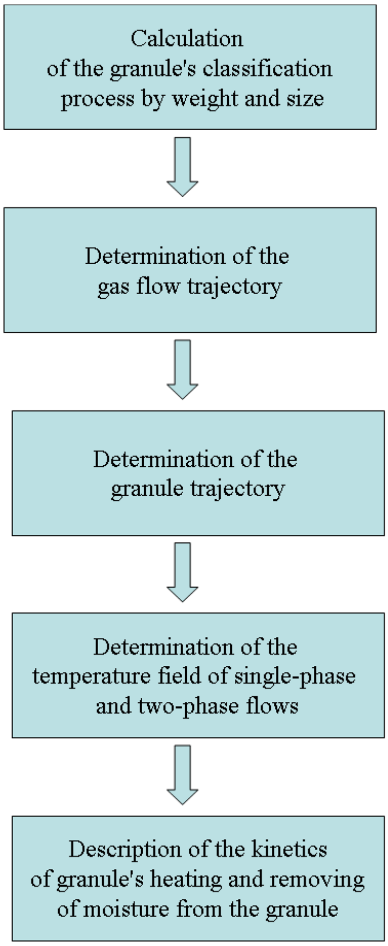

Fig.14. Algorithm of calculation of process of receiving porous surface layer on granule of ammonium nitrate.

Algorithm of vortex granulator engineering calculation consists of separate blocks that are logically connected to each other (fig. 14). The feature of algorithm is presence of optimization calculation block with selection of optimal hydrodynamic vortex granulator working conditions, that make possible to remove moisture from the granules for the minimum required time. In order to automate the calculations and facilitate optimization calculation each blocks of algorithm is implemented in copyright software products. Software products have the function of the output of research results as files *.xls for further transfer to the program of creation of design and technological documentation.

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