The Simulation of Alumina Feed in the Reactor of Dry Gas Treatment Plant

Vyacheslav G. Grigoriev[1], Sergey V. Tepikin[2], Yaroslav A. Tretyakov[3], Aleksey V. Knizhnik[4] and Yuriy V. Zhiltsov[5]
1. CEO
2. Chief Technical Officer
SibVAMI JSC, Irkutsk, Russia
3. Head of the Mathematical Simulation and Measurement Department
RUSAL ETC LLC, Krasnoyarsk, Russia
4. Head of the Technical Department
5. Lead Engineer of the Technical Department
SibVAMI JSC, Irkutsk, Russia
Corresponding author: Aleksey.Knizhnik@rusal.com

Abstract

The specialists of SibVAMI at UC RUSAL have developed a modern technology for the dry treatment of waste gases from the production of aluminium by electrolysis. This technology is complex and includes various processes and technical solutions. Today, the dry gas treatment plants (DGTP) designed by UC RUSAL are successfully operated at the Irkutsk and Bratsk aluminium smelters.

The gases treated at the DGTP of UC RUSAL comply with environmental requirements. At the same time, given the complexity and diversity of the processes within the DGTP, there remains the opportunity for the further enhancement of the individual process solutions and further improvement of its economic and technological efficiency. One of the units successfully functioning today, but having the potential for additional optimisation, is the alumina feed unit to the DGTP reactor. The design of this unit affects the uniform distribution of alumina in the gas flow.

In order to optimise the design of the alumina feed unit for the DGTP reactor, the ability to reliably simulate the alumina feed process into the gas flow is necessary. The aim of this paper is to select a computational model for this process. The paper compares the results obtained using the Euler-Euler medium interaction model and the Euler-Lagrange model in the ANSYS CFX software package. The paper analyses the compliance of the calculated models of the motion of solid particles in gases with the experimental patterns of the motion of solid particles. As a result, it was proposed to use the Euler-Euler model to simulate a unit for alumina feed into the gas flow

Key words: Alumina feed reactor, dispersed system, particle, Euler-Euler model, Euler-Lagrange model.

1. Introduction

The improvement of mathematical simulation tools of hydrodynamic processes in dispersed systems is triggered by the need for a detailed study of the physical processes that occur in dry gas treatment plants (DGTP). DGTP plants are used for the purification of process waste gases from the production of aluminium by electrolysis. The purification of gases in DGTP is carried out by the adsorption process, the intensity of the adsorption depends on the distribution of the adsorbent (alumina particles) in the gas flow. The introduction of alumina into the gas flow is carried out through a nozzle installed in the neck of the reactor. The design of the nozzle affects the uniformity of the alumina distribution in the gas flow.

The aim of this work is to develop a computational model that will reliably predict the effect of the structure on the distribution of alumina in the flow in the DGTP.

Our paper focuses on a three-dimensional (3D) stationary mathematical model, making it possible to carry out the computational analysis of the movement of alumina particles from the reactor to the tilting chamber of the DGTP. The paper compares the results obtained using either the **Euler-Euler model** of media interaction or the **Euler-Lagrange model**. To solve the problem, the CFD (Computational fluid dynamics) ANSYS CFX software package has been employed, which allows simulating dispersed systems.

The layout of the studied computational model is shown in Figure 1.

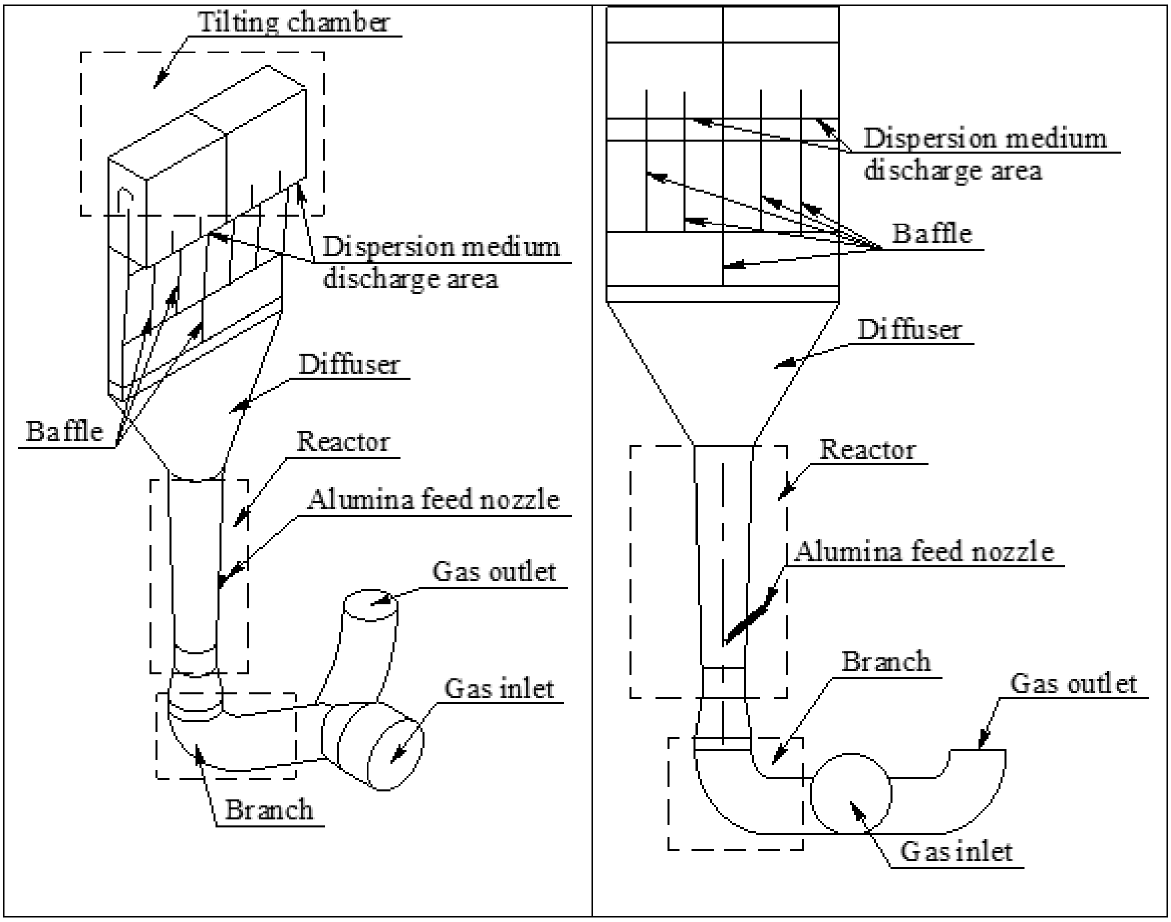


Figure 1. Layout of the studied computational model.

2. Setting Up the CFD Software

Modern CFD software makes it possible to use several mathematical models to simulate the motion of the solid particles in a gas flow. Such models describe the various effects and processes occurring during the motion of a two-phase medium:

- Particle distribution in the flow (media interaction model);
- Accounting for particle resistance (model of the exchange of momentum between the particle and the gas medium);
- The motion of the gaseous phase, taking into account turbulence (model of the motion of the gaseous medium).

The first step in the simulation of the DGTP is the correct choice of these models. In particular, it is important to choose a media interaction model.

2.1. Media Interaction Model

In the computational model, the dispersed system consists of two phases: gas and solid particles. A simulation of the dispersed system in ANSYS CFX is performed according to the block diagram shown in Figure 2 [1].

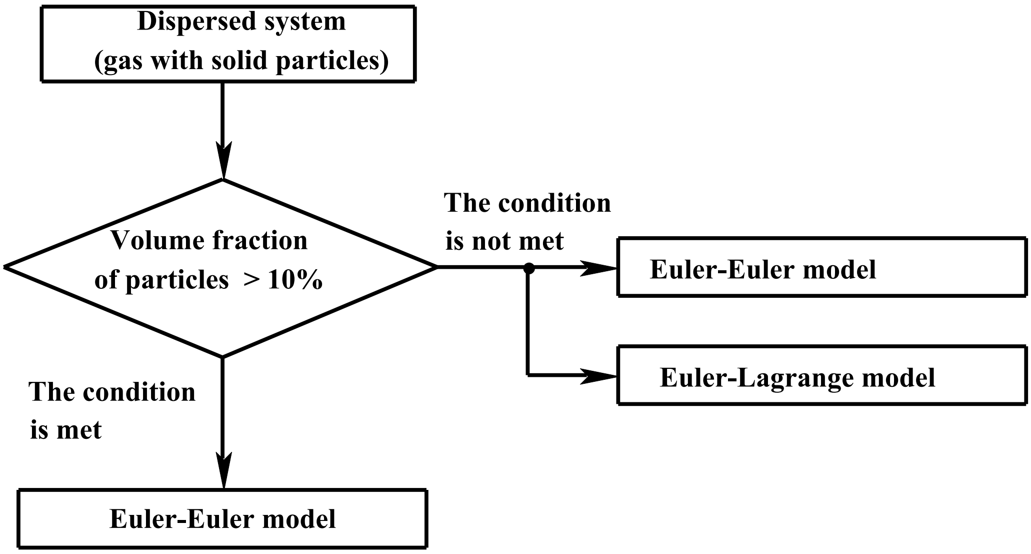


Figure 2. Block diagram of the calculation of the dispersed system in ANSYS CFX.

From the block diagram above, it can be seen that the dispersed system can be calculated using two models of interaction between the different media:

- Euler-Euler model:
    - The phases are regarded as interpenetrating continuums. The interaction of media through pressure and interphase exchange coefficients is calculated, taking into account the calculation of Euler variables [4];
- Euler-Lagrange model:
    - The gaseous medium is defined similarly to the Euler-Euler model. The solid particles are represented as point masses which move in the gaseous medium, taking into account the calculation of Lagrange variables. This model is recommended for use in calculations where the content of the volume fraction of solid particles in the gas medium varies from 0 to 10 % [4].

In DGTP, the volume fraction of alumina at the outlet of the alumina feed nozzle exceeds 10 % (and, therefore, the Euler-Euler model should be used). In the reactor and filter, the volume fraction of alumina is reduced (and, therefore, either model could be used). The main objective of this work is to determine which mathematical description gives more reliable results when combining the alumina feed nozzle and the reactor in only one domain.

2.2. Model of the Exchange of Momentum Between Particles and Gas Medium

The choice of other computational models in the DGTP simulation is simpler, but no less important. The Schiller-Naumann model should be used to describe the exchange of the quantity of motion between the particle and the gas medium [2]. According to the model, the drag coefficient, C_D, [-], of particles is described as a function of the particle's Reynolds number [1]:

$$C_D = \frac{24}{Re} \cdot (1 + 0.15 \cdot Re^{0.687}) \tag{1}$$

$$Re = \frac{\rho_\alpha \cdot |U_\beta - U_\alpha| \cdot d_\beta}{\mu_\alpha} \tag{2}$$

where:

ρ_α	Gas density, kg/m^3
U_α	Gas velocity, m/s
U_β	Particle velocity, m/s
μ_α	Dynamic viscosity of gas, Pas
d_β	Particle diameter, m.

2.3. Model of the Motion of the Gas Medium

The motion of solid particles can be traced taking into the account the turbulence of the gaseous phase. In order to accomplish such a task, RNG (re-normalisation group) version of the k-ε model is used. Of all the turbulence models available in CFX, it is the most suitable one for simulating flow with highly curved particle trajectories [3].

2.4. Boundary and Initial Conditions

The set of boundary conditions shown in Figure 1 consists of:

- Branches and gas duct at the base of the calculated geometry:
    - The elongation of the duct at the Inlet and the addition of whole bag filter to the model do not significantly affect the distribution of gases in the reactor, according to preliminary results obtained during the early stages of work while ignoring the motion of particles. This allowed for the gas Inlet and Outlet ducts to be modeled without observing the traditional 1:10 diameter-to-length ratio enabling the fully development of the flow for the application of boundary conditions;
- Reactor and alumina feed nozzle;
- Diffuser (the element connecting the reactor to the DGTP housing);
- Baffles;
- Tilting chamber.

The input parameters for the dispersion medium are shown in Table 1.

Table 1. Input parameters of the dispersion medium.

Parameter description	Value and unit
Temperature of the gas mixture	130 °C
Flow rate of the gas mixture entering the DGTP	65 000 m^3/h
Mass flow rate of the alumina entering the DGTP	6 000 kg/h

2.5. Computational Grid

The computational domain is a segment of the DGTP design under consideration. On the basis of a preliminary analysis of convergence, a discrete mathematical model was constructed (Figure 3) consisting of 5 755 000 tetrahedral control volumes. The size of the control volumes in the near-wall layers was set taking into account the criterion y^+, which must satisfy the condition $30 < y^+ < 300$, as the gas mixture moves in a highly developed turbulent flow.

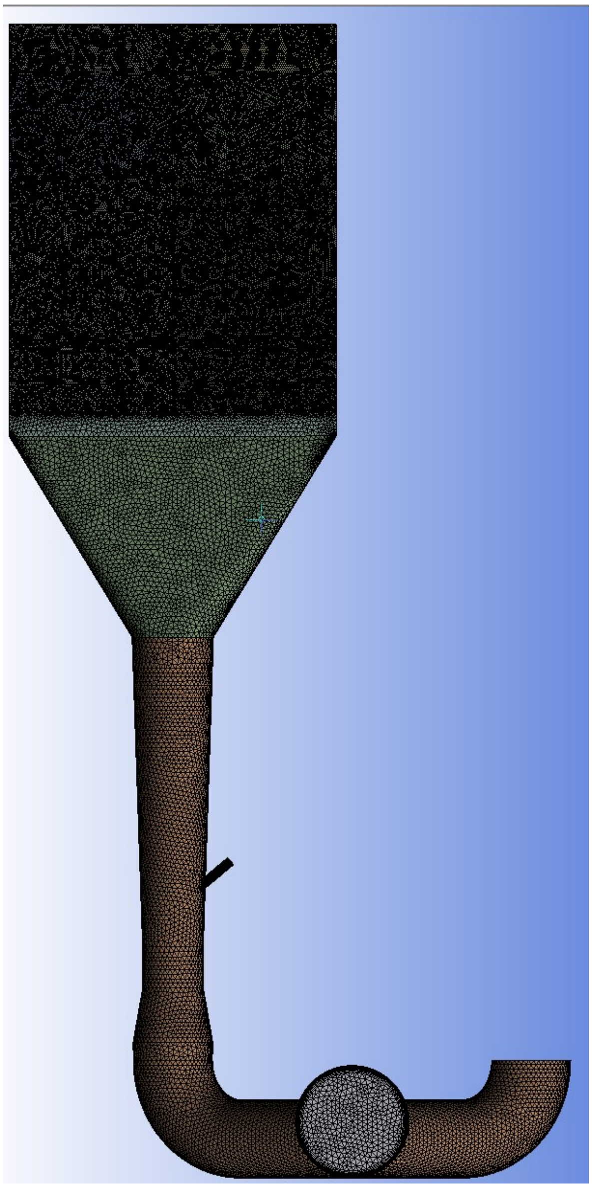


Figure 3. Fragment of the computational grid of the DGTP model.

2.6. Conducting a Numerical Analysis

Before starting the calculation, some settings were specified to control the numerical solution scheme:

- First order advection scheme (HighResolution):
    - The advantage of this scheme is its stability and good rate of convergence;

- The time scale was set by a piecewise linear function, which gradually decreases while the iteration number increases – refer to Table 2:
    - This approach was employed due to a significant difference in the scale of the simulated processes in the different components of the DGTP. The large scale at the beginning of the solution helps to accelerate the convergence of the equations.

Table 2. Used timescales.

Iteration number	0 - 100	100 - 200	200 - 300	300 - 400	400 - 500
Timescale, (s)	0.15	0.10	0.08	0.06	0.04

The system of equations was solved iteratively. The magnitudes of the calculated variables in each control volume were changed from a certain initial distribution (based on the given initial conditions) to the converged solution

In the course of the solution process, two main indicators of the convergence level were monitored, namely:

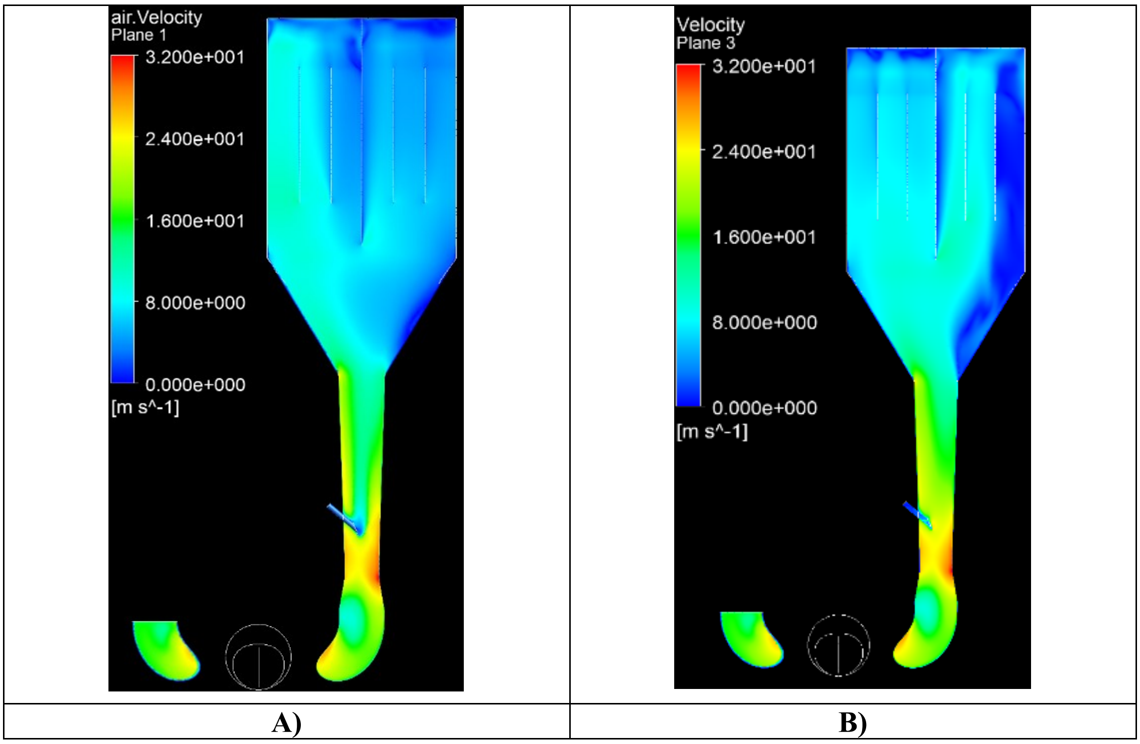
- The RMS residuals of the calculated variables;
- The global imbalances of the calculated variables.

The solution process was stopped when all the indicators met the convergence criteria (residuals < 10^{-3}… 10^{-5}, imbalances < 1 %, the target parameters do not change during the last 100 iterations by more than 1 %).

3. Calculation Results

As a result of the calculations, the velocities of the motion of the media, the flow lines of the motion of the gas medium and the changes in the volume fractions of the solid particles in the computational model were determined. The colour maps of the gas mixture velocity distribution in a cross-section of the computational geometry for two media interaction models are shown in Figure 4.

As can be seen from the color map of the gas mixture velocity distribution for the **Euler-Euler model**, the alumina particles in the area of the alumina feed nozzle have a disturbing effect on the gas medium. Such an effect is absent in the **Euler-Lagrange** media interaction model, which leads to significant differences in the distribution of gas flows in the models under consideration.

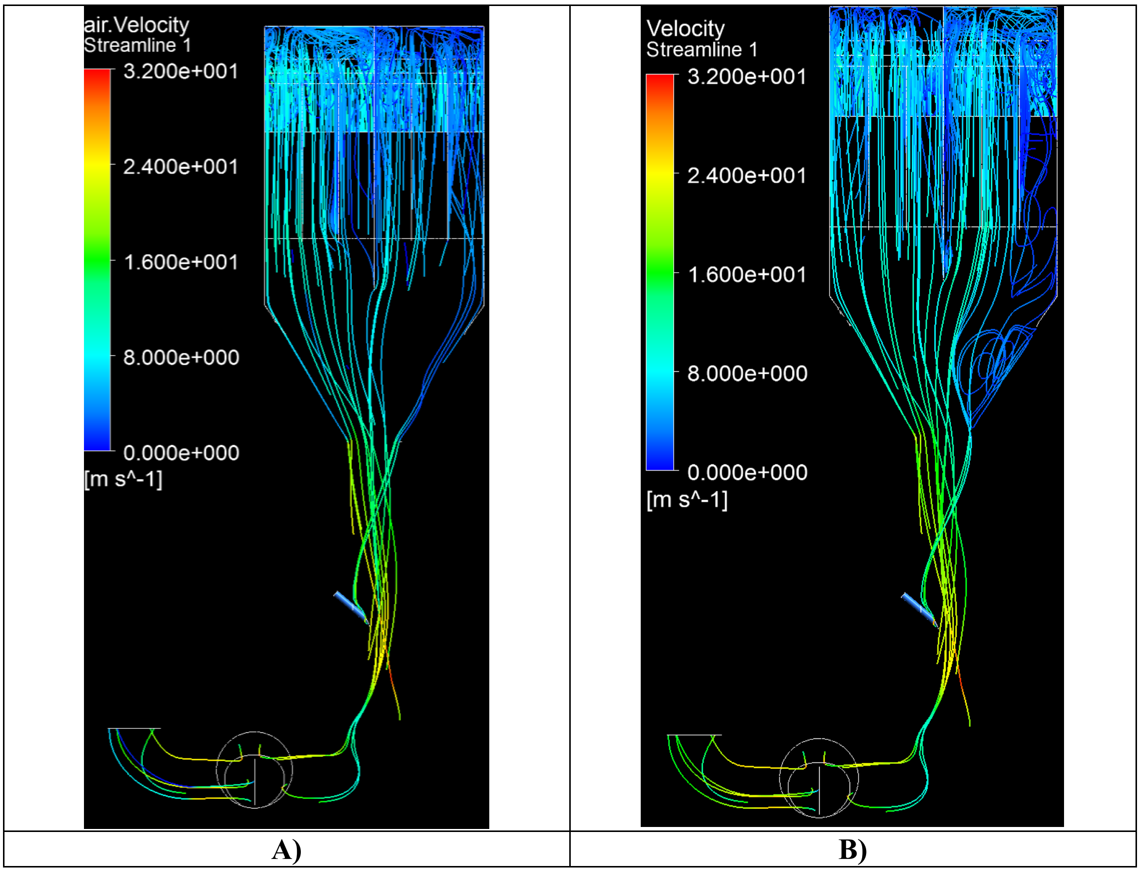


A) **B)**

Figure 4. Magnitude of the gas mixture velocity distribution computed with A) Euler-Euler model and B) Euler-Lagrange model.

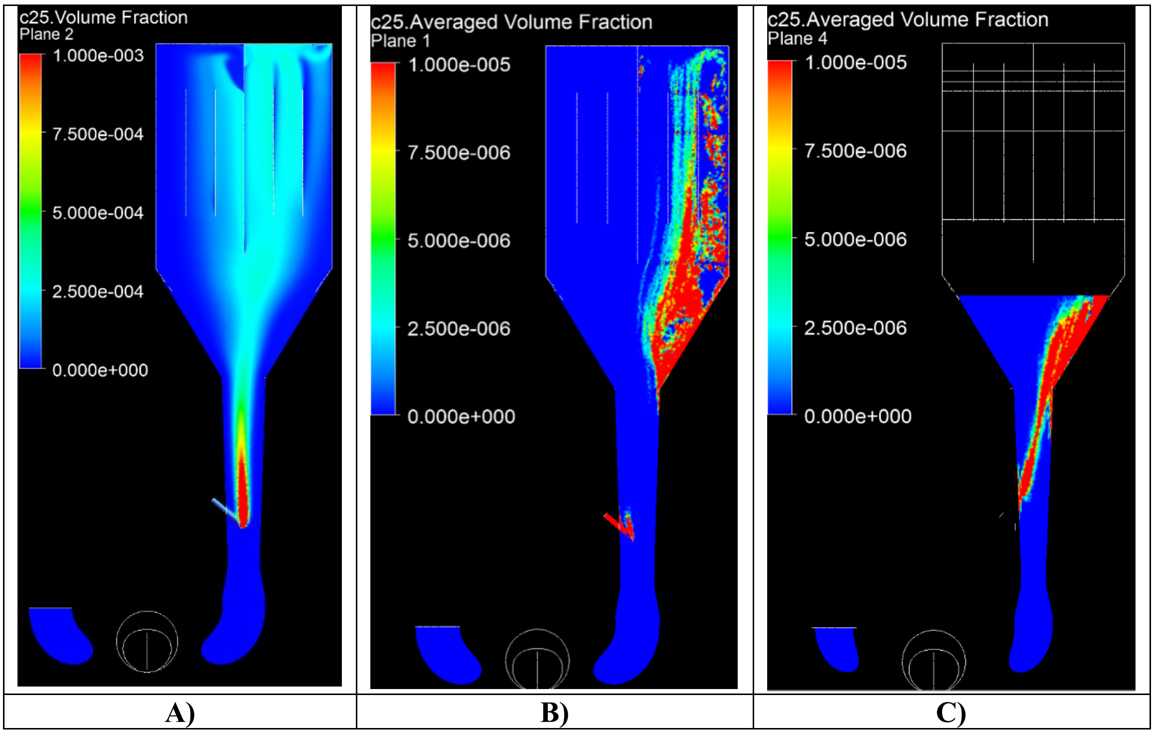
Figure 5 shows the stream line velocity maps for the gas medium in a cross-section of the computational domain. It can be observed that, in the vicinity of alumina feed nozzle, the flow is directed to the right corner of the diffuser. In the area where the diffuser is located, the streamlines show that the vorticity densities in the **Euler-Lagrange model** and the **Euler-Euler model** differ significantly. It has to be stressed that the **Euler-Euler model** takes into the account the influence of particles on the gas flow in the area of the alumina feed nozzle and, therefore, it is considered as the most suitable option.

Figure 6 shows volume fraction of solid particles in a cross-section of the computational domain, where it can be seen that the volume fraction of particles in the outlet area of the alumina feed nozzle is above 10 % thus suggesting that the **Euler-Euler** model should be considered – refer to aforementioned block diagram in Figure 2. The particles in the **Euler-Lagrange** media interaction model do not disturb the gas flow, and, as a result, fall into a region where the gas flow lines are directed into the right corner of the diffuser. Consequently, the patterns of particle distribution in each of the models under consideration differ from each other.



A) **B)**

Figure 5. Gas streamlines computed with A) Euler-Euler model and B) Euler-Lagrange model.



A) **B)** **C)**

Figure 6. Volume fraction of solid particles computed with A) Euler-Euler model, and B) and C) Euler-Lagrange model in two different planes.

Figure 7 shows the distribution of solid particles at the alumina feed nozzle outlet in an operating 'dry' gas treatment plant. Upon comparison of this image with the colour maps in Figure 6, it was found that the **Euler-Lagrange** media interaction model yields an unreliable distribution of solid particles in the area of the alumina feed **nozzle**.

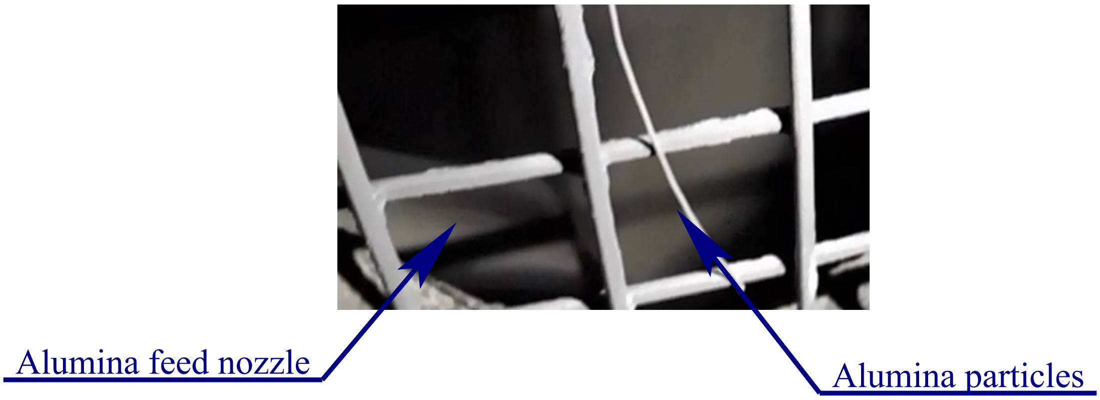


Figure 7. Distribution of solid particles at the outlet of the alumina feed nozzle in an operating DGTP.

4. Conclusions

The developed mathematical model makes it possible to estimate at the design stage the local disturbances associated with the distribution of smelter-grade alumina in the flow in the DGTP. Moreover, the study of the media interaction models has made it possible to establish that the use of the **Euler-Euler model** allows for the qualitative prediction the distribution of solid particles in the area of the alumina feed nozzle while the **Euler-Lagrange model** does not yield a reliable alumina distribution of alumina in this particular region – refer to Figure 6-B).
Since ANSYS-CFX supports only two media interaction models, it is clear that, in the future, SibVAMI JSC and RUSAL ETC LLC will use the **Euler-Euler model** of media interaction when performing computational work on DGTP simulation.

5. References

1. Manual ANSYS CFX-Solver Modeling Guide. ANSYS CFX Release 14.5. – Canonsburg: ANSYS, Inc., 2013.
2. M.S. Selim, A.C. Kothari, R.M. Turian, Sedimentation of multisized particles in concentrated suspensions, *AlChE Journal*, Vol. 29, No. 6, November 1983, 1029-1038.
3. Robert W Lyczkowski, Jacques X. Bouillard, State-of-the-art review of erosion modeling in fluid/solid systems, *Progress in Energy and Combustion Science,* 28, Issue 6, 2002, 543-602.
4. P.V. Kondrashov, Mathematical modeling of gas dynamics of powder jet in the implementation of technology «Rapid prototyping», *East European Advanced Technology Journal*, 5/7 (65) 2013.