

# Granular flow in static mixers by coupled DEM/CFD approach

Lato Pezo<sup>1</sup>, Milada Pezo<sup>2</sup>, Aca Jovanović<sup>1</sup>, Nenad Kosanić<sup>3</sup>, Aleksandar Petrović<sup>3</sup>, Ljubinko Lević<sup>4</sup>

<sup>1</sup>University of Belgrade, Institute of General and Physical Chemistry, Belgrade, Serbia

<sup>2</sup>University of Belgrade, Laboratory for Thermal Engineering and Energy, Institute of Nuclear Sciences "Vinča", Belgrade, Serbia

<sup>3</sup>University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia

<sup>4</sup>University of Novi Sad, Faculty of Technology, Novi Sad, Serbia

## Abstract

The mixing process greatly influences the mixing efficiency, as well as the quality and the price of the intermediate and/or the final product. Static mixer is used for premixing action before the main mixing process, for significant reduction of mixing time and energy consumption. This type of premixing action is not investigated in detail in the open literature. In this article, the novel numerical approach called Discrete Element Method is used for modelling of granular flow in multiple static mixer applications (1–3 Komax or Ross mixing elements were utilized), while the Computational Fluid Dynamic Method was chosen for fluid flow modelling, using the Eulerian multiphase model. The main aim of this article is to predict the behavior of granules being gravitationally transported in different mixer configuration and to choose the best configuration of the mixer taking into account the total particle path, the number of mixing elements and the quality of the obtained mixture. The results of the numerical simulations in the static mixers were compared to experimental results, the mixing quality is examined by *RSD* (relative standard deviation) criterion, and the effects on the mixer type and the number of mixing elements on mixing process were studied. The effects of the mixer type and the number of mixing elements on mixing process were studied using analysis of variance (ANOVA). Mathematical modelling is used for optimization of number of Ross and Komax segments in mixer in order to gain desirable mixing results.

**Keywords:** DEM/CFD, prediction, static mixer, Komax, Ross, particle tracking.

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Static mixers are low energy consuming equipment (due to the gravitational flow of the material) and efficiently mixing devices, that can handle a wide range of applications. Detailed review on static mixers, concerning the mechanisms, applications, classification and characterization methods focusing on mixing process and mass transfer performance is given by various researchers [1–3]. The mixing process is very complex and sensitive, and it must be optimally configured. Too long mixing process may cause deformation of the particles that are mixed, to reduce the quality of the mixture and may also cause the increase in the price of technological process and the final product. The mixing process is a result of diffusion, convection and shear, which are the main mechanisms of the homogenization [3–6].

The problems related to the optimization of the mixing processes can be overcome by using a mathematical modelling. Experiments are usually complex and require more financial resources. The models can

drastically reduce the empirical work necessary for predicting parameters of the mixing process.

Models based on Discrete Element Method (DEM) have been developed in the past and shown to be reliable and efficient in catching particle interactions and predicting mixing process for investigation of particle mixing. The soft-sphere method originally developed by Cundall and Strack [7], was the first granular dynamics simulation technique published in the open literature. They developed the linear spring and the dashpot model whereby the magnitude of the normal force between two particles was the sum of spring force and damping force. Lagrangian tracking techniques have been used in many studies in order to characterize the mixing performance in different systems [8–11]. A detailed review and definitions of the quality of a mixture, the mixing mechanisms, the possibilities for the choice of solid mixer, the experimental assessment of homogeneity and mixing indexes are presented in Poux *et al.* [12].

The computational expense of the DEM is very high owing to the extensive contact detection algorithm, and solid time step limitations to resolve particle interactions *via* collisions. Numerical simulations and mathematical modelling are very powerful tools for optimization.

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Correspondence: L. Pezo, University of Belgrade, Institute of General and Physical Chemistry, Studentski trg 12/V, 11000 Beograd, Serbia.

E-mail: [latopezo@yahoo.co.uk](mailto:latopezo@yahoo.co.uk)

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The focus of this paper was to optimize the geometry and to compare different static mixer devices. Komax and Ross are commercial products, with known geometry, used widely in various branches of industry.

In this paper, experimental and numerical comparison between various multiple Komax and Ross mixing configurations has been performed. The fluid is treated as a continuum while the solid phase is modelled using the DEM. The fluid (air) velocity and pressure field are computed by using the Computational Fluid Dynamic (CFD) approach. In the DEM, particle–particle and the particle–wall interactions are resolved and the time integration is performed using Newton’s second law of motion. DEM modelling gives information about particle–particle interactions, particle–wall interactions, position, velocity and acceleration of particle and forces acting on the particle. This information can be useful for construction and design of the mixing devices. Appropriate modelling can contribute better mixing quality and overcome defects and problems that can occur during the mixing process. The quality of the mixing process is analysed using relative standard deviation (RSD) criteria [13]. The effects of the mixer type and the number of mixing elements on mixing process were studied using analysis of variance (ANOVA). The main aim of this study was to demonstrate the use of DEM/CFD simulation coupling in planning the number of Komax or Ross elements in order to gain desirable mixing results.

**MATERIALS AND METHODS**

**Mathematical model**

This paper studies the flow in two types of twisted-blade static mixers (Komax or Ross mixing elements, linked in a series of 1–3 pieces). It evaluates the mixing performance by calculating the trajectory of suspended particles through the mixer. The mathematical model is solved in two stages, first the fluid velocity and pressure field are determined by CFD, and then, using a separate study, the particle trajectories of the granular materials are computed by DEM. The conservations of mass and momentum in terms of the local mean variables over a computational cell are given by Navier–Stocks equations [14]:

$$\frac{\partial(\rho_f \varepsilon)}{\partial t} + \nabla(\rho_f \varepsilon u) = 0$$

and

$$\frac{\partial(\rho_f \varepsilon u)}{\partial t} + \nabla(\rho_f \varepsilon u \cdot u) = -\nabla p - F_{p-f} + \nabla(\varepsilon \tau) + \rho_f \varepsilon g$$

(1)

where  $\varepsilon$ ,  $u$ ,  $t$ ,  $\rho_f$ ,  $p$ ,  $F_{p-f}$ ,  $\tau$  and  $g$  are: porosity, mean fluid velocity, time, fluid density, pressure, volumetric fluid–particle interaction force, fluid viscous stress tensor, and acceleration due to gravity. Fluid particle interaction force is defined by:

$$F_{p-f} = \frac{1}{V_{\text{cell}}} \sum_{i=1}^{k_i} \rho_{p-f,i} \tag{2}$$

where  $F_{p-f,i}$  is the total fluid force on particle  $i$  and  $k_i$  is the number of particles in a CFD cell. The solid phase is treated as a discrete phase and described by the so-called DEM [13]. According to this model, the translational and rotational motions of a particle at any time  $t$ , can be described by Newton’s law of motion:

$$m_i \frac{dv_i}{dt} = f_{p-f,i} + \sum_{j=1}^{k_j} (f_{c,jj} + f_{d,jj}) + m_i g$$

and

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^{k_j} (T_{ij} + M_{ij}) \tag{3}$$

where  $m_i$ ,  $I_i$ ,  $v_i$  and  $\omega_i$  are: the mass, moment of inertia, translational and rotational velocities of particle  $i$ , respectively. The fluid flow field can be obtained by solving Eqs. (1) by use of a standard CFD method. The particle behaviour can be obtained by solving Eq. (3) by an explicit time integration method.

The modelling technique is based on the assumption that the particle is soft (soft particle method), and that particles are allowed to overlap [7]. The amount of overlap is labelled as  $\Delta x$ , and the normal and tangential relative velocities determine the collision forces ( $F_n$  and  $F_t$ ), based on the Kelvin–Voigt model [10,15]. Figure 1 illustrates the collision force as the result of normal and tangential forces. The normal force  $F_n$  is considered as the repulsive force that pushes the particles apart (or particle from bounding geometry), depicted as the action of the spring, and also dissipation action, resulting in an effective coefficient of restitution, shown as dashpot action. Tangential component is considered as an incrementing spring action and dashpot action that is subject to frictional limits.

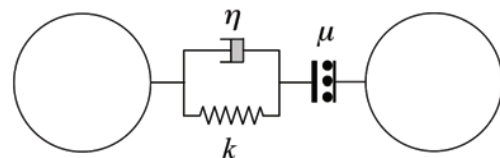


Figure 1. Kelvin–Voigt contact model.

The contact forces in normal and tangential direction are defined as:

$$F_{ij}^n = (-k_n \delta_{ij}^n - \eta_n v_{ij}^n) \quad \text{and} \quad F_{ij}^t = (-k_n \delta_{ij}^t - \eta_n v_{ij}^t) \quad (4)$$

The modelling of the fluid flow by CFD is performed at the computational cell level, whilst the modelling of the solids flow by DEM is accomplished at the individual particle level. Coupling DEM and CFD is achieved as follows: DEM gives information about positions and velocities of individual particles at each time step, for the evaluation of porosity and volumetric fluid–particles interaction force in a computational cell. Incorporation of the resulting forces into DEM will produce information about the motion of individual particle for the next time step [15].

### Experimental method

The experimental apparatus was specially designed for this study, using transparent Plexiglass consisted of three segments (Ross and Komax configurations), Fig. 2a. The upper segment of the mixer (marked with 0) is divided into the two compartments with a barrier and a mobile panel. Spherical painted synthetic zeolite 4A granules (approx. 2.5 mm) are placed in both compartments, red granules in the first compartment and blue granules in the second compartment. The characteristics of the zeolite granules are given in the literature [16]. This compartment is used only for the initial separation of the granules before the premixing. The first and last compartments are used to collect the granules before and after the premixing is done. These compartments are also made of transparent plexiglass with a

height of 60 mm. The second compartment is a premixing device, with 3 segments (marked as 1, 2 and 3), each with a height of 60 mm, and the outlet diameter of 60 mm. The segments are connected in the way that the outlet of the first right-handed segment is connected with second, left-handed segment, at an angle of 90 degrees relative to the vertical axis, Fig. 2b–d. Figure 2b shows the computer model of Ross mixer.

Fig. 2c presents the special design of the Komax static mixer used for this experiment. It consists of three mixing elements, two right-handed Komax segments and one left-handed Komax segment. The elements are made of white plastic (ABS), in thickness of 1.5 mm, by using a 3D printing device (CubePro Trio, used for rapid prototyping). The tube in which the segments are placed is made of 3 mm transparent plexiglass. After passing through three segments of the static mixer, granules fall at the bottom of the lower compartment of the premixer.

Fig. 2d presents the computer model of Komax mixer. Fig. 2e shows Komax mixing element and Fig. 2f presents Ross mixing element computer model. These computer models were used in numerical simulation.

The conditions under which the experiments were conducted are the same as in the numerical simulation conditions.

### Numerical model

Numerical evaluations were performed for observed Ross and Komax static mixer configurations. The

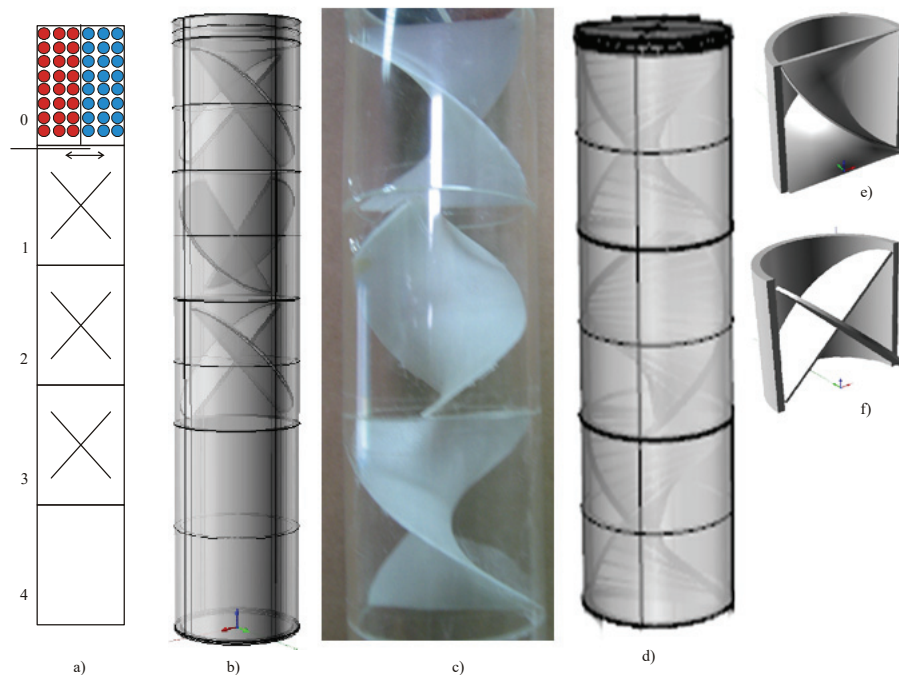


Figure 2. a) Scheme of the static mixer used in the experiment, b) static mixer, type Ross with three elements (3d computer model), c) Komax mixer with three elements used in the experiment, d) static mixer type Komax with three elements (3d computer model), e) mixing element type Komax (3d computer model) and f) mixing element type Ross (3d computer model).

first segment of the mixer is filled with 30,000 spherical particles, diameter 2.5 mm. The inlet compartment filled with 15,000 red particles and a second compartment filled with 15,000 blue particles, outlet-pressure outlet (atmospheric pressure) and wall – the other side of the mixer and the blades of the mixer (Fig. 2a). No slip condition is adopted at the wall. The adiabatic conditions at the walls are applied. It is assumed that the surface roughness is ideal with fresh surface. The influence of the gravity is taken into account and it represents the force which leads the particles to the bottom. The density of the particles released is normalized to the magnitude of the fluid velocity at the inlet. This means that there are more particles released where the inlet velocity is highest. It is assumed that the gas (air) velocity is close to zero, and the impact of fluid on particle movement is minimal. Particle density was  $650 \text{ kg/m}^3$ , fluid density was  $1.2 \text{ kg/m}^3$ , viscosity  $1.8 \times 10^{-5} \text{ kg/ms}$ , particle friction coefficient was 0.3, Young's modulus was  $10^7$ , Poisson's ratio of particles was 0.25, while CFD time step was  $5 \times 10^{-5} \text{ s}$  and DEM time step was  $5 \times 10^{-6} \text{ s}$ .

The set of balance equations (Eq. (1)–(3)) is solved by using the control volume based finite difference method. Semi Implicit Method for Pressure-Linked Equations (SIMPLE) numerical method is used for solving pressure-correction equation from the momentum and mass balance equations [14]. The elements used in numerical mesh are tetrahedral and size of an element is less than  $10^{-8} \text{ m}^3$ . A discretization of partial differential equations is carried out by their integration over control volumes of basic and staggered grids. The convection terms are approximated with upwind finite differences, while diffusion and source terms are approximated with central differences [14]. The calculation error for every balance equation and every control volume is kept within limits of  $10^{-5}$  by iterative solution of sets of linear algebraic equations. CFD time step is ten times larger than the DEM time step. The DEM time step is limited by the natural oscillation period of spring-mass system used to model contacting particles. It should satisfy the following equation ( $m$  is particle mass and  $k$  is stiffness coefficient):

$$\Delta t_{\text{DEM}} \leq \frac{1}{10} 2\pi \sqrt{\frac{m}{k}} \quad (5)$$

### Colour image analysis

In order to check the quality of the mixing process, using *RSD* criteria, colour image analysis is performed. Colour images of experimental and computer simulation results were captured by a Sony PowerShot A550, which is a common digital camera for home use. The macro function of the digital camera has been used, to cover a scene area of approximately  $\varnothing 60 \text{ mm}$ . Samples were placed on a white paper napkin set on a flat white

painted surface, inside the closed chamber, 15 cm below the digital camera. Paper napkins were used in order to avoid undesired reflection effects from chamber's walls. With this setup, it was possible to capture images with negligible shadows and without specular reflections.

### Response surface methodology

The RSM method was selected to estimate the main effect of the process variables on the mixing process. The independent variables were the type of the mixing element (Ross or Komax) and the number of elements (1–3), and the dependent variable observed was *RSD* criteria. A model was fitted to the response surface generated by the experiment. The model used was a function of the variables:

$$Y = \beta_0 + \sum_{i=1}^2 \beta_i X_i + \sum_{i=1}^2 \beta_{ii} X_i^2 + \beta_{12} X_1 X_2, \quad k = 1, 2, \dots, 8 \quad (6)$$

where:  $\beta$  are constant regression coefficients.

Analysis of variance (ANOVA) and response surface regression method (RSM) were performed using Stat-Soft Statistica, for Windows, ver. 10, program.

### RESULTS AND DISCUSSIONS

The results of the DEM/CFD simulation are compared with experimental results. The mechanical properties of zeolite granules are taken from [16]. CFD modelling is used to determine the fluid velocity field and the pressure field, and DEM is used for determining the particle behaviour and particle trajectories during the mixing process. In the following, we consider two different representative cases (1, 2 and 3-segment Ross element configuration and 1, 2 and 3-segment Komax elements configuration). The velocity and the pressure field of the fluid phase were obtained *via* CFD calculations, as well as particle trajectories, Fig. 3a–f presents the mixing results, performed with three-segmented Ross and Komax configuration. Fig. 3a–d refer to the fluid phase. The influence of fluid phase on particle behaviour can be significant, especially in the case of forced or turbulent flow. Fluid phase can influence the velocity and acceleration of the particles and that can affect on the trajectory of the particles and forces acting on the particles.

Fig. 3e and f show the trajectory of 8,000 particles through one pass of the mixer. Particle trajectory has influence on the mixing quality. Optimal prolonging of the trajectory contributes better homogeneity of the mixture [3].

DEM analysis is the most reliable and most convincing method to optimize the mixing process according to mixing quality. The results of the numerical simulations of the movement of one representative par-

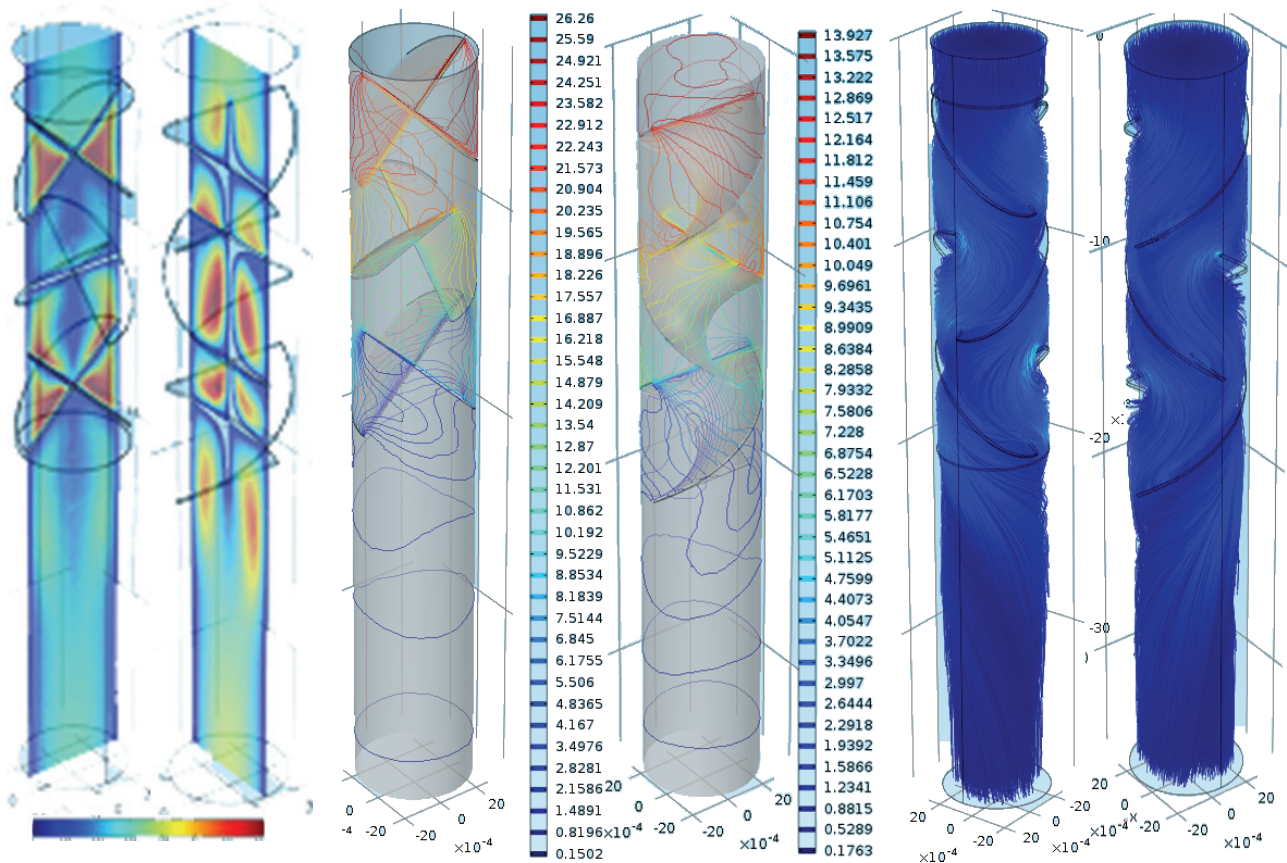


Figure 3. Velocity field of fluid phase, axial direction section (Pa) for: a) Ross and b) Komax mixers configuration; pressure fields in static mixer for: c) Ross and d) Komax mixers; particle trajectories for: e) Ross and f) Komax mixers.

title are shown on Fig. 4 – trajectory, velocity and acceleration in  $x$ ,  $y$  and  $z$  direction of one particle during the mixing process (inside the Komax mixer). The position of the representative particle is dramatically changed within the mixer, with significant turn-overs in particle velocity and acceleration, which greatly contributes to the possibility of increased mixing quality [3].

Overall particle trajectory for three-segmented Komax and Ross configurations, gained by numerical simulations were: 436 and 430 mm, respectively.

In this work, RSD was used to follow the evolution of mixing uniformity for the static mixers with different configurations, explained above, [12]:

$$RSD = 100 \frac{\sigma}{\bar{x}}, \quad \sigma = \sqrt{\sum_{i=1}^M (\bar{x} - x_i)^2 (M-1)^{-1}} \quad (7)$$

where  $M$  is the number of samples,  $x_i$  the concentration of sample  $i$ , and  $\bar{x}$  the average concentration of all samples. For instance, concentration of red particles in a sample is calculated as the ratio of the number of red particles and the total number of particles.

The results of numerical simulations of mixing processes in Ross and Komax mixers are presented on Fig.

5. The mixing process begins after particles leave the upper segment (marked as 0, Fig. 2a, as soon as the mobile panel is removed, enabling the granules to fall toward the static mixer). The particles are rapidly blended in the first section, as seen from the figure, reaching the mixing degree of 20–27% at the outlet. Because of the twisted surface geometry, Komax mixing element shows better mixing results in this section (20–22%) compared to Ross (24–27%). Particle velocities are greater in Komax mixer, especially between segment 1 and 2, as seen from Fig. 5. Both mixers shows more effective mixing after second and third section. Komax mixing elements reaches the mixing degree of 6–8% and 4–5% at the outlets, while the mixing quality of 11–13% and 5–6% were obtained at the outlets of section 2 and 3, using Ross elements. This is expected, because of the higher particle velocities in the Komax mixer. The small, but steady decrease in the mixing degree was observed for both Komax and Ross blending elements during DEM/CFD simulation, Fig. 5 (after segment 4). This is due to centrifugal force affecting the motion of granules that exit the mixing compartment. The use of the quadratic grid divider could enable the mixing degree to remain constant after granules left the third mixing element.'

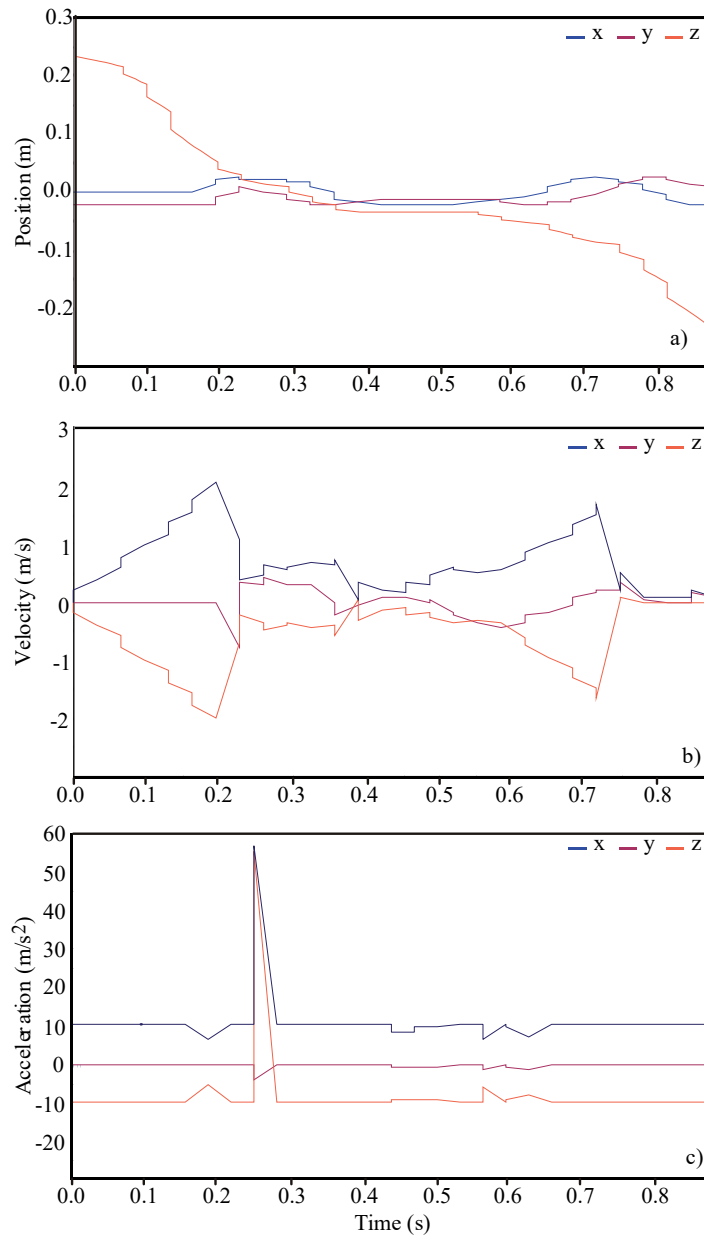


Figure 4. Trajectory, velocity and acceleration in x, y and z direction of one particle during mixing process in Komax mixer.

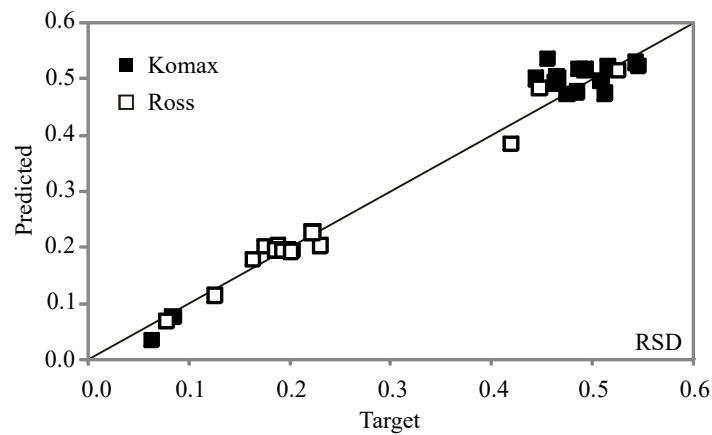


Figure 5. RSD criteria for experimental and numerical results in Ross and Komax mixers.

Table 1 shows the influences of process variables on observed response, for numerical simulation of mixing in Ross and Komax mixers. The analysis revealed that the linear terms of both variables contributed substantially to generate a significant SOP model. The influence of mixing element type (MET) was significant in SOP model, statistically significant at  $p < 0.10$  level, while the influence of the number of elements (NE) was the most important in the SOP model calculation ( $p < 0.01$ ). The quadratic term of NE was also very influential (statistically significant at  $p < 0.01$  level), as well as the interchange term MET  $\times$  NE ( $p < 0.10$ ).

Table 1. Analysis of variance (ANOVA) for experimental and numerical results in Ross and Komax mixers; <sup>+</sup>significant at  $p < 0.01$  level, <sup>\*\*</sup>significant at  $p < 0.10$  level, MET – mixing element type, NE – number of mixing elements, df – degrees of freedom, SoS – sum of squares, F – F test

	df	SoS	F	p
MET	1	0.002 <sup>**</sup>	3.41	0.08
NE	1	0.397 <sup>+</sup>	646.70	<0.01
NE <sup>2</sup>	1	0.107 <sup>+</sup>	174.49	<0.01
MET $\times$ NE	1	0.002 <sup>**</sup>	3.79	0.06
Error	27	0.017		
$r^2$		0.968		

A high  $r^2$  is indicative that the variation was accounted and that the data fitted satisfactorily to the proposed model. The  $r^2$  value was found very satisfactory and showed the good fit of the model to experimental results.

## CONCLUSION

Coupled DEM/CFD approach was used to investigate mechanisms of fluid flow and particle tracking for granular flow. In the DEM, particle–particle and the particle–wall interactions are resolved and the time integration is carried out using Newton's second law of motion. Mixture model was used in CFD analysis for the determination of the characteristics of the fluid phase. DEM analysis was used to determine the particle trajectories and the history of particle positions in order to determine the quality of the mixture. The mixing quality was estimated by a mixing criterion, named RSD (relative standard deviation). The effects of the mixer type and the number of mixing elements on mixing process were studied using analysis of variance (ANOVA). The aim of this study is to predict the behaviour of granules in different mixer configuration and to optimize the number of mixing elements taking into account the price of the final product, the duration of the mixing process and the quality of the mixture. It is obvious that the mixer based on Komax elements enables better mixing quality, compared to Ross, espe-

cially when the height of installation is low. However, the use of Ross is more financially acceptable, due to its simpler geometry. According to the results, the number of mixing elements is more influential parameter than the type of mixing elements. It seems that this type of device can be used only as premixing device and additional mixer is necessary to gain the good quality of the mixture. However, the premixing process can contribute better quality of the mixture and can significantly reduce the mixing time and the cost of the mixing process.

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## IZVOD

### PROTOK GRANULISANOG MATERIJALA U STATIČKOJ MEŠALICI – DEM/CFD PRISTUP

Lato Pezo<sup>1</sup>, Milada Pezo<sup>2</sup>, Aca Jovanović<sup>1</sup>, Nenad Kosanić<sup>3</sup>, Aleksandar Petrović<sup>3</sup>, Ljubinko Lević<sup>4</sup>

<sup>1</sup>Univerzitet u Beogradu, Institut za opštu i fizičku hemiju, Studentski trg 12/V, 11000 Beograd, Srbija

<sup>2</sup>Univerzitet u Beogradu, Institut za nuklearne nauke Vinča, Laboratorija za termotehniku i energetiku, p. pr. 522, 11001 Beograd, Srbija

<sup>3</sup>Univerzitet u Beogradu, Mašinski fakultet, Kraljice Marije 16, 11000 Beograd, Srbija

<sup>4</sup>Univerzitet u Novom Sadu, Tehnološki fakultet, Bulevar Cara Lazara 1, 21000 Novi Sad, Srbija

(Naučni rad)

Proces mešanja veoma utiče na kvalitet krajnjeg poluproizvoda i/ili krajnjeg proizvoda, a parametri procesa mešanja i dizajn opreme veoma utiču na efikasnost mešanja, kvalitet proizvoda i cenu proizvoda. U ovom radu, prikazana je upotreba metode diskretnih elemenata (engl. Discrete Element Method – DEM) na modelovanje mešanja granula u različitim konfiguracijama statičkih mešalica (korišćene su različite Komax i Ross konfiguracije za mešanje). Za modelovanje protoka fluida primenjena je metoda numeričke mehanike fluida (engl. Computational Fluid Dynamic – CFD), korišćenjem Ojlerovog dvofaznog modela. Povezivanjem rezultata ove dve metode dobijaju se pouzdan, dovoljno tačan i adekvatan model koji daje rezultate koji odgovaraju eksperimentalnim merenjima. Statičke mešalice se široko koriste u industiji prerade hrane, farmaceutskoj ili hemijskoj industriji. Ovaj tip mešalice se koristi uglavnom kao predmešač, pre glavnog mešanja, pri čemu se značajno smanjuje vreme mešanja i štedi energija. Ova vrsta mešanja nije dovoljno ispitivana u literaturi. Kvalitet mešanja granula zeolita u ovom radu je ispitivan dobro poznatim kriterijumom za kvalitet mešanja, pod nazivom relativna standardna devijacija. Uticaj tipa mešalice i broja elemenata za mešanje ispitivani su analizom varijanse (ANOVA). Cilj ovog rada je bio da se predvidi ponašanje granulisanog materijala u različitim konfiguracijama mešalica i da se optimizuju parametri procesa uzimajući u obzir trajanje procesa mešanja, kvalitet mešavine i cenu finalnog proizvoda. Za potrebe ovog rada, napravljene su statičke mešalice tipa Ross i Komax od providnog pleksiglasa, dizajnirane u CAD paketu, napravljene korišćenjem CNC glodalice. Pošto su napravljene elementi bili prozirni, praćenje procesa mešanja granula je bilo i vizuelno. Praćene su i analizirane trajektorije, brzine i ubrzanja čestica, u cilju procene kvaliteta procesa mešanja. Dobro poznati kriterijum za kvalitet mešanja, pod nazivom relativna standardna devijacija (RSD) je korišćen za ovu svrhu. Optimizacija dimenzija i parametara mešanja u statičkoj mešalici je izvedena korišćenjem matematičkog modeliranja. Cilj ovog rada je bio da se predvidi ponašanje granulomog materijala u različitim konfiguracijama mešalica i da optimizuje parametre procesa uzimajući u obzir trajanje procesa mešanja, kvalitet mešavine i cenu finalnog proizvoda mešanja. U istraživanju je primećeno da su Komax elementi primenljiviji, u poređenju sa Ross elementima, posebno kada je visina instalacije mala. Međutim, upotreba Ross je finansijski prihvatljivija, zbog njegove jednostavnije geometrije. Dodatni pregrada sa kvadratnim otvorima, koja se postavlja na izlazu iz statičke mešalice, koristi se da bi se umirilo kretanje granula na obodu cevi, kao i da smanji segregacija granula.

*Ključne reči:* DEM/CFD • Statički mikser • Komax • Ross • Trajektorije čestica