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Prediction slurry reactor design under uncertainty using CFD model

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Abstract:

Mechanically agitated reactors find wide range of applications for solid suspension and mixing in the chemical, biochemical, and mineral processing industries. Understanding the solids dynamics in these reactors is necessary to improve the design and operation of such reactors. Computational fluid dynamic (CFD) models are often useful in this regard, as it can provide significant insights into the flow and mixing of the phases involved. However, the model predictions need extensive evaluation with experimental results before they can be confidently used for the scale-up and optimization of large scale reactors. In the present work the predictive capabilities of CFD techniques as applied to solid-liquid stirred vessels are investigated. Suspensions of sand (diameter equal to 327 μm) in water are studied. Eulerian-Granular multiphase model was simulated using FLUNT 6.3.26 to predict the slurry reactor design under uncertainty. The profiles obtained with the Eulerian-Granular approach coupled with the Eulerian, Granular models, and experimental data for comparison purposes. The present model provides an improvement of the predictions in the lower part of the vessel, with respect to the Eulerian model; while the same results can be observed in the rest of the tank where the solid concentration is lower. It seems that the interaction phenomena between the solid and the liquid phases and those among the solid particles do not vary appreciably for low solid concentrations, while at higher concentration some effects become noticeable. It was found that the quasi-steady state behavior of the sand in the mixing tank reached after 20 sec, also after 10 sec were the free surface of the static pressure will be growth until reach peremptory shape after 20 sec. The present model provides a proper representation for the solid distribution, by adopting particle drag coefficient.

Keywords: Slurry Reactor, CFD, Fluent, Multiphase model.

استخدام تقنية حركة الموائع الحسابية لمعالجة نموذج مفاعل الملاط تحت ظروف غير محددة

الخلاصة

وجدت المفاعلات ذات الخلط الميكانيكي المدى الواسع في التطبيقات في مجال الهندسة الكيمياوية والبايوكيمياوية وهندسة المعادن. ان فهم ديناميكية المواد الصلبة العالقة ضروري لتحسين تصميم وتشغيل هكذا نوع من المفاعلات. وغالبا ما تستخدم نماذج ديناميكية الموائع الحسابية (CFD) لتوفير صورة واضحة حول الجريان والخلط للأطوار المتعددة. على أي حال فان عملية التنبؤ بالنموذج تحتاج إلى نتائج تجارب عملية واسعة قبل الشروع بتصميم المفاعل الصناعي وكذلك استخدام طرق الأمثلية (Optimization) لإيجاد أفضل التصاميم.

تم خلال هذا البحث تحري إمكانية تقنية (CFD) لمعالجة نموذج مفاعل ذو خلاط يحتوي على طورين (صلب- سائل)، الطور السائل متمثلاً بالماء والطور الصلب متمثلاً بالرمل الحبيبي بقطر (327 μ m). وقد تم اعتماد نموذج يوليرين-الحبيبي المتعدد الاطوار لتحري تصميم مفاعل الملاط (slurry) تحت ظروف غامضة، وتمت مقارنة النموذج الحالي مع نماذج ونتائج عملية سابقة مستخدمة من قبل باحثين سابقين، وقد أعطى النموذج المقدم في هذا البحث تنبؤ مقبول عن الجزء الأسفل من المفاعل بالمقارنة مع نموذج (Eulerian)، كما بين ان ظاهرة التداخل بين الأطوار المختلفة أو بين جسيمات المادة الصلبة ذاتها لم تتغير عند التراكيز الواطئة للمادة الصلبة وكانت اقل وضوحاً، بينما في التراكيز العالية تصبح هذه الظاهرة قابلة للملاحظة. وقد تم الاستعانة ببرنامج (FLUNT 6.3.26) لحل المعادلات الخاصة بهذا النموذج . تم التوصل في هذا البحث الى ان عملية الخلط للرمل داخل الخزان تصل الى حالة خلط شبه مستقرة بعد(20) ثانية، كما ويبدأ السطح الحر للضغط الساكن بالنمو بعد مرور(10) ثانية الى ان يصل الى شكله النهائي بعد مرور(20) ثانية. ان النموذج الحالي يوفر صورة دقيقة عن طبيعة توزيع تركيز المادة الصلبة وذلك بالأخذ بنظر الاعتبار معامل الإعاقة (drag coefficient) للجسيمات الصلبة.

Symbol	Notation	Symbol	Notation
English symbols		T	Tank diameter
C	Impeller clearance	*UDF*	User define function
C_D , C_L	Drag and lift coefficient	V_{dr}	Drift velocity
CFD	Computational fluid dynamic	d_p	Particle diameter
D_l,D_s	Turbulent diffusivity for liquid , solid	u	Axial velocity
D	Impeller diameter	v	Radial velocity
EGM	Eulerian Granular Multiphase	v_q	Velocity of the phase q
F_q	Gravitational force	v_s, v_l	Velocity of the solid, liquid phases
F_{lift}	Lift mass force	w	Angular velocity
F_{vm}	Virtual mass force	***Latin symbols***	
H	Liquid level	α_l, α_s	Volumetric fraction of liquid, solid phase
LDV	laser Doppler velocimetry	α_q	Volumetric fraction of phase q
N	Shaft speed	α_s	Volumetric fraction of solid
Njs	just-suspended speed	$\kappa-\varepsilon$	Dispersed turbulent model
P_q	Pressure of the phase q	μ	Viscosity
R_{pq}	Interface momentum transfer	σ	Turbulent shimdt number
		τ_s , τ_q	Shear stress in the solid, q phases

Introduction:

Slurry reactors, in which solid–liquid suspensions are agitated using one or more impellers, are one of the most important unit operations in the chemical, biochemical, and mineral processing industries, because of its ability to provide excellent mixing between the phases. The flow pattern and turbulence prevailing in the reactor ensures good heat and mass transfer properties for the system, apart from providing good solid suspension within the vessel. Relevant examples of solid–liquid industrial systems include multiphase catalytic reactions, crystallization, precipitation, leaching, dissolution, coagulations, and water treatment (1). Despite its widespread use, the design and operation of these reactors still remain a challenging problem because of the complexity of three dimensional circulating and turbulent multiphase flow encountered in the tanks. With the improvement in computational capabilities, computational fluid dynamics (CFD) has emerged as a viable option to study turbulent multiphase flows and gain insights on the hydrodynamic behavior of complex systems. Guha et al (2008)(2) showed that there are a variety of approaches to modeling the solids transport and include Lagrangian or homogenous techniques with the liquid phase influencing the particle motion but not the particles influencing the liquid (one-way coupling). Of particular interest is the Eulerian multiphase model, which uses separate sets of Navier-Stokes equations for the liquid and solids (or granular) phases. In this approach, the interactions between the phases are coupled. Micale et al. (2000) (3) predicted particle distributions of low particle concentrations in single and multiple impeller stirred vessels using Eulerian-Eulerian models. . Lanre M. et al. (2002) (4) their simulations were in reasonably good agreement with experimental axial measurements of solid concentration. However, some uncertainty in the results predicated the authors to use correction factors to fit the numerical predictions to experimental data. Their conclusions were that improved single-phase simulations and incorporation of so-called four-way interactions (fluid-particle, particle-fluid, particle-particle, and particle-turbulence interaction) would improve the applicability and reliability of the modeling work.

Modeling Liquid-Solid Multiphase Flow

There are a number of multiphase models that can be used to model the solids suspension in an agitated vessel. The Lagrangian Eulerian model solves the equation of motion for the discrete particle trajectories. The coupling between the phases through drag terms can be modeled but accumulation of particles cannot be modeled. The drift flux and ASM models are homogeneous mixture models for modeling multiphase flows.

ASM models

The ASM models introduce slip between the phases through an algebraic relationship. These models are ideally suited to modeling particles with relaxation times less than 0.001-0.01 seconds and in low concentrations.

The Eulerian models

The Eulerian models are the most rigorous of the multiphase models and model the multiple phases as interpenetrating continua. A separate set of momentum equations is solved for each phase.

The interaction between the phases is modeled through the momentum exchange terms and includes the drag exerted by the continuous phase on the dispersed phase. Coupling is achieved through the pressure and interphase exchange coefficients. The manner in which this coupling is handled depends upon the type of phases involved; granular (fluid-solid) flows are handled differently than nongranular (fluid-fluid) flows. For granular flows, the properties are obtained from application of kinetic theory. Momentum exchange between the phases is also dependent upon the type of mixture being modeled. Applications of the Eulerian multiphase model include bubble columns, risers, particle suspension, and fluidized beds (5).

Model Comparisons

Selection the appropriate model based on the following (5)

1. For bubbly, droplet, and particle-laden flows in which the phases mix and/or Dispersed-phase volume fractions exceed 10% either the mixture model or the Eulerian model is used.
2. For fluidized beds the Eulerian model for granular flow is used.
3. For slurry flows and hydrotransport the mixture or Eulerian model is used.
4. For sedimentation the Eulerian model is used.

Approaches to Multiphase Modeling

Currently there are two approaches for the numerical calculation of multiphase flows: the Euler-Lagrange approach and the Euler-Euler approach (6).

1. The Euler-Lagrange Approach

The Lagrangian discrete phase models in FLUENT follows the Euler-Lagrange approach. The fluid phase is treated as a continuum by solving the time-averaged Navier-Stokes equations, while the dispersed phase is solved by tracking a large number of particles, Bubbles or droplets through the calculated flow field. The dispersed phase can exchange momentum, mass, and energy with the fluid phase. A fundamental assumption made in this model is that the dispersed second phase occupies a low volume fraction, even though high mass loading ($\overset{\bullet}{m}_{particles} \geq \overset{\bullet}{m}_{fluid}$) is acceptable. The particle or droplet trajectories are computed individually at specified intervals during the fluid phase calculation. This makes the model appropriate for the modeling of spray dryers, coal and liquid fuel combustion, and some particle-laden flows, but inappropriate for the modeling of liquid-liquid mixtures, fluidized beds, or any application where the volume fraction of the second phase is not negligible.

2. The Euler-Euler Approach

In the Euler-Euler approach, the different phases are treated mathematically as interpenetrating continua. Since the volume of a phase cannot be occupied by the other phases, the concept of phasic volume fraction is introduced. These volume fractions are assumed to be continuous functions of space and time and their sum is equal to one. Conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases. These equations are closed by providing constitutive relations that are obtained from empirical information, or, in the case of granular flows, by application of kinetic theory. In FLUENT, three different Euler-Euler multiphase models are available: the volume of fluid (VOF) model, the mixture model, and the Eulerian model.

Gidaspow (1993) (7) described that in the EGM model, the granular momentum equation includes in a solids stress tensor that is modeled based on the kinetic theory for granular flow. Massah, H. and Oshinowo (2000) (8) proposed an additional transport equation for granular temperature (or solids fluctuating energy), which is proportional to the mean square of the random motion of particles. The Eulerian Granular Multiphase (EGM) model provides a fully predictive solution of the solids transport in the process vessel. The EGM model accounts for four-way coupling between and within the phases that applies to systems with dense granular flows. The strongly coupled momentum equations of the granular and liquid phases require a transient solution. Just-suspended speed historically, the characterization of the suspension of solids in stirred tanks is through the parameter of the just-suspended speed *Njs*. The concept of *Njs* was introduced more than forty years ago and is the primary design parameter used today by engineers involved in the sizing, scaling and overall design of stirred tanks for the purpose to suspending, dissolving and reacting solids. The famous correlation by Zwietering (1958) (9) correlates the *Njs* to the particle and fluid properties, the mass ratio percentage of the solids, and the impeller diameter. The parameter *S* in the Zwietering correlation incorporates the influence of the tank bottom shape, impeller clearance and blade characteristics. This lumped parameter can be evaluated from tables developed by many workers and scattered over the literature.

Experimental data

Experimental data from the literature was chosen to validate the two-phase flow field for the distribution of solid particles is one important feature of solid-liquid stirred tanks whose experimental behavior has been mainly described with simple fluid-dynamic models over the years. Very dilute solid-liquid suspensions have been considered in most experimental investigations. Brucato et al. (10) applied CFD methods to the simulation of solid-liquid stirred tanks and developed different models for predicting the behavior of the solid phase, either based on Lagrangian or

Eulerian approaches. Bakker et al.(11) showed that all operating above *Njs* and system shows a different level of solids distribution. In this study it is interesting to note that the cloud height is not uniform across the tank diameter as the simulations show the funneling of the solids being drawn towards the impellers. The 3D CFD results qualitatively predict the extent of the solids distribution in the tanks. The need for further analysis and development of modeling techniques and comparison of the simulations with experimental data arises from several reasons. Black box methods for the treatment of baffled stirred tanks are often adopted, thus leading to not entirely predictive procedures. In addition, a number of modeling techniques have been proposed and implemented in commercial codes, whose choice is not straightforward for the normal user. Moreover, the consistency of the simulation predictions with the actual flow field and solid particle distribution has been demonstrated only in few cases. A. Ochieng (2005) (12) employed the CFD simulation with a four blade Mixtec HA735 propeller in a fully baffled Perspex tank with a diameter (T) of 0.378 m. The impeller diameter was 0.33 T and the four baffles were 0.1 T wide. The impeller bottom clearance was 0.15 T and the impeller speed was in the range of 200–700 rpm. Ochieng, and Lewis (2006) (13) employed in this work the same impeller-tank configuration as that reported in earlier work. The nickel solids loading by mass were in the range of 1–20% w/w, and subsequent references to solids loading are percentages by mass, unless stated otherwise. All the flow profiles were taken at the middle of two baffles. Three particle sizes of nickel were used: 230 μm, 400 μm and 750 μm, which were denoted by Ni230, Ni400 and Ni750, respectively. Ochieng and Onyango (2008) (14) studied the influence of drag models on the prediction of solids suspension in a tank stirred by a hydrofoil impeller using computational fluid dynamics (CFD) and experimental techniques they compared between the drag models based on Reynolds number only and those that take solid volume fraction into account or those that account for the effect of the free stream turbulence.

Fluent CFD model:

The stirred tank models (computational grids of quad elements) are set-up automatically using Fluent 6.3.26 from Fluent Inc. The commercial CFD code FLUENT6.3.26 is used with the EGM model in the solution of the solid-liquid multiphase flows. The granular viscosity model of Syamlal & O'Brien (15) is used in this work. The granular bulk viscosity model of lun et al. (6) is used also. Turbulence in the liquid phase is modeled using the standard $\kappa-\varepsilon$ model and secondary phase turbulence generation is neglected. The EGM model calculations are performed as time-dependent. No-slip boundary conditions (u=v=w=0) for both phases are applied on the tank walls and shaft with the latter having a prescribed rotational velocity. The free surface of the suspension is described by zero gradients of velocity and all other variables. Since the shear stress is zero, the free surface can be interpreted as a slip wall. The impellers are modeled implicitly using internal boundary conditions based on laser Doppler velocimetry (LDV) data supplied by the impeller manufacturers. LDV impeller data can also be obtained from a number of sources(16).The impellers can also be modeled explicitly in three-dimensions using the multiple reference frames or sliding mesh models but add to the computational expense of the calculations.(3)

Due to the simplicity of the mixing tank geometry and the explicit treatment of the impellers, the stirred tanks are set up as 2D axisymmetric models with a transport equation for swirl. By modeling the mixing tank in two dimensions, the simulation runtime is considerably accelerated. The computational grids consisted of approximately 2250 cells in the 2D models. After obtaining the continuous (liquid) phase steady-state flow field, the time-dependent solids suspension calculations are performed. Typically, the multiphase flow fields reached “near-steady-state”are 20 Sec.

Mathematical model

The CFD simulations of the stirred tank are performed by adopting Eulerian-Granular that based on an Eulerian treatment of the two phases. With that approach, the continuity and momentum equations are solved for each phase, thus obtaining separate flow field solutions for the liquid and the solid phases simultaneously. The continuity and momentum equations for a generic phase q, based on the Eulerian treatment, are:

$$\frac{\partial}{\partial t}(\alpha_q) + \nabla.(\alpha_q \vec{v}_q) = 0^{(6)} \qquad \text{…Eq.(1)}$$

$$\frac{\partial}{\partial t}(\alpha_q p_q \vec{v}_q) + \nabla.(\alpha_q \vec{v}_q \vec{v}_q) = -\alpha_q \nabla p + \nabla.\overset{=}{\tau}_q + \vec{R}_{pq} + \alpha_q p_q (\vec{F}_g + \vec{F}_{lift,q} + \vec{F}_{vm,q})^{(6)} \qquad \text{…Eq.(2)}$$

Where α_q is the volumetric fraction of the phase q, F_g is the gravitational force and F_{lift} and F_{vm} are the lift and virtual mass force, respectively. These last two forces have been neglected in the calculations, as it is already found that they give a minor contribution to the solution with respect to the other terms(11). The inter-phase momentum transfer term, R_{pq}, is modeled *via* the drag coefficient, C_D, as:

$$R_{s1} = \frac{3}{4}\frac{\alpha_s p_s}{d_p} C_D |\vec{v}_s - \vec{v}_1| (\vec{v}_s - \vec{v})^{(11)} \qquad \text{…Eq.(3)}$$

The last parameter is calculated by using the standard correlation implemented as a default in Fluent 6.0 (17) that refers to a particle falling in a still fluid. Also, the effect is investigated of a correction to take into account the increase in the drag coefficient due to free stream turbulence (18,19,).

The Granular model differs from the Eulerian one for the momentum equation of the solid phase, which is modified with respect to **Eq (2)** as

$$\frac{\partial}{\partial t}(\alpha_s p_s \vec{v}_s)+\nabla.(\alpha_s p_s \vec{v}_s \vec{v}_s)=-\alpha_s \nabla p-\nabla p_s+\nabla \overset{=}{\tau_s}+F_g+K_{1s}(\vec{v}_1-\vec{v}_s)+\alpha_s p_s(\vec{F}_s+\vec{F}_{lift,s}+\vec{F}_{vm,s})^{(11)}$$

…Eq.(4)

As can be observed, this equation is identical to the previous one **Eq.(2)**, except for one additional term that introduces a "solid pressure" contribution. This term has been modeled according to the kinetic theory of granular flows(20) as implemented in Fluent 6.0. In the present case of turbulent two-phase flow, the momentum transfer due to the turbulent fluctuations of the volumetric fraction is taken into account by adding to both **Eq. (3)** and **(4)** the additional term:

$$R^t{}_{s1}=\frac{3}{4}\frac{\alpha_s p_s}{d_p}C_D\left|\vec{v}_s-\vec{v}_1\right|v_{dr}{}^{(20)} \qquad \text{…Eq.(5)}$$

Where the drift velocity vdr is defined as:

$$v_{dr}=\frac{D_s}{\sigma_{s1}\alpha_s}\nabla\alpha_s-\frac{D_1}{\sigma_{1s}\alpha_1}\nabla\alpha_1 \;{}^{(20)} \qquad \text{…Eq.(6)}$$

In **Eq (6)**, D is the turbulent diffusivity and σ is the turbulent Schimdt number.

In order to close the problem, a suitable turbulence model has to be coupled with the Reynolds Averaged Navier-Stokes equations. Three different extensions of the standard k-ε model to multiphase systems have been developed. In the simplest case, referred to as "Mixture Model", only a couple of k and ε equations are solved, where the physical properties of the mixture are adopted. Therefore, the two phases are assumed to share the same k and ε values. A more advanced modification of the single phase k-ε model, named "Dispersed Turbulence Model", is based on the solution of the k and ε equations for the liquid phase, while the turbulence quantities for the solid phase are calculated on the basis of a simplified treatment(21).

Reactor Geometry and Liquid-Solid Property Data

A summary of the stirred tank geometry and liquid and solid property data are listed in **Table (1)** Godfrey and Zhu(22). The problem involves the transient startup of an impeller-driven mixing tank. The primary phase is water, while the secondary phase consists of sand particles with a

327 micron diameter. The sand is initially settled at the bottom of the tank, to a level just above the impeller. A schematic of the mixing tank and the initial sand position is shown in **Figure (8)**. The domain is modeled as 2D axisymmetric.

Problem Description:

The Eulerian multiphase model it is used to solve the particle suspension problem. The Eulerian multiphase model solves momentum equations for each of the phases, which are allowed to mix in any proportion. The steps of the work are:

- Use the granular Eulerian multiphase model
- Specify fixed velocities with a user-defined function (UDF) to simulate an impeller
- Set boundary conditions for internal flow
- Calculate a solution using the segregated solver
- Solve a time-accurate transient problem

The problem is involved the transient startup of an impeller-driven mixing tank. The primary phase is water, while the secondary phase consists of sand particles with a 327 micron diameter. The sand is initially settled at the bottom of the tank, to a level just above the impeller. The domain is modeled as 2D axisymmetric. The fixed-values option is used to simulate the impeller. Experimental data are used to represent the time-averaged velocity and turbulence values at the impeller location. This approach avoids the need to model the impeller itself. These experimental data are provided in a user-defined function (UDF). A (UDF) is used to specify the fixed velocities that simulate the impeller. The values of the time-averaged impeller velocity components and turbulence quantities are based on experimental measurement. The variation of these values may be expressed as a function of radius, and imposed as polynomials according to **Eq.(7)**:

$$Variable = A_1 + A_2 r + A_3 r^2 + A_4 r^3 + A_5 r^4 + A_6 r^5 \, ^{(23)} \qquad \ldots\text{Eq.(7)}$$

The order of polynomial to be used depends on the behavior of the function being fitted , the polynomial coefficients is shown in **Table (2)**(23). The segregated solver, axisymmetric, unsteady and implicit formulations are used for multiphase calculations. The Phase Interaction is calculated using Gidaspow for the Drag Coefficient.

Results and discussions

Experimental measurements and Numerical models from Montante *et. al*(23) are used for comparison with the CFD simulations.

Water and Sand velocity for fixed-zone

In this work, for the Granular model it is found that the vector velocity for both sand and water velocity at initial time, are the same in the fixed-zone as shown in the **Figures 1(a,b)** because of the mixing starting in this zone.

Sand volume fraction distribution

Figure (2a) gives accurate image about the sedimentation state and the cloud height make about (26%) of vessel height as a settled sand bed, in another way 26% of the vessel height is predicted as the settled sand bed. In order to assess whether better spatial solid distribution could be obtained while taking into account the effect of the 'solid pressure' term in the two-phase model, **Eq. (4)** so that **Figure 2(b,c,d)** show the effect of eddy growth on the sand volume fraction distribution after three times (1 sec , 10 sec , 20 sec). It is found that the quasi-steady state behavior of the sand in the mixing tank reached after 20 sec But after 20 sec there is no discernible differences can be observed in the profiles obtained with the Granular equations in the vessel (CFD Iteration is made for 30 sec and gave same profiles). **Figure 2(b,c,d)** show decreasing the bold red region (high sand volume fraction) gradually till reaches the smallest in the **Figure 2(d)** because of the solid pressure effect increasing until reaching quasi-steady state behavior for the sand in the mixing tank**.** Because of the high velocity effect on the sand particles, the particles accumulate in the vicinity of the tank wall and some of the sand accumulates below the impeller where the velocity equal to zero. With time the sand accumulation grow until reach the final height after 20 sec where the equilibrium reached.

Liquid-solid velocity distribution

Figure 3(a,b,c) show presence a region in which water velocity largest value, started below the impeller and decreases until reach the vessel base, and this region will be expanded (increasing velocity) radially until reach the interior wall of the vessel, and that confirm the results shown in **Figure 2(a,b,c,d)**, but after 20 sec ideal mixing will be eventuated for the present system. Resembling results can be noticed for solid distribution as shown in **Figure 4(a,b,c)**.

Mixture static pressure distribution

The fixed-zone have largest static pressure and the region between fixed-zone and the bottom of the vessel will be decreased gradually and near the bottom will be largest secondly .also there is another high static pressure region near the edge of the vessel base. This enucleating the eddy motion touching to points out of the regions that mentioned above. And its effectiveness don't accessible these regions till after 20 sec as shown in the **Figure 5 (a,b)**.Where **Figure 5(a)** show the static pressure after 10 sec , the free surface will be growth until reach peremptory shape after 20 sec as in **Figure 5(b)**, where the pressure are equal in over all points in this surface.

In the region of higher concentration, i.e. from the tank bottom to the region just above the lowest impeller, an improvement in the simulated profiles with respect to the Eulerian-Granular profile can be observed. However, the agreement with the experiment is still unsatisfactory and sedimentation is over-predicted for both the solid-liquid systems. The data-processing is completed after about 5250 iterations, as in **Figure (6)**. Where the fluent package solve conservation equations in iterated steps for each equation until reach a flatness in the curve of the equation data with the number of iteration which means the final corrected data.

Comparison the Eulerian-Granular model with experimental data

The profiles obtained with the Eulerian-Granular approach coupled with the Eulerian, Granular models, and experimental data of Montante et. al(23) are reported in the **Figure (7)** for comparison purposes. In the region of higher concentration, i.e. from the tank bottom to the region just above the impeller, an improvement in the simulated profiles with respect to the Eulerian profile can be observed. On the contrary, no discernible differences can be observed in the profiles obtained with the Eulerian- Granular equations in the upper part of the vessel, where the concentration is lower because of the highly mixing level, which means that the Eulerian-Granular model is more accurate than the Eulerian model for the dilute system of solid-liquid. However, the agreement with the experiment is still unpersuasive and sedimentation is over-predicted for both the solid-liquid systems. There is error still in the model in the description of the eddies accurately.

Conclusion

1. The application of CFD to modeling unit operations in the slurry reactor to improve and enhance process design is a reality. Recent advances in the capabilities of commercial CFD software, in particular FLUENT, has enabled engineers to understand the performance of the design and perform pre-construction optimization based on the results of CFD analysis.
2. A practical application of CFD to model the low to high concentration solids suspensions in stirred tanks and predict the distribution of solids, the velocity distribution of the solids and liquid, the cloud height of the suspension, and the blending of the liquid phase, has been described in the present work.

3. The Granular modification of the Eulerian model for the solid phase provides an improvement of the predictions in the lower part of the vessel, with respect to the Eulerian model; while the same results can be observed in the rest of the tank where the solid concentration is lower.
4. It seems that the interaction phenomena between the solid and the liquid phases and those among the solid particles do not vary appreciably for low solid concentrations, while at higher concentration some effects become noticeable.
5. None of the models provides a fair representation of the solid distribution, unless a proper particle drag coefficient is adopted.
6. Based on the observations presented in this work, it can be concluded that more fundamental understanding of the flow field and the associated interactions close to the impeller are necessary to resolve and predict the complex two-phase flow in a solid– liquid stirred tank reactor. In such models for single phase flow the CFD computed flow field is used to couple the compartmental model with kinetics of the desired reaction system.

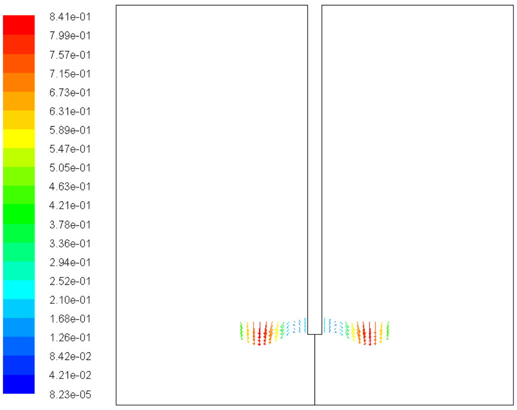

Figure 1 (a): Initial Sand velocity at fixed zone. (m/s)

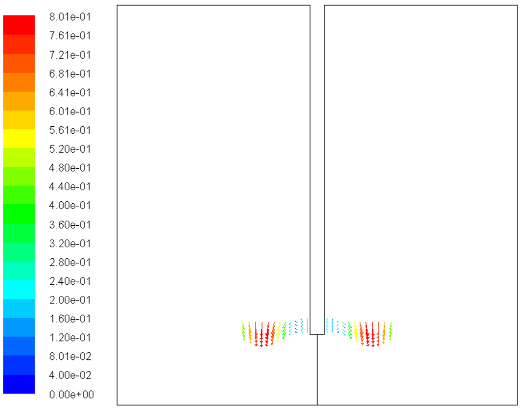

Figure 1 (b): Initial Sand velocity at fixed zone. (m/s)

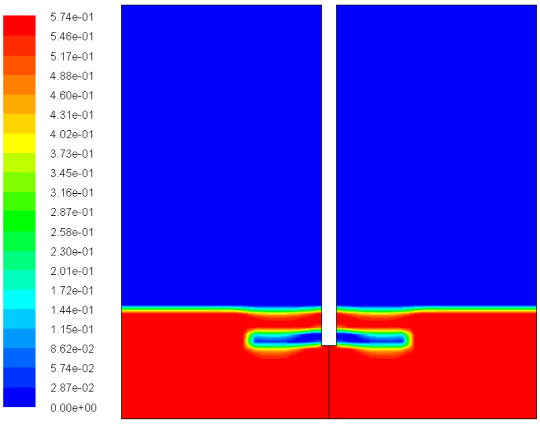

Figure 2 (a): Initial Sand volume fraction at t=0. (v/v)

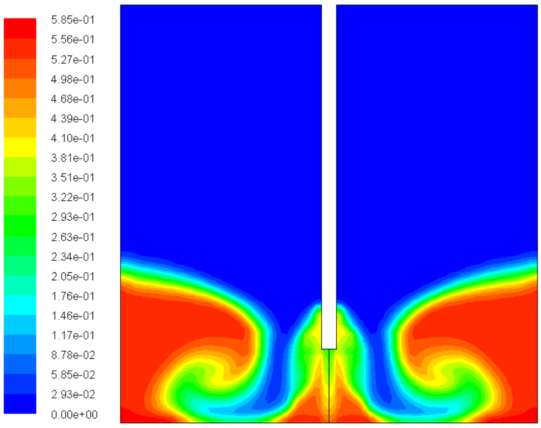

Figure 2 (b): Sand volume fraction after 1 Sec. (v/v)

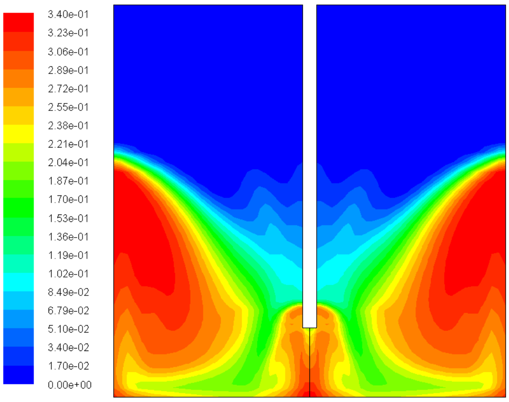

Figure 2 (c): Sand volume fraction after 10 Sec. (v/v)

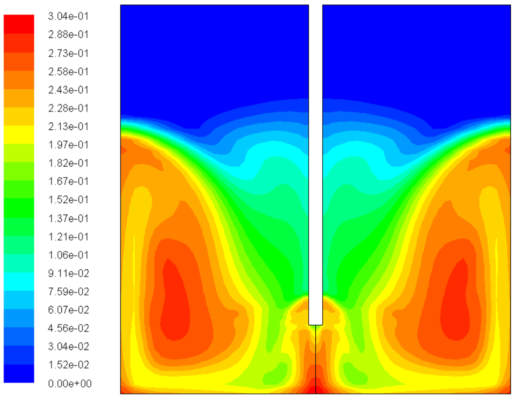

Figure 2 (d): Sand volume fraction after 20 Sec. (v/v)

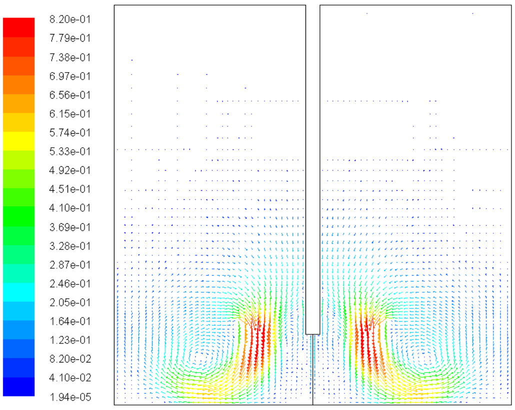

Figure 3 (a): Water velocity after 1 Sec. (m/s)

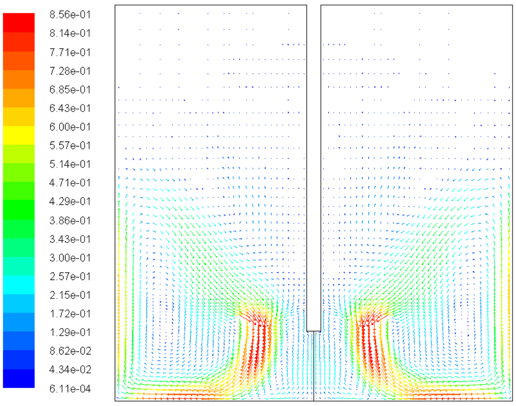

Figure 3 (b): Water velocity after 10 Sec. (m/s)

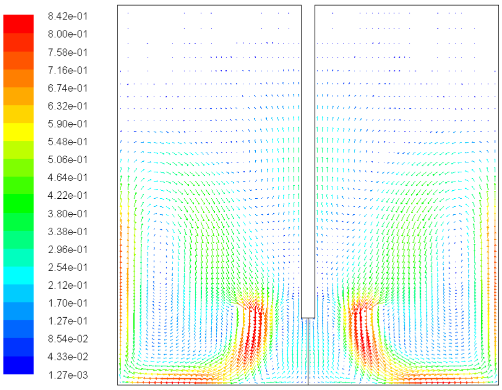

Figure 3 (c): Water velocity after 20 Sec. (m/s)

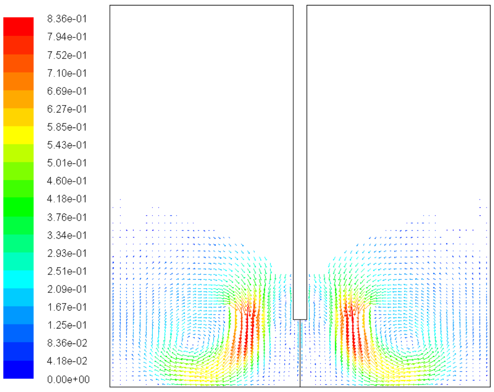

Figure 4 (a): Sand velocity after 1 Sec. (m/s)

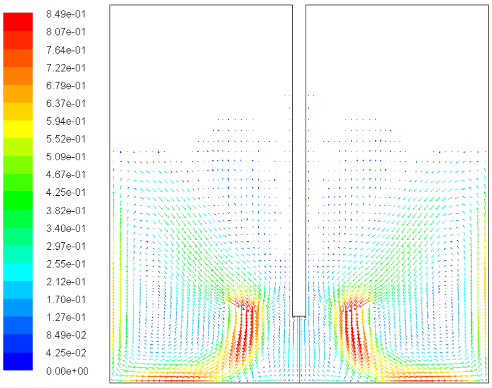

Figure 4 (b): Sand velocity after 10 Sec. (m/s)

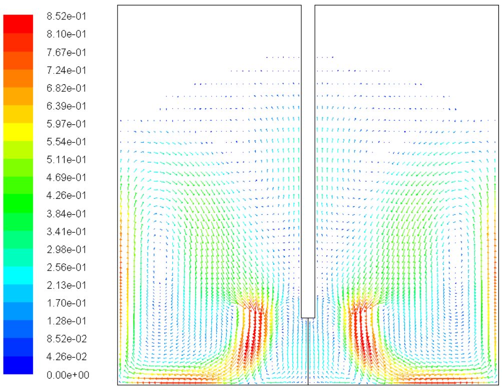

Figure 4 (c): Sand velocity after 20 Sec. (m/s)

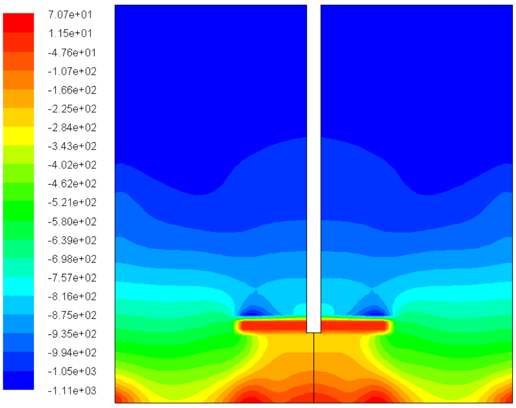

Figure 5 (a): Mixture static pressure after 10 Sec. (pa)

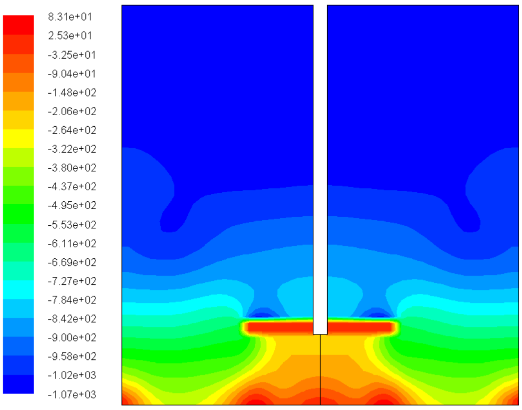

Figure 5 (b): Mixture static pressure after 20 Sec. (pa)

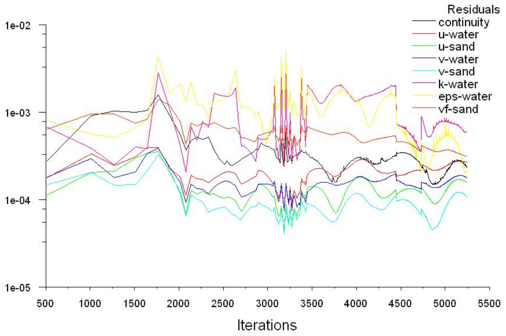

Figure (6): Scaled residuals of conservation equations for 20 Sec.

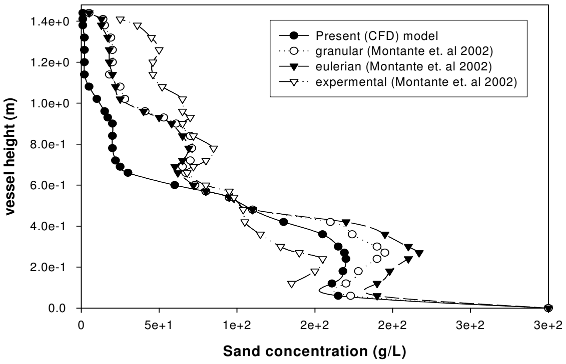

Figure (7): Comparison of the axial concentration profiles obtained with the Eulerian, the Granular , the experimental data (Montante et. al,2001), with the Present Granular-Eulerian model for (d_p=327 μm).

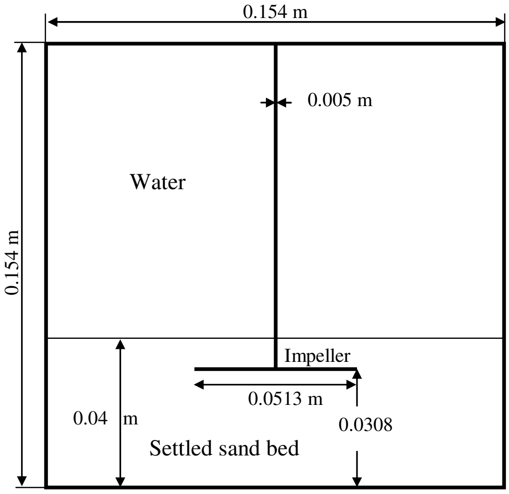

Figure (8): Problem Specification

Table (1): Tank, impeller and material properties. D – Impeller diameter, C –off-bottom clearance, T – tank diameter, N – shaft speed, H – liquid level.

Geometry	Properties	
Single , Pitched-blade turbine (four blades at 45°) D=T/3; C=T/5 N=1600 rpm T=H=0.154 m	Liquid	ρ =998.2 kg m^{-3} μ =0.001003 kg m^{-1} s^{-1}
	Solids	ρ =2500 kg m^{-3} μ = 0.001003 kg m^{-1} s^{-1} d_p =327 µm

Table (2): The polynomial coefficients for Eq.(7) [(23)].

Variable	***A1***	***A2***	***A3***	***A4***	***A5***	***A6***
u velocity	-7.1357e-2	54.304	-3.1345e+3	4.5578e+4	-1.9664e+5	-
v velocity	3.1131e-2	-10.313	9.5558e+2	-2.0051e+4	1.1856e+5	-
kinetic energy	2.2723e-2	6.7989	-424.18	9.4615e+3	-7.7251e+4	1.8410e+5
dissipation	-6.5819e-2	88.845	-5.3731e+3	1.1643e+5	-9.1202e+5	1.9567e+6

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