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# Investigation of the Flow Field Development Inside a Rotating Packed Bed with the Use of CFD

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In the present work numerical investigations of the two-phase flow field inside a Rotating Packed Bed (RPB) are performed with the use of Computational Fluid Dynamics (CFD). The RPB geometry will eventually be used for the production of nanoparticles of $CaCO_3$ and $4MgCO_3Mg(OH)_24H_2O$. In the respect, the development of appropriate numerical models for the optimization of the overall process is significant and the use of CFD methods and the development of representative CFD models can be of prime interest. For this reason, a computational grid modelling of the rotating packed bed geometry was created in which two fluids, one in gas phase and one in liquid phase, are flowing in co-flow alignment. For the gas phase fluid, properties of air were applied, while for the liquid phase properties of water were used. The Realizable k-ε turbulence model was used for the computations together with the volume of fluid (VOF) methodology in order to model the two-phase flow development and the gas-liquid interactions. The numerical analysis was performed using a steady flow assumption by applying a rotating frame of motion for the RPB geometry. The RPB geometry was modelled as an isotropic porous medium of predefined pressure loss formula taking into consideration the RPB core geometrical characteristics. The results from the computations provided a detailed view inside the RPB core revealing the various interactions between the gas and liquid phases in relation to the RPB operational conditions. The results of the computational study will provide appropriate information that will help in the development of simpler but accurate RPB computational models which will be able to provide rapid and reliable results regarding the two-phase flow field development and interaction inside the RPB core.

## 1. Introduction

Rotating Packed Bed (RPB) technology, which was invented by Ramshaw and Mallinson (1981), is of high interest in industrial applications that invlove high mixing of different phase fluids and it is widely used in these areas in order to increase the mass transfer and micromixing efficiency (Ouyang et al., 2018). In RPBs, flow is forced radially inside a rotating porous medium in order to intensify the two phase flow mixing and dispersion of various selected fluids. As a result, its usage intensifies separation and reaction processes, nanoparticle synthesis, separation efficiency of liquid mixtures in chemical industry (Qammar et al., 2018), and is also proposed for post combustion $CO_2$ capture. The generated flow pattern charasteristics inside a RPB are of high interest, however, difficult to be understood and modelled with accuracy. Various studies can be found in the literature that attempt to mathematically model the dispersion and the mixing of the liquid and gaseous phases of fluids inside an RPB. Among others, Yan et al. (2012) derived a mathematical model in order to describe the realistic flow conditions inside an RPB including pressure drop, turbulence mixing and liquid film thickness and Sang et al. (2017) established a mathematical model for the prediction of the mass transfer area. A computational approach that has been widely used in the last decade towards this goal is Computational Fluid

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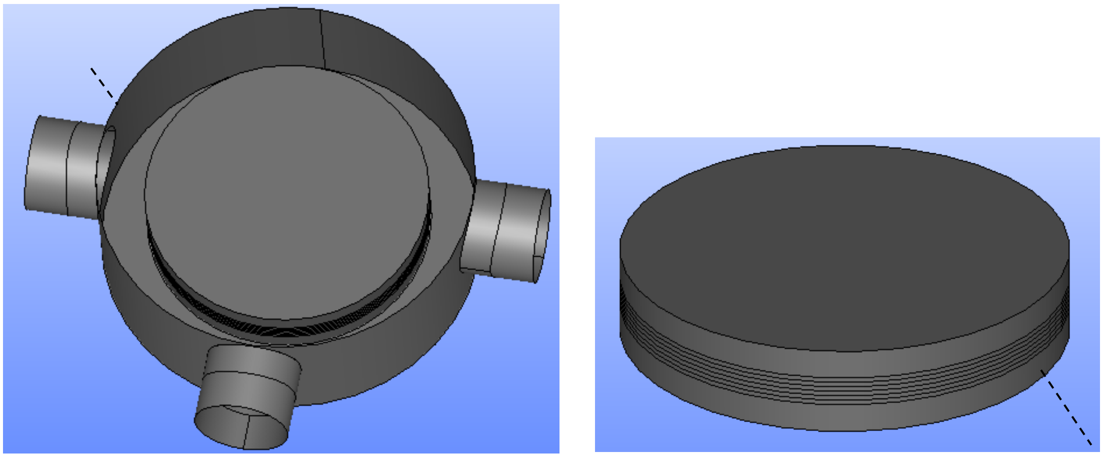
Dynamics (CFD), a fluid mechanics methodology that is able to shed light in the complex flow characteristics inside a RPB. Regarding RPB studies with the use of CFD, the following works can be mentioned.

Hugo and Larachi (2009) studied the impact of the air flow inlet variation on the flow distribution inside the RPB core, Hamedi et al. (2010) used three-dimensional CFD modelling in order to study the effect of the gaseous phase flow rate on the pressure drop inside a RPB with the use of RNG k-ε turbulence model. The RNG k-ε model is presented in Orszag et al. (1993). Peng et al. (2017) used two-dimensional CFD for analysing the effect of the rotating velocity on the fluid mixing inside RPB. Ouyang et al. (2018) modelled a two-dimensional fluid flow with the use of the Rializable k-ε turbulence model, which was introduced for modelling turbulent flows, by Shih et al. (1995). More advanced turbulence modelling approaches with the use of Reynolds stress turbulence models (RSM) were also adopted. For instance, Shi et al. (2013) used 2D CFD computations with a RSM adoption in order to identify the flow patterns inside the RPB. Guo et al. (2016) performed two dimensional CFD computations for modelling the micromixing efficiency in an RPB with a RSM model. They concluded that the rotating speed and the liquid inlet velocity can enhance the RPB micromixing efficiency.

An accurate RPB CFD model should include a turbulence model that is capable of capturing the complex turbulence flow characteristics, a proper implementation of a two phase flow model being able to describe the phases interaction and finally, a precise model of the RPB packing zone in order to model with accuracy the pressure drop inside the RPB core. In the current study, three-dimentional CFD, with FLUENT commercial software (Ansys® Academic Research, Release 16.2) was used, with the implementation of the RNG k-ε turbulence model. The widely used Volume of Fluid (VOF) methodology (Hirt and Nichols,1981), was applied for modelling the two phase flow interaction, which is a widely used method for modelling two phase RPB flows and the implementation of the the pressure drop law as described in Azizi (2019) inside the RPB core. The overall modelling approach is very challenging since it should combine the capturing of 3D flow characteristics with numerical stability and fine resolution of the flow structures. As a result, to the authors knowledge, no similar approach has been presented so far, in the literature and such an attempt is the significant contribution of this work. The proposed methodology and approach is able to provide the 3D flow and turbulent structures inside the RPB, incorporate all the geometrical characteristics of the packing material and help in the improvement of the overall RPB design, finding the optimal geometry and flow conditions. The final goal of the presented work which is a part of a bigger project is to derive a simple yet accurate mathematical model for rapid calculations for the production of $CaCO_3$ and $4MgCO_3Mg(OH)_24H_2O$ nanoparticles with the use of a RPB.

## 2. Rotating Packed Bed model development

For the CFD computations a computational grid for a 10-degrees sector of the overall cyclic RPB geometry, as presented in Figure 1, was created and used. The computational grid consisted of ~100,000 computational nodes. In the CFD computations rotational periodicity conditions were applied in the sector sides in order to significantly reduce the computational effort and time. The computational grid inlet region was splitted in two equal 5-degrees sub-sectors in order to apply the air and water inlet co-flow conditions inside the RPB. Typical views of the computational grid and the inlet regions are presented in Figure 2.



*a)* *b)*

*Figure 1: Typical views of the overall cyclic RPB geometry a) overall inside view (front cover not shown for clarity) b) filling material disk inside RPB*

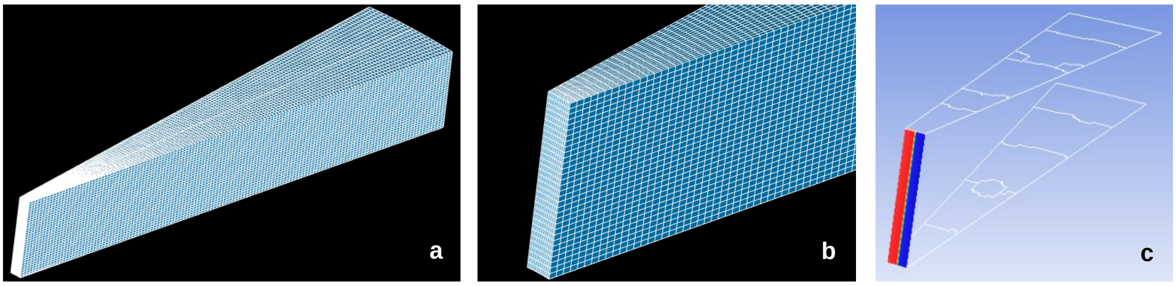



*Figure 2: a),b) Typical views of the computational grid, and c) the gas (red) and liquid (blue) phase inlet regions*

The CFD computations were performed in Ansys/Fluent CFD software with the use of the Volume of Fluid (VOF) method in which an additional transport equation of the volume fraction is being solved in order to determine the interface surface between the gas and liquid phases, as presented in Eq(1).

$$\frac{\partial}{\partial t}(\alpha_l\rho_l)+\frac{\partial}{\partial x_j}(U_i\alpha_l\rho_l)=0 \tag{1}$$

where the gas phase volume fraction, $\alpha_g$, and the liquid phase volume fraction, $\alpha_l$ , are connected by Eq(2).

$$\alpha_g=1-\alpha_l \tag{2}$$

For the turbulence modelling,the Realizable k-ε turbulence model with Enhanced Wall Treatment option was applied. The CFD computations were performed as pseudo-transient with the use of a rotating frame of motion. For the numerical discretization 2$^{nd}$ order discretization schemes were applied. The geometrical characteristics of the RPB packing were included in the numerical analysis by following an isotropic porous medium approach in which the pressure drop imposed by the RPB packing was taken into consideration by the addition of dedicated source terms in the Navier-Stokes momentum equations, as presented in Eq(3).

$$\frac{\partial}{\partial t}(\rho U_i)+\frac{\partial}{\partial x_j}(\rho U_i U_j)+\frac{\partial P}{\partial x_i}-\frac{\partial}{\partial x_j}\left[(\mu+\mu_t)\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)\right]=S_M+S \tag{3}$$

where $S_M=S_{cor}+S_{fg}$, $S_{cor}=-2\Omega\times U$, $S_{cfg}=-\rho\Omega\times(\Omega\times R)$, $S^T=\left(\frac{\partial P}{\partial x},\frac{\partial P}{\partial y},\frac{\partial P}{\partial z}\right)$, Ω is the angular velocity, R is the local radius, μ and $\mu_t$ the molecular and the turbulent viscosity.

The imposed pressure drop formulation was based on the conclusions of Azizi (2019) in which a generalized correlation of the pressure drop of fluids through woven screen meshes is presented. In this correlation the geometrical characteristics of the woven screen meshes are directly linked to the imposed pressure drop through Eqs(3) to (7). The hydraulic diameter and Reynolds number are defined by Eq(4).

$$D_h=4\frac{\varepsilon}{\alpha}\ [m] \rightarrow Re_h=\frac{\rho U_0 D_h \tau}{\mu\varepsilon} \tag{4}$$

The geometrical characteristics (ε, a, W, L, τ) of the filling material are defined by Eq(5).

$$\begin{gathered}\varepsilon=1-\left[\frac{\pi}{2L}\left(\frac{b}{M}\right)^2 W\right]\\ a=\pi\frac{W}{M^2}\\ W=\sqrt{b^2+M^2}\\ L=2b\\ \tau=1+1[(1-\varepsilon)/2]\end{gathered} \tag{5}$$

where b, M are defined in [m] as shown in Figure 3.

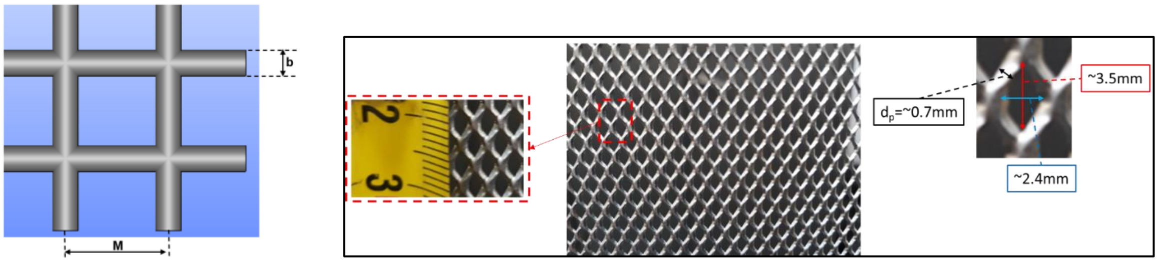
The pressure drop coefficient, f ,of the filling material is defined by Eq(6).

$$f=\frac{22.97}{Re_h^{0.8011}}+0.3079 \tag{6}$$

The pressure drop coefficient is correlated to the pressure drop by Eq(7).

$$f=\frac{\Delta p}{L}\frac{\varepsilon^2 D_h}{2U_0^2\rho} \tag{7}$$

The selection of the correlation of Azizi (2019) was based on the fact that the RPM filling material was similar to the one of a woven mesh as presented in Figure 3.




a) b)

*Figure 3: a) Geometrical characteristics of typical woven mesh and b) geometrical characteristics of the filling material of the RPB (right)*

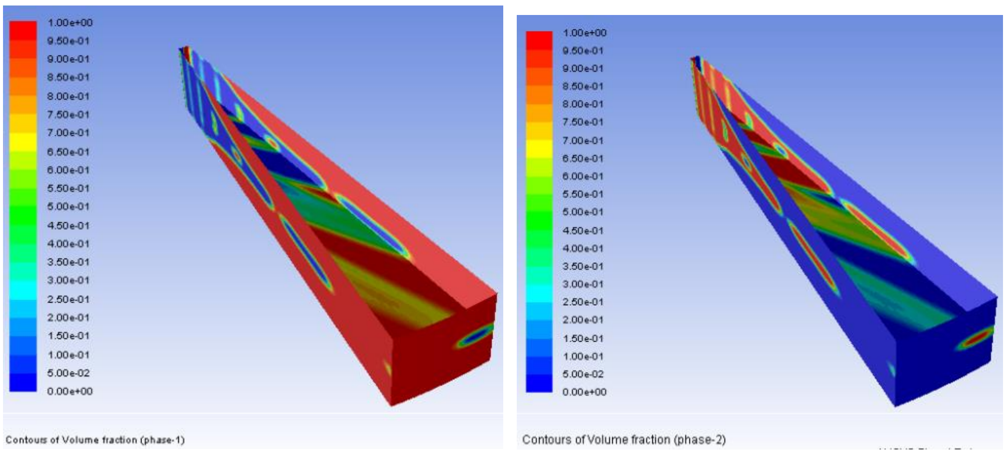
## 3. Results and discussion

The boundary conditions of the CFD computations are presented in Table 1.

*Table 1: Boundary conditions of the CFD computations*

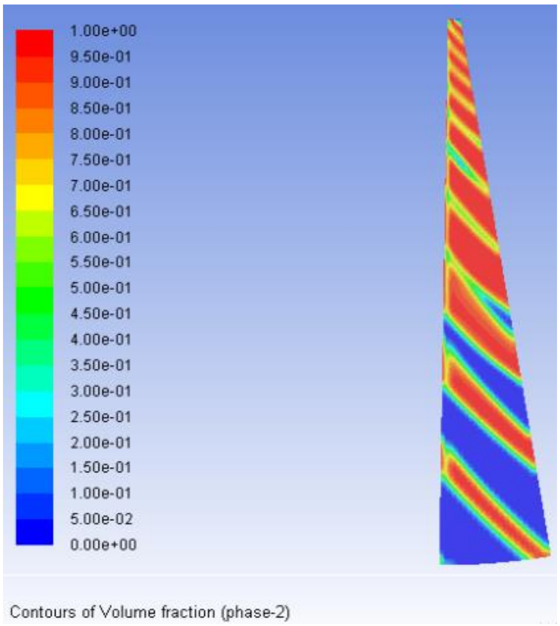
| | Gas phase | Liquid phase | Units |
|---|---|---|---|
| Density ($\rho$) | 1.225 | 998.2 | kg/m$^3$ |
| Inlet Velocity ($U_0$) | ~0.4 | 2 | m/s |
| Turbulent Intensity | 3 % | 3 % | - |
| Turbulent length scale | 0.00035 | 0.00035 | m |
| Outlet Pressure | 101,325 | | Pa |
| RPM rotational speed | 955 | | RPM |

Typical views of the CFD computations are presented in Figures 4 and 5, where the flow development of the gas and liquid phases is presented by illustrating the respective volume fractions. For a more comprehensive understanding of the interaction and mixing between the gas and liquid phases CFD computations were performed for two cases of different pressure drop conditions for the RPB filling material. In the first case the applied pressure drop followed the correlation presented in the work of Azizi (2019) while in the second case a correlation of significantly reduced pressure drop was applied.

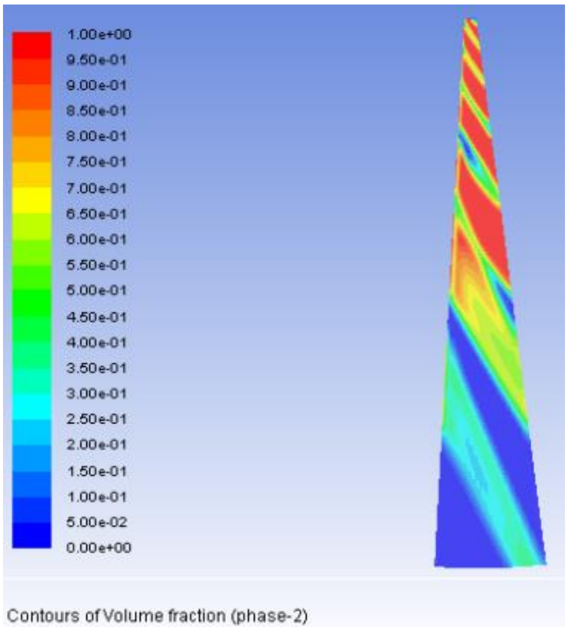



a) b)

*Figure 4: a) Gas phase and b) Liquid phase development inside the RPB*




*a)*




*b)*

*Figure 5: Liquid phase development inside the RPB middle plane with a) decreased and b) increased pressure drop (Azizi (2019)) inside the RPB packing*

From the presented application and the CFD analysis, the following findings were observed regarding the gaseous and liquid fluid phases inside the RPB:

- The incorporation of the RPB packing in the calculations, leads to increased mixing between the gaseous and the liquid fluid phases, as it can be seen in Figure 4 and mainly in Figure 5b. As a result, large areas where the volume fraction takes values between 0.3 to 0.7 are present inside the RPB core. On the other hand, for the case where a reduced pressure drop is applied (Figure 5a), the volume fraction takes distinct values either close to unity, which is the case of liquid phase, or closer to zero, which is the case of the gaseous fluid phase. This observation indicates reduced mixing for this case between the two fluid phases.
- The increased pressure drop that is induced from the RPB packing, enhances the overall diffusion process of the liquid inside the gaseous phases resulting in an increase of the mixing between the two phases.
- The proper choice of the packing material of the RPB is of critical importance since the latter significantly affects the pressure drop inside the RPB and consequently the mixing of the two phases. Different geometrical characteristics of the selected packing material can lead to different values of pressure drop, diffusion and mixing.
- The presented methodology has the potential to incorporate arbitrarily selected packing geometries based on woven meshes (Figure 3a) and can be easily used for the calculation of the overall mixing, pressure drop and efficiency of the RPB.

## 4. Conclusions

From the performed investigations, the main advantages and points that could be improved in the presented methodology can be summarized to the following statements. Regarding the advantages of the methodology:

- Rapid and accurate 3D solutions can be achieved with reduced demands in CPU power and memory requirements. The computational time is varying between 2 to 4 hours depending on the numerical difficulties resulting from the flow structures development. By using this modelling approach, which corresponds to a heavily dense computational grid for a 10-degrees sector of the RPB, the solution is accelerated by more than 50 times in relation to a similar computation for the overall RPB geometry with a computational grid of similar quality.
- With the use of a fine computational mesh the flow field structures and the phases mixing can be modelled with increased accuracy.
- The proposed methodology gives the ability to incorporate all the important geometrical characteristics of the RPB packing material and accurately model its impact on the overall mixing of the two phases.

- The proposed methodology describes in detail all the complex fluid phenomena together with the effect of turbulence on the overall RPB efficiency.

The points of imporvement can be summarized as follows:

- The use of periodic boundary conditions cannot include the effect of the gravitational force, although its impact may be insignificant especially in high rotational speeds.
- The computational domain does not take into consideration the overall RPB geometry and does not compute the interaction of the RPB core with the outer case of the RPB.

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## References

Azizi F., 2019, On the pressure drop of fluids through woven screen meshes, Chemical Engineering Science, 207, 464–478.

Guo T.Y., Shi X., Chu G.W., Xiang Y., Wen L.X., Chen J.F., 2016, Computational fluid dynamics analysis of the micromixing efficiency in a rotating-packed-bed reactor, Industrial & Engineering Chemistry Research, 55, 4856-4866.

Hamedi M., Haghshenas M.F., Esfahany M.N., 2010, Computational fluid dynamics analysis of fluid flow in a novel rotating packed bed. 13th Iranian National Chemical Engineering Congress & 1st International Regional Chemical and Petroleum Engineering, 25–28 October, Kermanshah, Iran.

Hirt C.W., Nichols B.D., 1981, Volume of fluid (VOF) method for the dynamics of free boundaries, Journal of Computational Physics, 39(1), 201–225.

Hugo L.C., Larachi F., 2009, Analysis of flow in rotating packed beds via CFD simulations - Dry pressure drop and gas flow maldistribution, Chemical Engineering Science, 64, 2113–2126.

Orszag S.A., Yakhot V., Flannery W.S., Boysan F., Choudhury D., Maruzewski J., Patel. B., 1993, Renormalization group modeling and turbulence simulations, In International Conference on Near-Wall Turbulent Flows, 15-17 March, Tempe, AZ, USA, 1031–1040.

Ouyang Y., Zou H.K., Gao X.Y., Chu G.W., Xiang Y., Chen J.F., 2018, Computational fluid dynamics modeling of viscous liquid flow characteristics and end effect in rotating packed bed, Chemical Engineering & Processing: Process Intensification, 123, 185–194.

Peng X., Xuesong L., Xin Y., Ingham D., Ma L., Pourkashanian M., 2017, Characteristics of liquid flow in a rotating packed bed for $CO_2$ capture: A CFD analysis, Chemical Engineering Science, 172, 216–229.

Qammar H., Hecht F., Skiborowski M., Górak A., 2018, Experimental investigation and design of rotating packed beds for distillation, Chemical Enigneering Transactions, 69, 655–660.

Ramshaw C., Mallinson R.H., 1981. Mass Transfer Process, US Patent No. 4283255.

Sang L., Luo Y., Chu G.W., Liu Y.Z., Liu X.Z., Chen J.F., 2017, Modeling and experimental studies of mass transfer in the cavity zone of a rotating packed bed, Chemical Engineering Science, 170, 355–364.

Shi X., Xiang Y., Wen L.X., Chen J.F., 2013, CFD analysis of liquid phase flow in a rotating packed bed reactor, Chemical Engineering Journal, 228, 1040-1049.

Shih T.H., Liou W. W., Shabbir A., Yang Z., Zhu. J., 1995, A New k-ε Eddy-Viscosity Model for High Reynolds Number Turbulent Flows - Model Development and Validation, Computers & Fluids, 24(3), 227–238.

Yan Z.Y., Ruan Q., Lin C., 2012, Hydrodynamics in a rotating packed bed II, A mathematical model, Industrial and Engineering Chemistry Research, 51, 10482–10491.