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MODELING AND ANALYSIS OF A NEW STIR GEOMETRY USING MULTIBODY DYNAMICS AND MOVING PARTICLE SIMULATION

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Abstract: *The present work aims to evaluate the agitation system of a homogenizer constituted by a non-conventional stir agitation geometry in a regular tank with baffles, through the modeling and computational simulation of a parameterized model, allowing the analysis of different geometries and the consequent optimization of time and resources. For the study carried out in this work, the non-conventional stir agitation geometry homogenizer was modeled using a CAD program; then, RecurDyn™, a multibody system program, was used for the dynamic analysis, where together with ParticleWorks™, a program based on MPS (Moving Particle Simulation Method), enabled the fluid dynamics of agitation to be simulated and the parameters necessary for the evaluation were extracted. The hydrodynamics that occurs within the agitation system is qualitatively measured by the particle velocities, where it was observed that for this work model a large high-speed recirculation zone caused only by the stir geometry, which is noticeably better for particle scattering than other literature when compared. From the power number ratio (Np) vs. the Reynolds number (Re), a curve was graphically generated and from it the amount of energy that would be needed to maintain the flow in a laminar regime is determined, and also how much energy would be needed to reach the turbulent regime; from the qualitative and quantitative comparison of the Np-Re curve in relation to the values obtained from other references, it was noticed that the new model of the agitator system requires less energy to obtain a high value of the Reynolds number. In addition, from the ratio of pumping number (Nq) vs. the Reynolds number (Ne), the corresponding curve was obtained, observing that the behavior of the present model has a low pumping ratio, that is, a low level of agitation caused by its large geometry, proving the expected result.*
Keywords: *non-conventional geometry, moving particle simulation method, fluid dynamics, power number, pumping number*

1. INTRODUCTION

Agitation systems are widely used in chemical and metallurgical industries in processes such as polymerization, catalytic reactions, precipitation and others, as established by Cheng *et al*. (2016).

Design of most types of process equipment generally involves defining and meeting a well-understood process objective. For example, the design of a distillation column would begin with a statement of the desired degree of separation.

In agitation equipment, a comparable procedure for specifying and designing has not been established in the published literature. The main reason of it is the wide range of applications for which agitators are used.

Provide technique for improving communication of agitation requirements as well as describing how this information can be converted into the proper hardware is the objective of the design procedure.

In industries driven by chemical process, the turbine agitators' applications involve one or more of the following purposes (Gates, 1975):

- Chemical reaction: distribute reactants and products aiming desired reactions;
- Heat transfer: increase convective motion adjacent to the transport surfaces;
- Bulk mixing: combine liquids of dissimilar composition and properties;
- Mass transfer: promote contacting between separate phases and different compositions;
- Phase interaction: promote suspension of solids or dispersion of gases and immiscible liquids.

Within the precipitation processes, the impeller tank assembly must be sized to ensure a homogeneous mixture of the reagents and the suspension of the precipitated. Some important parameters in this scenario are the power curve, which allows to determine the optimum speed of rotation of the impeller (Wang *et al.*, 2010), the pumping number that determines the system's ability to maintain suspended solids, as proposed by Olino (2010), and the hydrodynamic analysis of the fluid flow within the tank, which allows to analyze and understand the expected flow within the tank agitated (Cheng *et al*., 2016).

Trying to develop a real scale prototype to these problems could be hard, tiring and adding little value, because even with a lot of effort and expenses, this would not be sufficient to get the probably expected result.

So, in order to predict the results of these systems, the modern engineering is trying to focus its efforts in computational simulations involving static, dynamic, fluid dynamics and heat transfer analyses, among others.

The most used software in the engineering industry are CAEs that are able to predict with a certain degree of efficiency stresses, deformations, displacements, accelerations, flow velocities, heat transfer rate and topology behavior of a flowing fluid. As an example, we can cite Ansys™ software, it is well endowed with vast tools from end to end, and can count with Fluent, a fluid analysis software by variable volumetric mesh formed by finite elements, which, to summarize, requires a certain amount of time analysis of the mesh optimization so that the results are not harmed, in the case of fluid analysis, by the formation of vorticities or fields of poorly predicted speeds caused by improper meshes. Other examples of CAE are those focused on dynamics, both of multibody and fluids, this one represented by ParticleWorks™ and that one by RecurDyn™. ParticleWorks™ is a mesh free Moving Particle Simulation (MPS) method analysis software that does not require mesh formation for its objective to be achieved. RecurDyn™, on the other hand, is an easy-to-use multibody dynamics software capable of performing the simulation with more sophisticated boundary conditions and obtaining the outputs is simpler for relatively complex modeling compared with other conventional CAE.

Such software can be used concurrently (RecurDyn™ and Particleworks™) for various purposes. As examples we can mention bearings and gears lubrication phenomenon by the movement relative to the lubricant, the power generated by a given turbine geometry when it is subjected to the dragging of a fluid, the resulting pressure in the flow caused by the rotation of a rotor of a centrifugal pump and in the case of our current study, the power and pumping curves can be determined for a unconventional impeller and also, a hydrodynamic analysis in a stirred tank with baffles, using MPS tools, considering a three-dimensional flow, incompressible, isothermal, monophasic in steady state.

2. SYSTEM GEOMETRY

The geometry used in this work is a vertical tank, with a volume of 5,000 l and mechanically agitated. The walls of this tank are the boundaries. It has 1,853 (mm) radius and 2,300 (mm) height, with bottom radius 1,183 (mm) well rounded. The tank has 4 baffles 90 degrees apart with 154.7 (mm) width, it has a central shaft 80 (mm) diameter end-to-end. In the shaft's end has an unconventional geometry stir with 1,380.57 (mm) diameter, 597.49 (mm) height and 199.88 (mm) deep composed by 2 blades as shown in Figure 1. It's worth mentioning that the stir geometry was not created by a literature guided method proposed by Gates (1975), it's a simple model that was put to the test to show its efficiency, or the lack of it, for the applied resolution method.

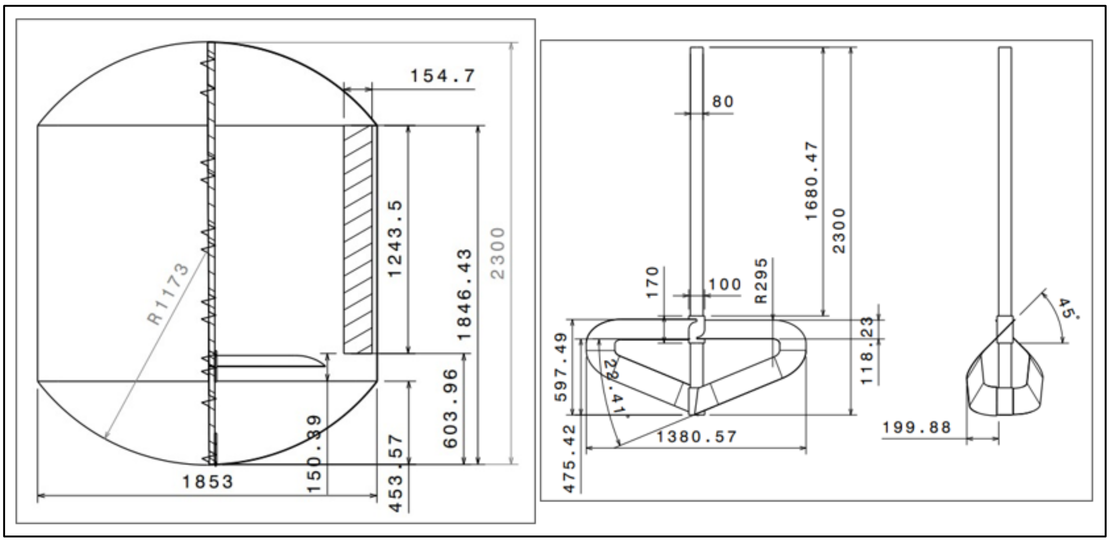


Figure 1. **Dimensions of the tank (left) and stir (right).**

Thus, the **D**stir/**D**tank ratio is equals to 0.745. This mechanical design was done in a conventional CAD software.

3. MODELING AND SIMULATION

This section discusses the step-by-step of the modeling and co-simulation performed by RecurDyn™ and Particleworks™ in order to achieve both dynamic and hydrodynamic behavior of the agitation model.

3.1. Multi-body dynamics on Recurdyn

Figure 1 model was exported to RecurDyn™ software interface with its original measures. Stir, shaft and tank were modeled as rigid bodies with constraints imposed at its respectively mass centers. The tank was fixed in the inertial reference frame [0,0,0], the stir was fixed in the shaft at stir's mass center point [-2.14, -7.66, -815.54] and the shaft is constrained with a revolute with the tank at shaft's mass center point, which coincides with inertial reference frame. So, the only body that is able to get motion is the shaft, which rotates along Y+ axes. Thus, the combined system of kinematic constraint is given by Eq. (1).

$$\Phi^k(q) = \begin{bmatrix} x_1 & y_1 & \phi_1 & x_2 & y_2 - c & \phi_2 & x_3 & y_3 \end{bmatrix}^T \tag{1}$$

And the driving constraint in the shaft is given by Eq. (2):

$$\Phi^D(q) = \phi_1 - \omega t \tag{2}$$

The kinematic equations that determine the motion of the system are thus Eq. (3):

$$\Phi(q,t) = \begin{bmatrix} x_1 & y_1 & \phi_1 & x_2 & y_2 - c & \phi_2 & x_3 & y_3 & \phi_1 - \omega t \end{bmatrix}^T \tag{3}$$

The equation of motion and the constraint equations, $\dot{q} = v$ and $\dot{v} = a$ constitute the following algebraic differential Eq. (4) (Recurdyn, 2017):

$$\begin{bmatrix} F(q,v,a,\lambda,t) & \Phi(q,t) & \dot{\Phi}(q,v,t) & \ddot{\Phi}(q,v,a,t) & \dot{q} - v & \dot{v} - a \end{bmatrix}^T = 0 \tag{4}$$

Applying Newton's method to solve non-linear equations, Eq. (5) and Eq. (6) are obtained:

$$H_p \Delta p = -H \tag{5}$$

$$p_n^{i+1} = p_n^i + \Delta p,\ i = 1,2,3,... \tag{6}$$

where H_p is shown by Eq. (7):

$$H_p = \begin{bmatrix} F_q & F_v & F_a & F_\lambda \\ \mathbf{\Phi}_q & 0 & 0 & 0 \\ \dot{\mathbf{\Phi}}_q & \dot{\mathbf{\Phi}}_v & 0 & 0 \\ \ddot{\mathbf{\Phi}}_q & \ddot{\mathbf{\Phi}}_v & \ddot{\mathbf{\Phi}}_a & 0 \\ U_0^T & \beta_0 U_0^T & 0 & 0 \\ 0 & U_0^T & \beta_0 U_0^T & 0 \end{bmatrix} \tag{7}$$

Since F and $\boldsymbol{\Phi}$ are a high non-linear degree function of q, v, a and λ, cares must be taken when obtaining the nonzero expressions in H_p, so that they can be efficiently calculated (Recurdyn, 2017).

Where body one is the shaft, body two is the stir, body three is the tank, c is a constant number that means the linear distance between stir and shaft mass center and ω is the angular velocity input that will going to rotate the shaft. The model exported to RecurDyn™ interface can be seen in Figure 2, each body with its respectively coordinate axis and constraints.

To do this work, it was conducted 10 simulations, each one with a different Reynolds number, varying for this the kinematic viscosity of the fluid or angular velocity of the stir.

3.2. MPS Method on Particleworks

The Moving Particle Simulation (MPS) is an analytical method dealing with incompressible flow, in which continuum mechanics is discretized using particles. The fundamental governing equations of the MPS method are the continuity equation and Navier-Stokes equations, as we can see in the Eq. (8) and (9) (Prometech Software, 2016).

$$\begin{gathered} \cancel{\frac{\partial \rho}{\partial t}} + \cancel{\rho}\left(\vec{\nabla} \cdot \vec{v}\right) = 0 \\ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \end{gathered} \tag{8}$$

$$\frac{D\vec{u}}{Dt} = -\frac{\nabla P}{\rho} + v\nabla^2\vec{u} + \vec{g} \tag{9}$$

The Navier-Stokes equations are divided into two stages and all terms are solved explicitly, except for the pressure term, which is solved implicitly.

Explicit calculation terms except pressure terms, implicit pressure calculation and correction of position and speed by pressure gradient are shown respectively in Eq. (10), (11) and (12) next:

$$\frac{\vec{u}^* - \vec{u}^k}{\Delta t} = v\nabla^2\vec{u}^k + \vec{g} \tag{10}$$

$$\nabla^2 P^{k+1} = \frac{\rho}{\Delta t^2}\frac{n^* - n^0}{n^0} = \tag{11}$$

$$\frac{\vec{u}^{k+1} - \vec{u}^*}{\Delta t} = -\frac{\nabla P^{k+1}}{\rho} \tag{12}$$

Particleworks performs the DES (detached eddy simulation) model for calculating turbulence, which has a good prediction for a high turbulence rate (Prometech Software, 2016).

The fluid has three-dimensional flow, incompressible, isothermal, monophasic in steady state.

The power number N_P and the pumping number N_Q, are dimensionless numbers which, when associated with the Reynolds number, facilitate the understanding of how much power is required taking in account the level of (turbulent or laminar flow). Both power and pumping number are represented in Eq. (13) and (14) respectively:

$$N_P = \frac{P}{N^3 D^5 \rho} \tag{13}$$

$$N_Q = \frac{Q}{ND^3} \tag{14}$$

Reynolds number, applied to rotational systems, is as shown in Eq. (15):

$$\mathrm{Re} = \frac{D^2 N \rho}{\mu} \tag{15}$$

Where P is the power input in the shaft (W), N is the angular velocity of the shaft (rad/s), D is the diameter of the stir (m) and Q is the flow rate of the stir (m³/s). The relation μ/ρ is equals to, kinematic viscosity.

Power and flow rate are obtained with the Eq. (16) and (17) respectively:

$$P = T_m \omega \tag{16}$$

$$Q = v_m A \tag{17}$$

The term $\boldsymbol{T_m}$ is the average torque that moves the shaft, $\boldsymbol{v_m}$ is the average velocity of the particles and A is the tank cross section area.

3.3. Convergence Criteria

This MPS mesh free software doesn't have an iterative method for allocating position, speed, acceleration, energy, etc. The pressure gradient calculation equation is taken only once and from there it makes the necessary corrections for the velocity and position of the particles. What can happen is a high discordant value of this pressure gradient causing the speed to take values excessively high, the time step decrease, making the simulation longer or causing errors, stopping the analysis.

However, in the analysis of the multibody dynamic software, since it is solved by Newton's method, it does have an error tolerance. The same was implemented as a standard of 0.005 and a maximum time step of 0.01.

3.4. Boundary Conditions

The conditions adopted in the problems were the no slip condition between the fluid and the agitators and between the fluid and the walls of the tank for the CFD software. The fluid dynamics analysis domain contains the interior of the tank since there is no flow outside of that domain. The fluid fills the tank up to the height of the baffle. The particles are 50 mm diameter, generating a total of 33,144 particles. The gravity was set as 9.81 m/s² downward Y axis in RecurDyn^{TM} software. More details can be seen in the Fig. 2.

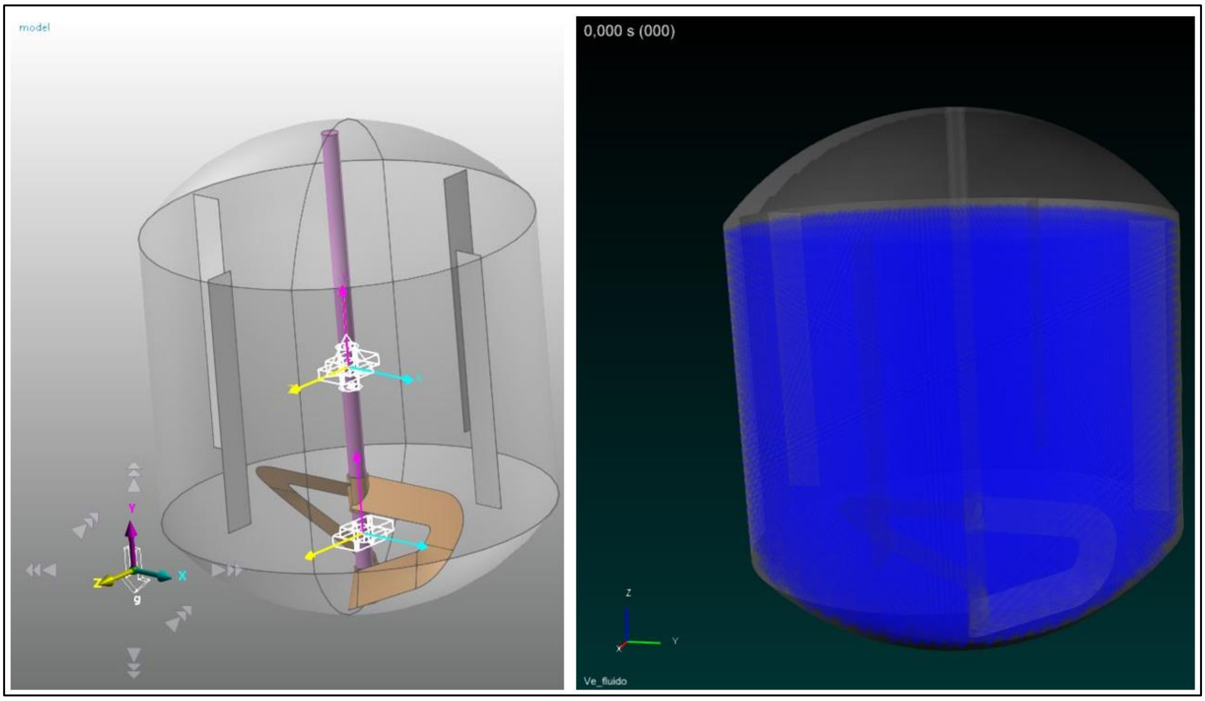


Figure 2. **Model exported to the multibody dynamic software (left), and to MPS mesh free software (right).**

4. RESULTS AND DISCUSSION

4.1. Particulate Fluid Dynamics Analysis

When it's about agitation systems, in general, it is important to keep in mind that low speed zones can cause different concentrations of solute causing the precipitation of compounds.

As shown in Figure 3 (left), a recirculation zone is caused by the concave ends of the stir geometry. It is relatively large and was obtained for a rotation N = 12 rad/s, in the observation plane YZ. We also see that this zone has high speeds, which is not really a problem for agitation phenomena. Note that the upper contour shows the formation of a central vortex, which drags the fluid from top to bottom and vice versa.

Figure 3 (center and right) is used to compare the fluid dynamics analysis of the different geometries of Sophia (2010) and Ferreira et. al. (2019), respectively.

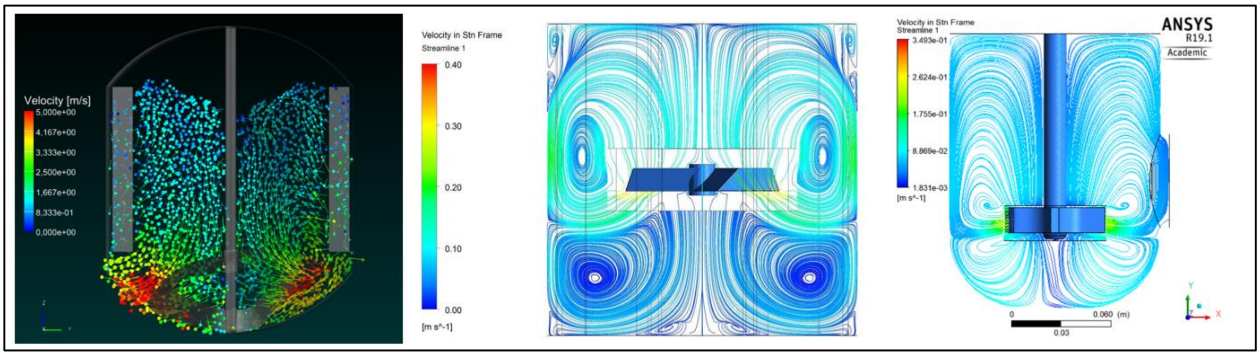


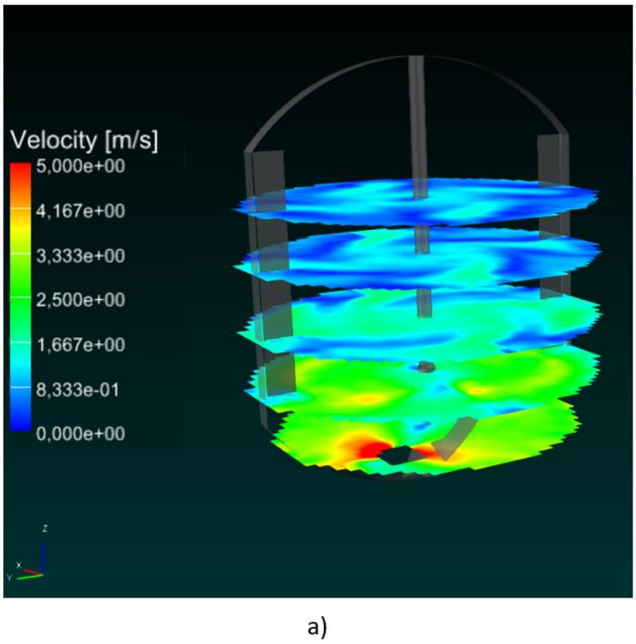
Figure 3. **Hydrodynamic analysis of this work impeller N = 12 rad/s (left); Flow pattern obtained by the frozen rotor model N = 30 rpm (Sophia, 2010) (center); Flow pattern obtained by the frozen rotor model N = 100 rpm (Ferreira, 2019) (right).**

We notice that Sophia's model (2010) has several recirculation zones, with the zone right below and right above the impeller being the big ones, but smaller ones, which we can call secondary, more susceptible to precipitation. An important cause of these zones is the flat bottom tank geometry.

The model by Ferreira (2019) has two distinct and less dangerous recirculation zones, as they are close to the impeller and have relatively high speed. Note that the secondary zones that existed in the model of Sophia (2010) do not occur in this model because the bottom of the tank is well rounded instead of flattened, turning this effect smoother.

The comparison between these models of homogenizers will be very difficult to carry good precision, since the differentiation between the type of rotor, the geometries of the rotor and the tank as well as it's relation between diameters and the impeller rotation model, in addition to other factors in relation to the models by Sophia (2010) and Ferreira (2019) for example. You can see that, in this current work, the graphic representation of the flow was made by vectors, the other two works used stream lines instead for an example.

Figure 4 shows the speed profiles obtained in the simulation of this work.



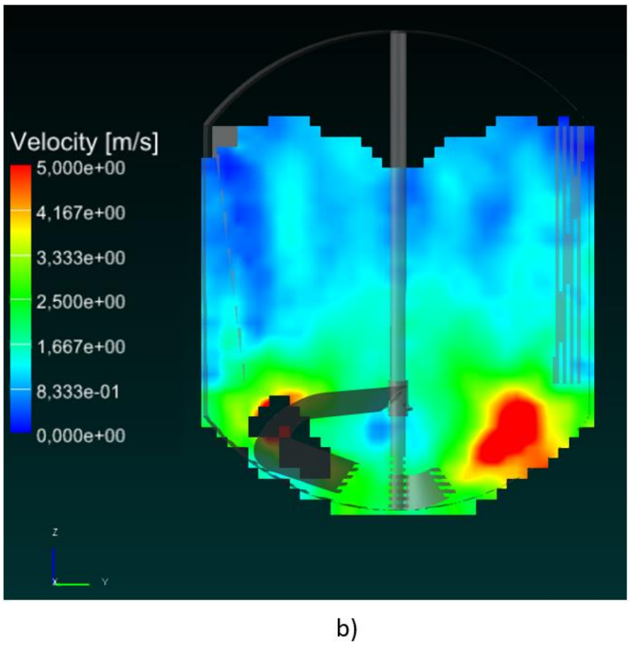
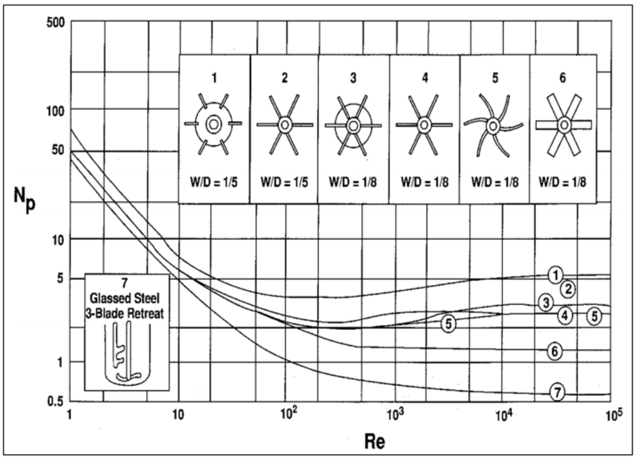


Figure 4. **Speed profiles obtained by the analysis: a) 5 top planes, b) the front view.**

4.2. Power Number

Conducting the analysis of our work with respect to the power number correlated to the Reynolds number, we compared it with respect to the literature to better understand if our analysis had a realistic character through the graphic analysis.

Figure 5 (left) shows the number of N_P *vs.* Re for different geometries and impeller width/impeller diameter ratio. We see next, in Figure 5 (right), that the present model follows the patterns already seen in the literature, but with a peculiar shape in the region Re = 10^5, which comes to be a characteristic of the geometric model.



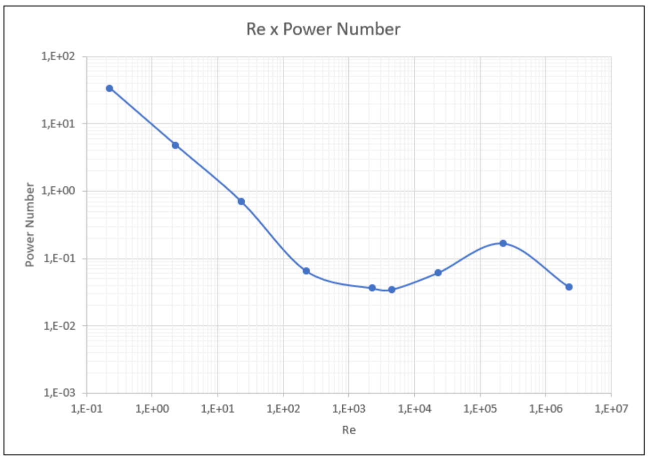


Figure 5. **N_P *vs.* Re for different geometries and impeller width / impeller diameter ratios (left) Uhl (1996) and N_P *vs.* Re for this current work impeller width / impeller diameter ratios = 0.745 (right).**

We note, by interpretation the graph in Figure 5 left and right that:

- Even in the laminar regime, which is where it requires the most energy consumption to maintain itself, the unconventional geometry model showed that it needs low energy, and when it is in the turbulent zone, its main application, has a lesser power number;

To achieve the turbulent regime, when the objective is suspended solids (Sophia, 2010), the results of N_P, are the most efficient among those compared in the literature, by Tab. 1:

Table 1. **N_P *vs.* Re for various geometries.**

Author	Radial impeller type	Power number variation Re > 10^3	D/T
Uhl (1996)	Figure 5 (left)	1 to 5	0.3 to 0.5
Oldshue (1983)	4 flat blades	1	-----
Nagata (1995)	8 flat blades, 4 flat blades @45°	1.2 to 1.4	0.6
Ferreira (2019)	Non-conventional	0.2 to 0.3	0.5
Sophia (2010)	4 flat blades	more than 1	0.5
Current work	Non-conventional	0.04 to 0.16	0.745

We notice from Tab. 1 that there are many factors to compare when we try to put alongside the power number required for the turbulent regime, such as the type of radial impeller, the number of blades, as well as their angles and sizes relations regarding to the diameter. Besides that, the relation between the diameter of the impeller regarding to the diameter of the tank itself, making comparisons for an impeller of unconventional geometry it's a tough work. However, after conducting the computational studies, we realized that this work model is that less consumes energy to reach a high Reynolds value.

4.3. Pumping Number

Another important number for system agitation analysis is the pumping number, considering that in some systems, in order to speed up the homogenization, we could only increase the speed of rotation of the impeller. However high numbers of Reynolds provided by high rotation speeds do not necessarily result in high pumping rates. Yet, the pumping number is presented so that next to the power number, a geometry efficiency limit is imposed, as can be seen better in Figure 6 (left).

We see from the study of this graph that from the turbulent regime, the ability of an impeller to supply flow to the fluid becomes constant regardless of the number of Reynolds.

Comparing this work to the literature, Paul, Obeng and Kresta (2004), found N_Q values around 0.6 and 0.9 for different diameter ratios, from $D/T = 0.25$ to 0.5, in that the higher the ratio of diameters, the lower the N_Q. This fact can be confirmed by the results of the simulations made in this work. We see that for this model, where $D/T = 0.745$, as shown in Figure 6 (right), there is little gain in the pumping rate by increasing the rotation speed of the homogenizer.

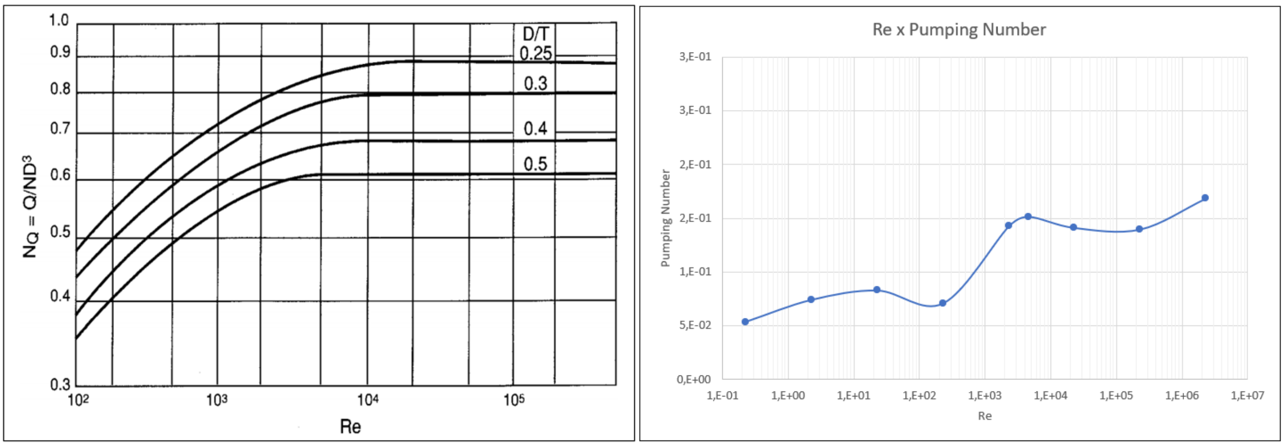


Figure 6. **N_Q *vs.* Re for different impeller width / impeller diameter ratios (left) (Morton, 1976) and N_Q *vs.* Re for this current work impeller width / impeller diameter ratios = 0.745 (right).**

Comparing Figure 6 left to right, we see that the current model pumping number is poorer than the others, which indicates a low level of agitation, however expected, considering that its D/T ratio = 0.745.

5. CONCLUSION

This work evaluated a radial non-conventional stir geometry with baffled regular tank. The geometry evaluated was modeled using a CAD software, after this, RecurDyn™ together with ParticleWorks™. Furthermore, a comparison was taken with literature models to evaluate the non-conventional stir geometry with a commercial stir geometry. We observed that our model presents similar behavior, but with a peculiar shape in the region $Re = 10^5$, which comes to be a characteristic of the geometric model. On the laminar regime, the unconventional geometry stir model showed that it needs low amount of energy, because our application has a lesser power number and presents the smaller consumes energy level to reach a high Reynolds number values, what demonstrate that it is a proficiency model. Besides that, the current model pumping number is very poor, which indicates a low level of agitation. However, it worth considering that its D/T ratio is 0.745, which is expected to cause low levels agitation.

6. ACKNOWLEDGMENTS

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