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A NEW APPROACH TO CHARACTERIZE SUSPENSIONS IN STIRRED VESSELS BASED ON COMPUTATIONAL FLUID DYNAMICS

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Abstract - Fluid dynamics simulations were applied for evaluating the suspension of particles in stirred vessels. The spatial distribution of particles throughout the vessel was characterized by a single parameter, here called the suspension quality (σ). Based on simulation results, a semi-empirical correlation was developed that correlated the suspension quality with the vessel geometry and solid and fluid properties, including a large variety of conditions, such as vessel and impeller diameters, impeller clearances, rotational speeds, particle densities and sizes. Comparison of the model with experimental data from the literature (Bohnet and Niesmak, 1980) suggests that the model can be extended to systems with different impeller geometries by adjustment of one single empirical parameter. The model can be used in the design of stirred vessels for the identification of the rotation speeds necessary to promote a specified suspension quality.

Keywords: Agitated vessel; Stirred tank; Solid suspension; Homogeneous suspension; Computational fluid dynamics.

INTRODUCTION

Two limiting situations can be distinguished for characterizing the distribution of solid particles dispersed in a liquid: just suspension and homogeneous suspension. The former occurs when the solid particles are in movement and no particle remains longer than 1 to 2 seconds at the bottom of the vessel. The latter is characterized by the uniform spatial distribution of the solid particles throughout the vessel. In practice, agitation systems operate between these two ideal situations, in conditions usually referred to as complete suspension. Complete suspension is important in industrial applications as diverse as suspension polymerization, dissolution, crystallization, extraction and in several catalytic processes.

Determination of conditions for just suspension is well documented, since it is simple to determine experimentally and gives sufficient information for several industrial applications. The most common approach is to experimentally determine the rotational stirrer speed that promotes just suspension (N_{js}). The following classic empirical correlation has been derived (Zwietering, 1958):

$$N_{JS} = \frac{S\nu^{0,1} d_p^{0,2} \left(g \frac{\Delta\rho}{\rho_L} \right)^{0,45} X^{0,13}}{D^{0,85}} \qquad (1)$$

Improved correlations have been presented which combine experimental evidence with various theories for stirred vessels in the just suspended condition (Musil and Vlk, 1978; Wichterle, 1988; Rieger and Ditl, 1994; Rieger, 2000; Murugesan, 2001; Rieger, 2002).

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For complete suspension, a correlation similar to Equation (1), which is valid for wide variety of suspension properties, vessel and impeller geometries, is not yet available. Earlier semi-empirical work is summarized in Table 1. In spite of this, much progress has been made in the understanding of the solids distribution throughout vessels. It is now established that computational fluid dynamics (CFD) provides a reasonably good description of complete suspension if an appropriate drag coefficient is considered. For example, it has been shown that drag models based on solids volume fraction are better than those based on Reynolds number only (Ochieng and Onyango, 2008). Such CFD models are most often based on the Euler/Euler approach with the k-e turbulence model (Spidla et al., 2005; Tamburini et al., 2009), but the Eulerian/Lagrangian approach has also been reported (Srinivasa and Jayanti, 2007). Models are often in 3 dimensions, but when the vessel geometry permits, a two dimensional symmetry may be applied (Khopkar et al., 2006). In some cases, solids distributions calculated by CFD are used as a basis to model other processes such as mixing (Ranade, 2009) and crystallization (Kougoulos et al., 2005; Woo et al., 2006) or to derive an optimal design of the impeller (Spogis and Nunhez, 2009). Advanced CFD techniques such as large eddy simulations and direct numerical simulations have also been explored to simulate turbulent mixing in stirred vessels, in order to gain insight into the details of local processes and transient flow conditions (Van den Akker, 2006). Recently, a detailed experimental study using radioactive particle tracking has shown the possibilities and limitations of both the Euler/Euler and the Large Eddy Simulation approaches for a vessel provided with a 6-blade Rusthon turbine (Guha et al., 2008).

Since CFD reasonably describes the solids distribution throughout mixing vessels, it may be applied for design or scale-up with respect to the degree of homogeneity of the suspension. In such cases, new simulations have to be performed for each application, in order to determine the impeller rotation speed that provides a specified solids spatial distribution in a vessel-impeller of given geometry. The disadvantage of this procedure is that it is time consuming. Besides, it is cumbersome for seeking the optimal geometric configuration for a given task.

Therefore, attempts have been made to use CFD either in combination with theoretical arguments or empirical evidence in order to find trends of general value. For example, the scale up criterion "$ND^{0.93}$ = constant", derived from a turbulence intermittency theory, was proposed for preserving the solids vertical distribution (Montante et al., 2008) for high aspect ratio vessels stirred by multiple impellers. In another contribution, an empirical correlation for the cloud height in baffled tanks provided with a hydrofoil propeller was suggested on the basis of the mixing features identified by CFD and experiments (Ochieng and Lewis, 2006). It has been suggested that a mean suspension height of 90% of the liquid level assures a uniform solids vertical distribution inside the cloud for pitched blade turbines (Angst and Kraume, 2006).

In the present work, we have used CFD to describe the suspension of particles in water. The simulated spatial distribution of solids was characterized by a single parameter, here called the suspension quality. Based on simulations for particles of different density and size in vessels of various geometries and scales, a semi-empirical correlation was developed for predicting the suspension quality. Since literature data is mostly concerned with 45^{o} pitched blades and Rushton turbines, flat blade impellers were studied. Such impellers are commonly encountered when the stirring must both suspend the solids and provide a high shear rate, such as in processes for solids dissolution, solid-liquid reactions, particle dispersion and deaggregation. The proposed correlation was validated with literature experimental data (Bohnet and Niesmak, 1980).

Table 1: Early work on solid distribution in stirred tanks

Publication	**Impeller type**	**Criterion to evaluate solids homogeneity**	**Results concerning suspension quality**
Einenkel (1980)	Propeller	Variance	Suspension quality as a function of power consumption and Reynolds number
Bohnet and Niesmak (1980)	Propeller and pitched-blade turbine	Suspension quality	Suspension quality as a function of rotational speed
Buurman et al. (1986)	4-pitched blade impeller	Suspension quality	Criterion for homogeneous suspension
Barresi and Baldi (1987)	Various impellers and propellers	Suspension quality	Suspension quality as a function of rotational speed
Magelli et al. (1990)	6-bladed Rushton turbine	Peclet Number	Relation between Peclet number and solids content

PROCEDURE

The operation of solid-liquid vessels at steady state in the turbulent flow regime was considered. The vessel was filled with water and particles of uniform size and density. Stirring took place in a vertical cylindrical vessel by means of the rotation of a single impeller agitator axisymetrically mounted. The volumetric fraction of solids in the suspension was 5 vol%. Particle sizes were 10, 50, 100 and 500 µm. Particles densities were 1375 kg/m^3 and 2650 kg/m^3, representing, respectively, a polymeric resin and sand.

The stirred vessel dimensions are shown in Figure 1. The vessel was provided with a two-bladed flat impeller and 4 baffles spaced from each other at angles of 90°. Both blade width and baffle width corresponded to 10% of the vessel diameter. The liquid height had the same value as the vessel diameter. The simulations were performed in vessels with diameters of 1 m and 5 m, rotational speeds of 20, 34, 45 and 100 rpm. The D/T and C/T ratios investigated assumed the values of 1/4, 1/3 and 1/2.

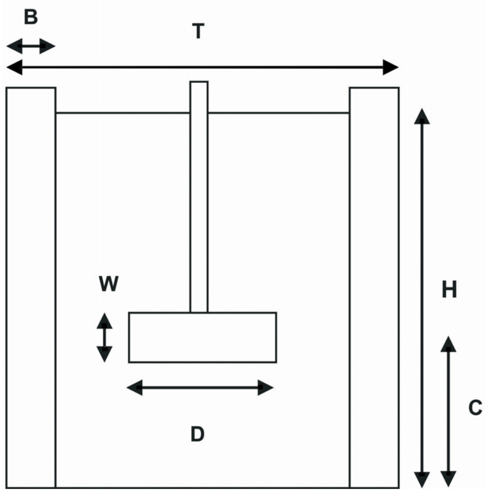

Figure 1: Main dimensions of stirred vessel. T = tank diameter; D = impeller diameter; C = clearance; W = impeller width; B = baffle width; H = liquid height.

The computations were conducted in Fluent version 4.5 in combination with the software MixSim version 1.7. Particles were treated as a single phase, shear forces within the particle and between solid and liquid phase were considered. The liquid surface was assumed to be flat. The k-ε turbulence model was used. The velocity profiles in the fluid adjacent to the agitator blades were obtained from three-dimensional single phase simulations (not shown). Two-phase simulations were conducted in a two-dimensional model due to limitations in the time needed for computations. For the 3D simulations of the vessel with 1 m in diameter, 80.000 computational cells were used. Mesh-independency was assured by repeating a simulation using 220.000 cells. For the 3D simulations with the 5 m vessel the number of cells was 400.000. The 2D simulations of the 1 m and the 5 m vessels were performed, respectively, with 2000 and 5000 computational cells.

Simulation results included the time averaged spatial distribution of the solids content, the energy dissipation, as well as the liquid and solid phase velocities (not shown).

Characterization of the Suspension Quality

The degree of homogeneity of the suspension was assessed through the ratio of the standard deviation to the mean of the particles volumetric fraction, defined by Equation (2) below:

$$\sigma = \sqrt{\frac{1}{n}\sum_{1}^{n}\left(\frac{c}{c_M}-1\right)^2} \tag{2}$$

The variable σ is called here the suspension quality. For a perfectly homogeneous distribution of particles throughout the vessel, the local and the mean concentrations, c and c_M, are identical everywhere, so Equation (2) gives a σ value of zero. However, a true homogeneous suspension is never realized, so a σ value of 0.25 is conveniently chosen to describe homogeneously distributed particles in situations of practical interest (if a specific application demands, other σ values can be chosen). As mixing becomes poorer, σ increases until solid settling at the bottom occurs, thereby characterizing the condition of just suspension. In the simulations, settling was clearly identifiable as a well defined region at the vessel bottom with a solids content of 40 vol%, which is characteristic of beds of particles at rest. It was considered that settling was negligible if less than 2% of particles present in the vessel settled. For most simulations, when this condition was observed, σ was found to be 0.8 or larger. Therefore, this value is chosen as characteristic of the just suspended situation. Complete suspension thus takes place for $0.25 < \sigma < 0.8$. Table 2 summarizes these choices. Another definition of the suspension quality, very similar to the one presented here, has been recently proposed (Kasat et al., 2008).

Table 2: Characterization of the degree of homogeneity in terms of the suspension quality (σ).

σ	Suspension quality
> 0.8	Portions of the solids settle at the bottom of the vessel
0.25 – 0.8	Complete suspension, with variable degree of homogeneity
< 0.25	Proximity to homogeneous suspension

In order to illustrate how the chosen limiting values for σ translate into the spatial distribution of particles throughout the mixing vessel, two simulation cases are shown in Figure 2 for a mean volumetric solids content of 5%. The right section of the figure shows the solids content distribution for σ close to the limiting value of 0.25. About 95% of the vessel volume assumes a concentration close to the desired mean value and the remaining 5% has very low solids content. The left section of the figure shows the solids distribution for a suspension quality of about 0.8: only a small fraction of the vessel has solids contents around the desired mean value of 5%. A condition of extremely poor mixing (not shown), with most particles settled at the bottom, resulted in a σ value of 2.8.

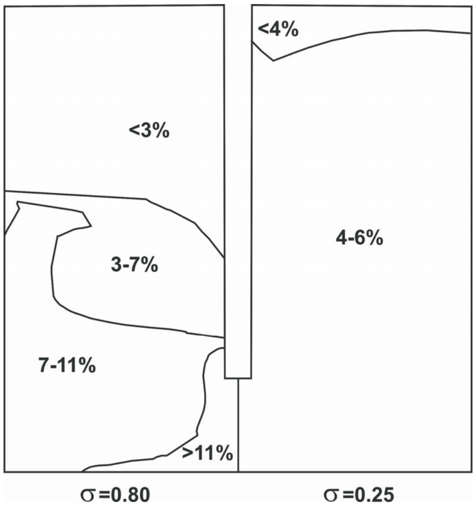

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Figure 2: Spatial distribution of solids content (in volume % units) in stirred vessels for two simulation cases with suspension qualities of 0.8 (left) and 0.25 (right). The mean solids content in both cases is 5%.

For each simulation the degree of homogeneity was therefore assessed by the suspension quality σ as defined above. In total, 94 simulations were performed.

RESULTS AND DISCUSSION

Influence of the Particle Size

Figure 3 shows the suspension quality σ as a function of the particle size for several vessel geometries. As expected, the degree of homogeneity decreases (i.e., σ increases) with particle size, due to the increased gravity action with size. It is also noteworthy that the vessel geometry (D/T and C/T) plays an important role in determining suspension quality. Only for very small particles, where the mixer is likely to be overdimensioned, does the suspension quality become insensitive to the vessel geometry.

Influence of the Impeller Diameter

For both types of particles, sand and resin, the best suspension qualities (lowest σ values) were achieved for the largest impeller diameters, as shown in Figure 4. This may be attributed to the strong influence of D/T on the energy input to the mixer, as shown in Table 3.

Influence of the Clearance

Figure 4 also shows how the relation C/T influences the suspension quality. For small values of D/T (1/3 and 1/4), placing the impeller close to the bottom of the vessel generally gives a better suspension quality. If D/T is large, however, the impeller in the middle of the vessel is preferable. This may be explained in terms of the spatial distribution of dissipated energy throughout the vessel. In the former case (D/T 1/3 and 1/4), the energy dissipated is relatively low, so gravity acting on the particles brings them to the lower part of the vessel. Therefore, placing the stirrer in this region is most effective in dispersing the particles. On the other hand, if the energy dissipation is sufficiently high (D/T 1/2), gravity plays a minor role, so placing the impeller at the center of the vessel (C/T 1/2) is sufficient to suspend the particles. Since this configuration gives the most uniform distribution of energy dissipation (see Figure 5), σ is the smallest for this condition.

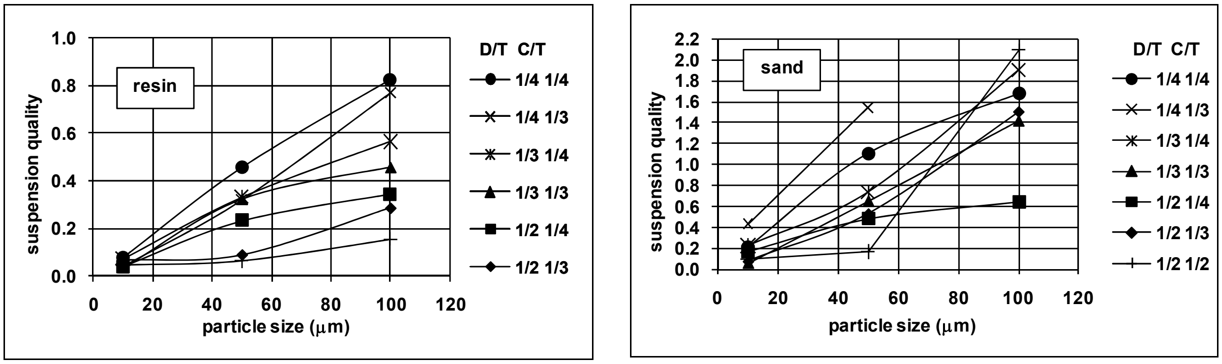

Figure 3: Suspension quality versus particle size for simulations with resin (upper figure) and sand particles (lower figure). Tank diameter T = 1m and rotation speed N = 100 rpm.

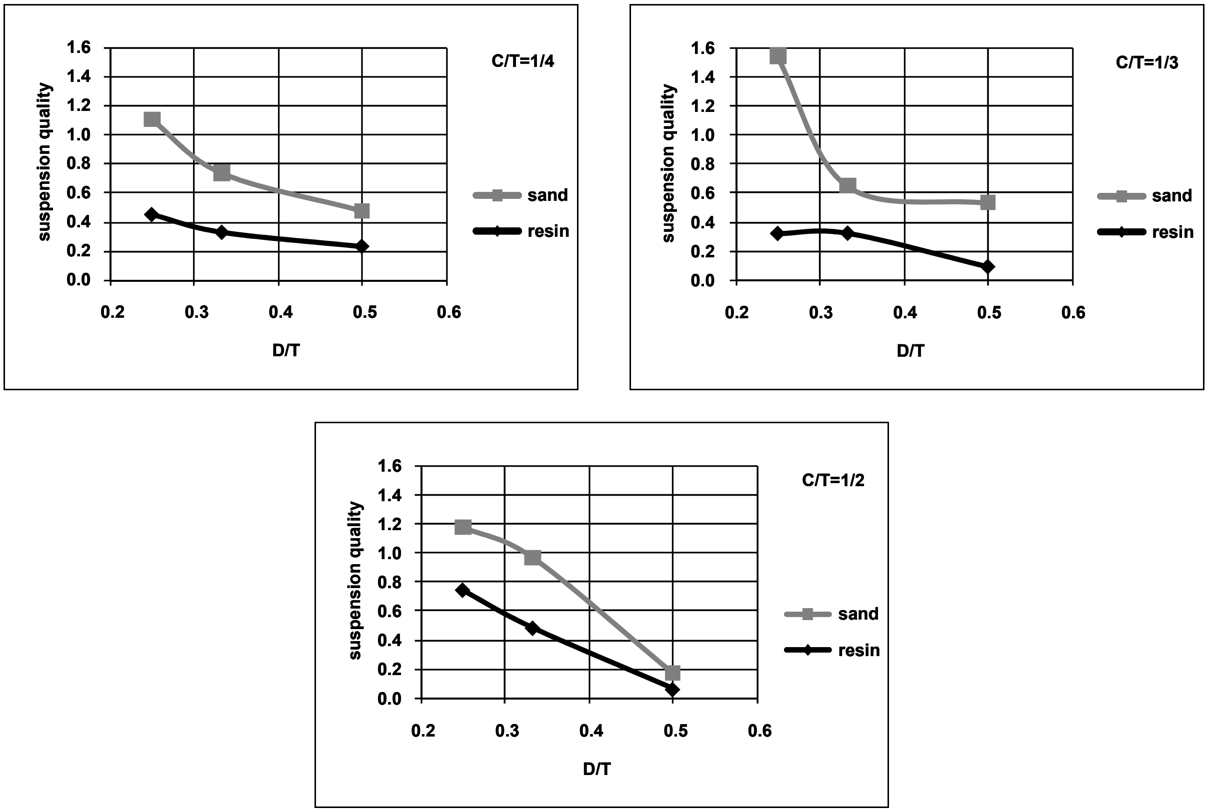

Figure 4: Influence of impeller diameter and clearance on the suspension quality (d_p = 50 μm). Tank diameter T = 1m and rotation speed N = 100 rpm.

Table 3: Energy dissipation as a function of impeller diameter D and clearance C in the mixing tank. For the sake of comparison, the highest values of energy dissipation in single phase flow fields are shown.

D/T (-)	C/T (-)	Highest energy dissipation (W/kg)
1/4	1/4	0.072
1/3	1/4	0.236
1/2	1/4	1.132
1/4	1/3	0.080
1/3	1/3	0.311
1/2	1/3	1.117
1/4	1/2	0.090
1/3	1/2	0.171
1/2	1/2	0.934

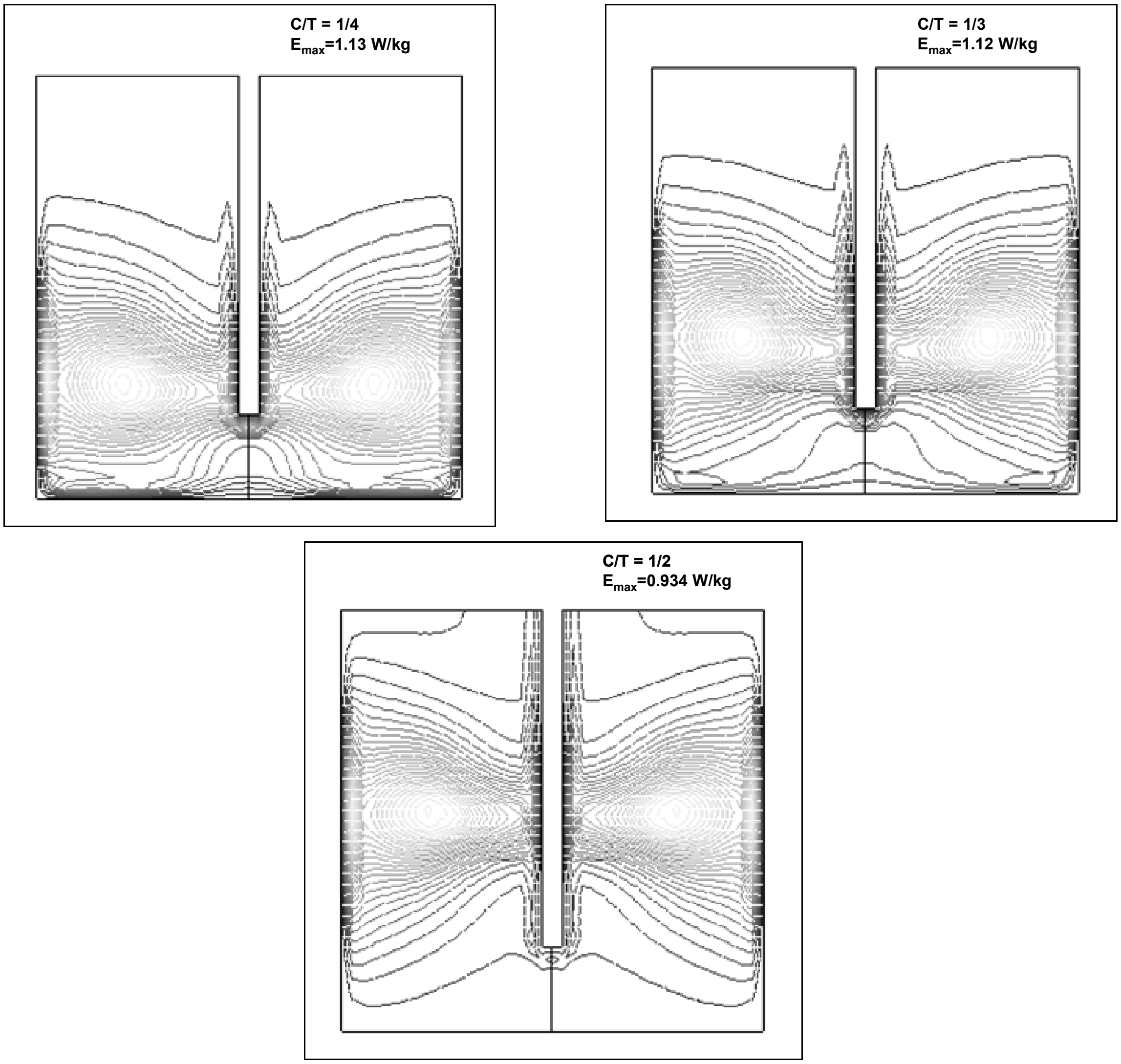

Figure 5: Spatial distribution of the energy dissipated (E) into the fluid for D/T =1/2, T = 1m. Lighter lines indicate higher values of E. The highest value of E, E_{max}, in the vessel as well as the C/T value are indicated in the upper right corner of the figures.

A Mathematical Model for Particles Suspension

A mathematical model based on dimensionless parameters is sought that correlates the simulated σ values to the mixing conditions, solids and fluid properties. Possible dimensionless parameters for such a correlation are taken from previous work on theories for stirred vessels in the just suspended condition (Musil and Vlk, 1978; Wichterle, 1988; Rieger and Ditl, 1994; Rieger, 2000; Murugesan, 2001; Rieger, 2002). Such theories often predict that the suspension of particles in stirred vessels depends on certain dimensionless numbers, such as the Froude number (Fr'), the modified Froude number (Fr*), the Archimedes number (Ar), the Reynolds number (Re), the particle Reynolds number, as well as other dimensionless ratios such as d_p/T, D/d_p, CD^2/T^3, $\rho_L/\Delta\rho$, D/T and the solids content, with the following definitions:

$$
\begin{aligned}
&Fr' = \left(N^2 D / g\right) \cdot \left(\rho_L / \Delta\rho\right) \\
&Fr^* = Fr' \cdot \left(\frac{D}{d_p}\right) \\
&Re = N \cdot D^2 \cdot \rho_L / \mu_L \\
&Ar = d_p^3 \cdot g \rho_L \Delta\rho / \mu_L^2
\end{aligned}
\tag{3}
$$

A simple model structure was considered, with the following general form

$$\sigma = a_0 \cdot \pi_1^{a_1} \cdot \pi_2^{a_2} \cdot \ldots \tag{4}$$

where $\pi_1, \pi_2, \ldots$ are dimensionless variables and a_0, $a_1, \ldots$ are model parameters that minimize the difference between model-derived values of the suspension quality (σ_{calc}) and values determined by CFD simulations (σ_{sim}). Minimization was achieved by linearization of Equation (4) (by taking the natural logarithm of both sides of the equation), followed by multilinear regression.

Several different combinations of dimensionless variables were investigated. A suitable correlation was selected based on three criteria. First, the model should fit well to CFD simulations. Second, the model parameters should be consistent, that is, the model should correctly predict trends for all variables (for instance, a model that predicts that a higher density leads to a better degree of homogeneity is rejected). Third, the model should be simple, that is, excessive or redundant dimensionless numbers are avoided. A correlation that fulfills these criteria is

$$\sigma = a_0 \cdot Fr'^{\,-0.446} \cdot Ar^{0.132} \cdot (d_p / T)^{0.382} \tag{5}$$

with $a_0 = 6.127$. The coefficient of correlation (multiple R) for the natural logarithm-based linearized correlation between σ_{sim} and σ_{calc} is 0.81 when the 94 CFD simulations are considered.

In Figure 6 values of the suspension quality determined with this correlation (σ_{calc}) are plotted against our simulation data (σ_{sim}). The dotted line gives the $\sigma_{sim} = \sigma_{calc}$ condition. The correlation reasonably predicts the suspension quality for the whole range of stirring conditions investigated.

Model Validation with Experimental Data

So far we have shown how CFD modeling can be applied to support the development of a mathematical model for particle suspension over a wide range of conditions. In order to validate this procedure, the proposed correlation was applied to laboratory scale experimental data obtained from the literature (Bohnet and Niesmak, 1980).

The model did not match the experimental data, as expected, because of the different range of conditions in the experiments and in our simulations, particularly the impeller type and particle densities and sizes, as given in Table 4. However, fitting was easily obtained, as shown in Figure 7, by adjusting the pre-exponential term a_0 of the correlation (Equation (5)), while keeping unchanged the dimensionless parameters and their powers:

$$\sigma = a_0 \cdot Fr'^{\,-0.446} \cdot Ar^{0.132} \cdot (d_p / T)^{0.382} \tag{6}$$

with $a_0 = 1.102$. This result indicates that the model represented by Equations (5) or (6) can be extended to systems with different impeller types and particle and fluid properties by the mere adjustment of the pre-exponential parameter a_0.

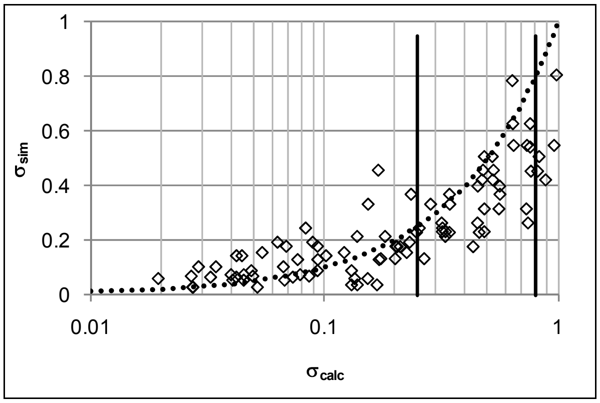

Figure 6: Suspension quality obtained by CFD simulations σ_{sim} (markers) versus values calculated with the correlation of Eq. (5), σ_{calc}. The dotted line represents the $\sigma_{sim} = \sigma_{calc}$ condition. The vertical lines indicate the limits for complete suspension ($0.25 < \sigma_{calc} < 0.80$) and for homogeneous suspension ($0 < \sigma_{calc} < 0.25$).

Table 4: Range of validity for the correlations developed for CFD simulations in this work and for laboratory scale data of Buurman, 1986.

Variable	Units	This work	Buurman, 1986
impeller	-	flat	4-pitched blade
N	1/min	20 - 100	60 – 1000
T	m	1 - 5	0.39
D/T	-	1/2 - 1/4	1/3
C/T	-	1/2 - 1/4	0.17
H/T	-	1	1
d_p	μm	10 - 500	70 – 1150
ρ_{solid}	kg/m^3	1375 - 2750	1050 – 8850
ρ_L	kg/m^3	1000	1000
C	vol%	0.05	0.05
Model parameters			
a_0		6.1270	1.1017
a1		-0.4459	-0.4459
a2		0.1322	0.1322
a3		0.3818	0.3818

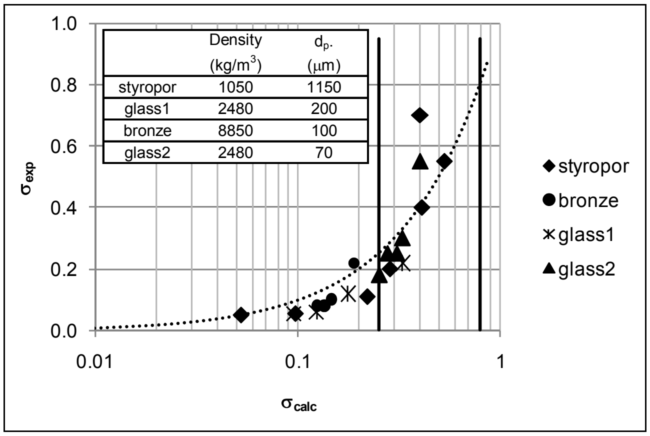

Figure 7: Suspension quality obtained experimentally by Bohnet and Niesmak (1980) versus calculated values with the correlation of Eq. (7). The dotted line represents the correlation outputs, and symbols the experimental values. The vertical lines indicate the limits for complete suspension ($0.25 < \sigma_{calc} < 0.80$) and homogeneous suspension ($0 < \sigma_{calc} < 0.25$).

Design of Solid-Liquid Mixers with Respect to Suspension Quality

Equations (5) and (6) can be rearranged into a more suitable form for the process designer. Isolating Fr' in the equation, one gets:

$$Fr' = a_0 \cdot \sigma^{-0,446} \cdot Ar^{0.296} \cdot (d_p / T)^{0.856} \quad (7)$$

where $a_0 = 2.244$ for the simulations with a flat blade impeller and $a_0 = 1.044$ for the experiments with a pitched blade turbine. For given vessel geometry and particle and fluid properties, the appropriate value of suspension quality σ is chosen, depending on whether homogeneous suspension ($\sigma = 0.25$) or complete suspension ($\sigma = 0.8$) is desired. Using the chosen value of σ in Equation (7), the Froude number Fr' is calculated. From this quantity the required rotation speed corresponding to the chosen suspension quality is derived.

CONCLUSIONS

Fluid dynamics simulations were used for the development of a simple semi-empirical correlation for suspension of particles in stirred vessels provided with flat blade impellers. The model correlated the suspension quality to the vessel geometry and solids and fluid properties for a large variety of conditions, such as vessel and impeller diameters, impeller clearances, rotational speeds, particle densities and sizes. By adjusting one single parameter, the model fit to experimental data of Bohnet and Niesmak (1980), indicating that the model structure is suitable for describing systems with different impeller types and materials properties. The model can be used in the design of stirred vessels for identification of the rotation speeds necessary to promote a specified suspension quality.

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NOMENCLATURE

B	baffle width	m
C	clearance	m
c	solids volumetric fraction	m^3/m^3 mixture
c_{AV}	mean solids volumetric fraction	m^3/m^3 mixture
D	impeller diameter	m
d_p	particle size	m
Fr*	modified Froude Number	(-)
g	gravitational constant	m/s^2
H	vessel height	m
N	stirrer rotational speed	1/s
N_{JS}	minimum rotational speed	1/s
Pe	Péclet Number for the solid	(-)
S	geometric constant	(-)
T	vessel diameter	m
W	impeller width	m
X	weight of solid per weight of liquid	kg/100 kg

Greek Letters

ν	kinematic viscosity	m^2/s
σ	suspension quality	(-)
ρ	particle density	kg/m^3
ρ_L	liquid density	kg/m^3

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