Computationally Determined Just Suspended Speed using Multiphase Mean Age Theory

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ABSTRACT

Mean age theory was applied towards predicting just suspended speed in mixing tanks by evaluating multiphase mean age near the bottom surface through strategic zone selection. Multiphase mean age equations were solved only in a thin section along the bottom of the vessel ($\sim 1\%$ of the vessel height), allowing the mean age in proximity to the bottom to be computed. A rigorously defined method for open systems and a modified method for closed systems using modified boundaries provided equivalent results. The technique was accurate within 1-3% of experimental values across a range of solid densities, solid fractions, and particle sizes while using multiple impeller types and vessel geometries.

Keywords: Mean age, CFD, just suspended speed, advection diffusion, multi-phase flow

INTRODUCTION

Inefficient mixing, which leads to inefficient reactions, excessive power draw,¹⁷ etc., is estimated to cost tens of billions of dollars every year.¹⁴ Poor solid-liquid mixing is a culprit in mixing inefficiencies. Knowing the relative behavior of independent phases is crucial to improving performance. In most solid-liquid systems, suspension of the solid particle is essential to maintaining adequate mass transfer. The particle resting on the bottom of the tank does not have its entire surface area exposed, and thus transfer of mass between the solid and liquid phases is inhibited. Much research has focused on determining just suspended speed (N_{JS}), the minimum impeller speed necessary for all solid particles to maintain off-bottom suspension. Zwietering²⁵ first put forth the concept as the minimum impeller speed required to ensure no particle remained on the bottom of the tank for more than 1-2 seconds, determined visually in a glass vessel. This technique, while still commonly used today, is highly subjective, although the author²⁵ claims it to be reproducible to within 2-3% with an experienced observer. The method is highly useful within a narrow range of conditions, but opaque suspensions, high solids volume fractions, and non-transparent tanks, such as stainless steel widely used throughout industry, all render the method unworkable.

Numerous other experimental methods to determine N_{JS} have been developed to remove subjectivity and overcome other limitations.^{3,4,6,12,13,15} Each method has its strengths, such as objectivity,^{4,13} unobtrusiveness,⁶ or applicability to industrial vessels.^{3,13,16} Some methods still rely on a visual observation,⁶ which

requires a transparent system. Others require the use of an intrusive sensor,^{4,13} which might alter the flow regime. Still others are difficult to implement due to unclear criteria, hard to setup correctly, or high experimental variability.^{3,13,16} Thus far, no single method can combine wide applicability, high accuracy, and ease of use.

CFD methods have been developed that depend on mimicking these sorts of experiments require unsteady-state simulations that depend on the transient motion of solid particles. Additional CFD methods, which do not directly mimic experimental work, have also been reported. Tamburini²² proposed using an unsuspended solids criterion, which is defined by mesh cells exhibiting the maximum packing fraction of solids. Tamburini goes further²³ to suggest this as a metric for sufficient suspension, which allows for agitation at speeds somewhat lower than complete off bottom suspension.

Mean age theory has gained traction in recent years as a means of acquiring time dependent data from steady state CFD simulations.^{8-10,18} This technique redefines time in a passive, steady state scalar, which then allows for analysis of traditionally time based variables such as mean residence time while using a steady-state CFD solution. Even with the increasing prevalence of high performance and parallel computing capabilities, a steady state solution is more convenient in terms of convergence criteria and speed of computation, especially for long time scale problems and/or larger volume systems. It can therefore be highly useful for collecting information such as local residence time⁹ or mixing time.⁹ Mean age theory was originally only applicable to single phase systems, but was recently extended for use in multiphase systems by Russ and Berson.¹⁸

Multiphase mean age theory (MMA) was applied here to obtain local, time dependent data for solids in proximity to the bottom of mixing vessels, which can be used to define N_{js} . The objectives were: (1) apply MMA theory to predict N_{js} in mixing tanks, and (2) validate the technique by comparing computational and experimental N_{js} across a range of solid densities, solid fractions, and particle size.

THEORY

Mean age theory is a means of modeling the time dependent behavior of a passive scalar in a steady-state CFD simulation, providing the mean time elapsed for a parcel of material traveling from the system inlet to any other location in the system, accounting for all possible path lines from the inlet to each point. The full derivation has been given extensively elsewhere for single phase ^{10,19-20} and multiphase systems,¹⁸ while a summary of the theory is given here. The theory begins with the advective-diffusive equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot (uC) = \nabla \cdot (D\nabla C) \quad (1)$$

where C is concentration, t is time, u is velocity and D is the diffusion constant. In a multiphase system, C can be defined as:

$$C(x, t) = \rho \cdot \alpha(x, t) \cdot \phi(x, t) \quad (2)$$

where ρ is the phase density, α is the phase volume fraction, and ϕ is a dimensionless scalar value for modeling scalar transport. Mean age can be defined as:

$$a(x) = \frac{\int_0^\infty tC(x, t)dt}{\int_0^\infty C(x, t)dt} \quad (3)$$

Modifying Equation 1 and incorporating Equations 2 and 3 leads to:

$$\nabla(ua) = \nabla \cdot D\nabla a + 1 \quad (4)$$

where the velocity is that of the phase under examination. Boundary conditions for this system are as follows

$$a=0 \quad \text{Inlet} \quad (5)$$

$$\frac{\nabla a}{\nabla x_n} = 0 \quad \text{Outlet} \quad (6)$$

$$\frac{\nabla a}{\nabla x_n} = 0 \quad \text{Wall} \quad (7)$$

This passive, steady state equation is then solved secondary to the flow solution obtained by CFD to give a spatial distribution of the mean age scalar throughout the entire flow-field.

Because MMA gives time related data, this technique can be extended to analysis of just suspended speed. At its most basic definition, just suspended speed is dependent on the time solids spend in proximity to a vessel bottom (1-2s²⁵).

Model zone definitions can be applied in conjunction with MMA to allow specific analysis in regions of interest within a vessel. Figure 1 shows an example of such conditions for examining settling and N_{js} in a mixing tank.

Figure 1: Diagram of zone selection for measuring N_{js} . A is a moving reference frame, B is a stationary zone, and C exists for measuring age near the vessel bottom.

Zone A was set as a rotating reference frame to adequately accommodate impeller motion for the purpose of modeling. Zones B and C were set as stationary zones in the modeling. Zone C exists solely for examining the age in the bottom of the vessel. The height of Zone C was on the order of 1% of the total height of the vessel, since only the behavior at the very bottom is relevant for determining N_{JS} . The thinner this zone the better, though a lower limit may be reached due to particle size or meshing concerns. The ratio of zone height to particle diameter used here ranged from 15:1-60:1.

The scalar age measurement is confined to the solid phase particles. The age of suspended particles (residing anywhere above Zone C) will be relatively low since the transport of the scalar will be convection dominated. However, if the particle is settling (in Zone C), then convective transport of the scalar will go to zero while slow diffusive transport will dominate, which will generate higher order of magnitude age values. Figure 2 shows a theoretical result for such a condition. Each point represents the average of the MMA in Zone C for a given impeller speed.

Above N_{JS} , the age value is very low. Below N_{JS} , the age value is orders of magnitude higher. N_{JS} occurs at the discontinuity between the two regions of the graph. The transition from convection-dominated

Figure 2: Theoretical age of solids in Zone C for varying impeller speed. Above N_{JS} , age is low and steady due to convection dominance. Below N_{JS} , age is much higher, due to the absence of convection. The sharp transition marks N_{JS} .

transport to diffusion-dominated transport as impeller speed decreases results in a very sharp increase in age.

Just suspended speed applications are more typical in closed vessels, so the technique introduced here will be more widely useful if it can also apply to systems with no flow in or out of the vessel. For a closed system, the age transport equation only needs to be solved within Zone C. Both the inlet and outlet boundaries need to be defined at the surface of Zone C where material enters and leaves this zone.

Figure 3 shows how CFD can define where velocity is positive or negative, indicating flow into or flow out of the zone.

Figure 3: Contours of vertical velocity along the boundary between zones B & C. Negative velocity indicates an inlet to zone C, while positive indicate an outlet from zone C.

Anywhere the z-velocity is negative, the flow is into Zone C and the region can be viewed as an inlet. Anywhere the z-velocity is positive, the flow is out from Zone C and the region can be viewed as an outlet. Outlet boundaries are known to have a very weak effect on mean age.⁷

CFD MODELING

CFD simulations were performed with ANSYS Fluent, v 14. Impeller motion was modeled using multiple reference frames. Unstructured meshes with tetrahedral cells were generated using ANSYS ICEM. All models contained between 450,000-500,000 tetrahedral cells. Mesh density was refined along the vessel bottom, in the bottom zone. Mesh sensitivity was performed, beginning with a total mesh count of 90,000 cells. The cell count was increased by a ratio of 1.5 per mesh iteration, while the average mean age in the bottom region was tested. Mesh insensitivity was reached after 5 mesh iterations. The liquid phase simulated was pure water. The solid phase simulated was sand or resin particles with varying diameters and densities. Multiphase behavior was simulated using the granular, Eulerian model owing to the large number of secondary phase particles. Turbulence was modeled using the RNG k- ϵ model. Since particle size did not exceed 200 microns, the effect of the free stream turbulence on the particle was not considered. A correction to the drag force due to the free stream turbulence would be needed when particle size exceeds 500 microns.²² Granular viscosity was modeled according to Syamlal and O'Brien.²¹ Granular bulk viscosity was modeled according to Lun, et al.¹¹ Phase drag interactions were modeled according to Gidaspow.⁵ Lift forces were not considered, since the solid specific gravity was greater than 2 in the majority of cases.²⁴ Specific equations employed by the solver for these models can be found in the Fluent Theory Guide.¹ Flow solutions were obtained first, then the scalar tracer values were computed from the resulting steady state flow field. Scalar transport was modeled using a diffusion constant of $2.299\text{e-}9\text{ m}^2\text{s}^{-1}$, the self-diffusion constant for water. Significantly lowering this value by orders of

magnitude showed no impact on results, while significantly increasing it by orders of magnitude significantly under predicted N_{js} .

RESULTS & DISCUSSION

Mean age of solids in Zone C were determined in both an open and closed vessel for a sand-water system in a 97 cm, stirred tank with $H/T=1$, a pitched blade turbine, and particle size of 111 μm (Figure 4).

Inlets and outlets for the open system were arranged as in Figure 1.

For the closed system, the

Figure 4: Comparison of mean age of solids in Zone C between the open and closed systems. Both techniques predict the same N_{js} .

boundary conditions at the tank inlet and outlet were

specified to be no flux. For the closed system assumptions to be considered valid, the method must predict the same N_{js} as a conventional open system where material flows in and out of the vessel. For the open system, the flow rate was chosen arbitrarily low (mean residence time was on the order of 1000 s) to ensure impellers dominated the flow so that the open and closed systems were comparable. Further, the age transport equation was solved in all zones in the open system, including Zones A and B, since flow entered through a traditional tank inlet.

As predicted by Figure 2, age values in Figure 4 above N_{js} were relatively constant and low, consistent with a convection-dominated system in the bottom

region where particles have not settled. Below N_{js} , the values were ~ 4 -6 orders of magnitude higher, consistent with a diffusion-dominated system due to the presence of settled solids. At N_{js} there was a significant discontinuity between the two regions, which corresponds with the speed above which all particles are at least just suspended, and below which some are not suspended. While there was some noise present below N_{js} , the trend is indisputable, and the noise ceases sharply at N_{js} . Above that speed there was no noise on the order of magnitude seen at slower impeller speeds. Since the closed vessel had a smaller region where the scalar was calculated (in Zone C only), the magnitude of the values was smaller, but most importantly, the order of magnitude increase in age, which predicts N_{js} , occurred at the exact same agitation speed, validating the assumptions. Clearly the closed system predicted N_{js} just as well as the open system, and with the added benefit of isolating precisely the area of interest.

Two published studies were used for experimentally validating this computational N_{js} method for a range of solid densities, solid fractions, and particle sizes.^{2,15} Both studies determined just suspended speed using Zwietering's method, which remains the standard by which other techniques are compared.

Figure 5: N_{js} as a function of solids density. Experimental data from Armenante et al. (1998).

The method was tested for a range of solid densities between 1375-2500 kgm^{-3} (Figure 5). Two of the density values used for validation were actual experimental data,² and two were values calculated from a correlation presented in the same publication. The correlation was used for additional validation in lieu of more experimental data since density could be easily altered this way while holding all other particle properties constant. N_{js} determined computationally based on MMA deviated from the experimental data/correlation by an average of 3%.

When varying the solids concentration between 0.6%-12% and using a pitched blade turbine, computationally determined N_{js} deviated from published experimental results by an average of just 3% (Figure 6).

The solids concentrations tested represent a wide range of

concentrations from both laboratory and industrial applications. Figure 7 shows a comparison to experimental results across a range of particle sizes and with a

Figure 6: N_{js} as a function of mass fraction. Experimental data from Rao et al. (1988)

Figure 7: N_{js} as a function of particle diameter. Experimental data from Armenante et al (1998)

different system geometry than the data in Figure 6. When varying the solid particle size from 75-200 μm and using a Rushton turbine, computationally determined N_{js} deviated from experiments by an average of just 1%.

At present this technique has only been tested using Eulerian-Eulerian modeling to account for the large number of solid particles. Defining the thickness of Zone C is somewhat arbitrary and must be balanced between being thin enough to be considered the “bottom” of the vessel while being thick enough to account for particle size and accumulation of a bed a few particles thick. Boundary conditions typically used when implementing Mean Age Theory were modified to account for the closed system. Nevertheless, the very close agreement between computational and experimental results indicates that the technique is robust across a range of particle densities, mass fractions, and particle sizes. The testing covered tank sizes between 0.1 and 0.5 m and both Rushton and pitched blade impellers. This also provides further evidence that the modified boundaries are empirically accurate. Any discrepancy between this technique and experimental results may be attributed as much to difficulties inherent in experimental measurements as it is to computational accuracy. The overall deviation is 3% or less, which is similar to the error reported in Zwietering’s foundational study (2-3%),²⁵ and given the continued widespread use of Zwietering’s method, it is reasonable to conclude the error in this study is on par with that reported elsewhere.

CONCLUSIONS

A new technique has been developed for accurately applying MMA theory towards predicting the just suspended speed in mixing tanks. A closed system with modified boundaries generated results as reliably as the comparable open system. The MMA technique was shown to accurately predict N_{js} across a range of solid densities, solid fractions, and particle sizes with average deviation from published experimental data of just 1-3%. Furthermore, tests were performed in different size tanks with both Rushton and pitched blade impellers indicating accuracy across a range of size and geometries. This steady state CFD technique can predict just suspended speed results with less computational time compared to unsteady CFD methods, with error equivalent to experimental methods, and without inherent experimental drawbacks such as altering the flow regime, requiring transparency, or subjective experimental variability

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