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A SCALABLE MODEL FOR MIXING VESSELS

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ABSTRACT

Stir-tank reactors, which are tanks containing a variety of impellers, baffles and inlet/outlet ports, are notoriously difficult systems to scale up from laboratory and prototype test configurations to full scale production sizes. The problem is associated with the difficulty of simultaneously scaling free-surface, rotational, viscous and other dynamic processes in such a way as to maintain similarity in all flow features. In this presentation we describe a new computational model for impellers that may be economically used to simulate stir-tank reactor flow fields. The model is based on some simple, yet powerful, ideas and uses in its definition scalable geometric and rotation-rate data. An essential feature of the impeller model is that it allows the impeller flow it generates to be influenced by such things as the close proximity of a tank wall, other impellers or a free surface. In this sense, our impeller model is more capable of being accurately scaled than previously reported impeller models. Results for a pitched-blade impeller are compared with published experimental data. Some qualitative results are presented illustrating how the model may be used and how generalizations of the model may be made to include approximate time-dependent effects in the vicinity of individual impeller blades.

INTRODUCTION

Mixing vessels and stir-tank reactors are used in the process industry to mix materials together under a variety of thermal and mechanical conditions. These vessels typically contain one or more impellers placed on a central shaft that induce radial and axial flows in the tank [1].

Experience has revealed that it is difficult to scale successful laboratory or intermediate size tanks up to full production sizes [2]. The scaling problem is associated with the fact that it is often impossible to maintain physical similarity in all flow processes when scaling from a laboratory device a few inches in diameter to a full-scale tank that may be many feet in diameter.

Computer flow modeling appears ripe for application to mixing vessels. Indeed, there have been several modeling attempts, some of them showing relatively good comparisons with experimental data [3-6]. In these efforts, however, the impellers have usually been replaced by a specified velocity distribution over the surface of the region carved out by the impeller. Such models are not general and it is unlikely they can be accurately scaled up in size.

Research efforts are underway in several laboratories to see if the moving blades of an impeller can be directly modeled using some sort of moving-grid numerical scheme, e.g., one based on the Chimera grid embedding approach [7]. This approach is attractive but is not likely to be useful in the near future because it involves enormous computer resources to resolve details currently at or beyond present capabilities.

The situation, then, is that a new type of impeller model is needed that has the potential for scaling and that does not require excessive amounts of computer time to produce useful results. This goal is the subject of the current paper. In the next section we describe a simple concept that can be used to construct models of impellers or other types of flow agitation devices.

A NEW IMPELLER MODEL

The rotating blades of an impeller push on the surrounding fluid imparting net momentum to the fluid in one or more directions. Combining this observation with the fact that mixing times are usually very long compared to the time it takes for an impeller to make one rotation, we are led to consider an impeller model as some sort of momentum source distributed over the region swept out by the impeller blades.

The simplest momentum source is one proportional to the difference between the blade velocity and the fluid velocity,

$$\text{Fluid Momentum Change} = K\left(\vec{U}_b - \vec{U}\right) \tag{1}$$

where a subscript "b" indicates the blade velocity, and K is a "drag" or "accommodation" coefficient. In general, K is a function of space and time.

We may make this suggestion plausible in the following way. Immediately at the surface of a blade the fluid must have the same velocity as the blade. We can insure this velocity boundary condition at the blade if we make K a delta function [8]; that is, if we make K a function whose value is zero everywhere except at the surface of the blade, where its value is infinite. The infinite value must be chosen such that a spatial integration of the fluid momentum equation with the K term included leads to the result $\vec{U}_b = \vec{U}$ at the blade surface. In this limit, then, Eq.1 can be used to satisfy the correct boundary condition on the moving blade.

In practice, of course, we cannot deal with delta functions in a discrete numerical approximation. The function must be spread over a spatial distance of at least one volume unit (i.e., mesh cell in a control volume method). If we spread the function out over a greater region, its magnitude must decrease such that the spatial integral over the entire function has a constant value.

Now we can imagine an impeller with N blades, each of which is represented by a locally smoothed delta function. The limiting case of complete smoothing would be a uniform value of K spread over the disk swept out by the blades. This, in fact, is the simplest version of our impeller model. Only in cases where the number of blades is small, and they are moving slowly, is it necessary to retain the spatial and time dependence of the individual blade K values.

There is one refinement to Eq.1 that must be considered. As it stands, the proposed model will try to make both normal and tangential fluid velocities conform to the specified blade motion. In high Reynolds number situations the momentum imparted to the fluid will be mostly through form-drag effects, and we should only be imposing momentum changes associated with velocities normal to the impeller blades. In this case,

$$\text{Normal Momentum Change} = K\left[\vec{U}_b - \left(\vec{U} - \vec{U}_t\right)\right] \tag{2}$$

where $\vec{U}_t$ is the component of fluid velocity tangent to the blade (and $\vec{U}_b$ is assumed to be a normal velocity). The principal difference between Eq.1 and Eq.2 is that the first equation may retard some radial flow in the impeller disk region.

To complete our model, it is necessary to specify the blade velocity, U_b. We propose an azimuthal velocity, U_{rot}, equal to the rotation velocity of the blade,

$$U_{rot} = \Omega R, \qquad \text{for } R_{in} < R < R_{out} \quad .$$

where Ω is the impeller rotation rate in radians-per-second and R is the distance from the axis of rotation. This relation is limited to R values between an inner radius, R_{in} and an outer radius, R_{out}.

Axial velocities, U_{ax}, are set proportional to the rotation velocity, but with a multiplicative constant A,

$$U_{ax} = A\Omega R \qquad \text{for } R_{in} < R < R_{out}$$

Thus, purely radial impellers would be assigned A=0, while pitched-blade impellers have non-zero A values.

In its simplest form, then, our impeller model is specified by the five parameters:

K = accommodation coefficient
Ω = rotation rate in radians per second
A = ratio of axial to azimuthal velocity
R_{in} = inner radius of blades or hub radius
R_{out} = diameter of impeller.

COMPARISONS WITH TEST DATA

To test the new model, we have made comparisons with the experimental data of Jaworski, et al [9]. Their test consisted of a single 45° pitched-blade impeller in a right-circular tank. The impeller had six blades with a diameter equal to one third the diameter of the tank. The tank was filled with water to a depth equal to its diameter. Four radial baffles having a width of one tenth the tank diameter were located at the tank wall with 90° spacing. Two test configurations were studied: one with the impeller at mid height in the tank and the other with the impeller placed one fourth of the height up from the bottom. The existence of these two cases was considered especially valuable for validation purposes. Figure 1, reproduced from Ref. 9, shows the measured velocity distributions for the two cases.

Our new impeller model was inserted in the commercial fluid dynamics solver *FLOW-3D®* developed by Flow Science, Inc. [10]. The numerical representation of the tank consisted of a nearly uniform rectangular mesh 22 by 22 cells in the horizontal (x-y) plane and 30 cells axially. The cylindrical tank was cut out of the mesh using the fractional area/volume method FAVOR; see mesh plot in Fig.2. Using a rectangular mesh rather than a cylindrical one has the advantage of providing more uniform gridding over the entire flow region.

For our tests we chose the momentum term in Eq.1 with K equal to 10, the number of revolutions per second. This number was a guess based on a few preliminary calculations for a different tank that had no experimental data available for comparisons. For the ratio of axial to azimuthal velocity, a value of A=1.5 was selected on the basis of experimental observations made by Ranade and Joshi [3].

We used the viscous blade model, Eq.1, for simplicity even though the calculations were performed under the assumption of negligible fluid viscosity and wall-shear effects (Reynolds numbers were of order 24,000).

Figure 3 shows the computed flow fields in a vertical plane offset from the axis by one half mesh cell. Qualitatively, the computed flows are in excellent agreement with the observations, Fig.1. For example, there are large reverse (upward) core flows under the impeller, strong downward flows under the outer portion of the impeller blades and narrow, but strong, upward flows along the outside wall of the tank. Vortex center positions are accurately reproduced. The biggest discrepancy is in the mid-height case where observations show that the reverse flow core extends over the entire bottom of the tank, while in the computation it only extends over about half the bottom.

Quantitatively the computed results are also in good agreement with the data. For instance, in the mid-height case the computed maximum axial velocity was 50 cm/s compared to a measured 54 cm/s. The computed maximum radial velocity was 18 cm/s while the measured value was about 23 cm/s.

For the lower impeller position, the maximum axial velocity was stated in the text of Ref. 9 to be about 67 cm/s, but the plotted data (Fig.4 of Ref. 9) indicates this value is closer to 46 cm/s. The maximum radial velocity was measured to be 38 cm/s. Our computations gave a maximum axial velocity of 49 cm/s and maximum radial velocity of 35 cm/s. Upward flow velocities along the tank side wall were 38 cm/s in the experiment and the simulation.

Computed values for both impeller locations are within the reported experimental reproducibility range of plus or minus 6.12 cm/s. Because both locations were computed using the same model parameters, these results lend support to the model's ability to adjust to changing geometric conditions, hence to its potential for accurate scaling. More comparisons with experiments are certainly needed, of course, to ascertain the dependence of parameters K and A on impeller design (e.g., number and shape of blades).

GENERALIZATIONS

An example of how more detail can be added to the new model is provided by an approximation to a Phaudler vessel. This type of vessel consists of a cylindrical glass tank with an elliptically-shaped bottom. Three glass-coated blades rotate near the bottom of the tank. The blades are assumed to be of the radial variety (i.e., A=0) and are separated by 120° intervals. They are rotating at a relatively slow 0.333 revolutions per second. The fluid is assumed to be viscous, having a Reynolds number based on impeller tip speed and diameter of 839.

To approximate the motion of the blades, we replace the constant K value used in the previous calculations with a space-dependent K. That is, we set $K=K_o$ in mesh cells occupied by the three blades and K=0 everywhere else. The rotation of the blades is handled by a coordinate transformation that replaces the initial blade location by one that has been rotated by the angle Ωt, where t is the elapsed time and Ω is the rotation rate in radians per second. Because there are three localized blades instead of one smoothed-out disk, the accommodation coefficient must be given a much larger value. We used a value of K_o=7.92 for no particular reason other than to insure a strong mixing action.

Selected results obtained in this way are presented in Figs. 4-6. In Fig.4 we see the flow generated in the plane of the impeller at three times separated by 0.4 s. The contours, which indicate where the accommodation coefficient is non-zero, are a little ragged because of the low resolution (i.e., each blade is only about two mesh cells in width). Figure 5 shows the flow in a central, vertical plane through the tank at the time corresponding to the first plot in Fig. 4.

The computed flow reaches a steady, periodic condition, Fig.6, and shows good mixing over the entire volume of the tank.

SUMMARY

We have presented a new, yet simple, model for impellers that is less restrictive than previous models. Because of its formulation as a momentum source, it is not sensitive to the presence of tank walls or other nearby impellers. Generalization of the model to include space and time dependencies for slow moving blades is easily accomplished. We expect that the model will be capable of more accurate scaling without the need for expensive calibration procedures.

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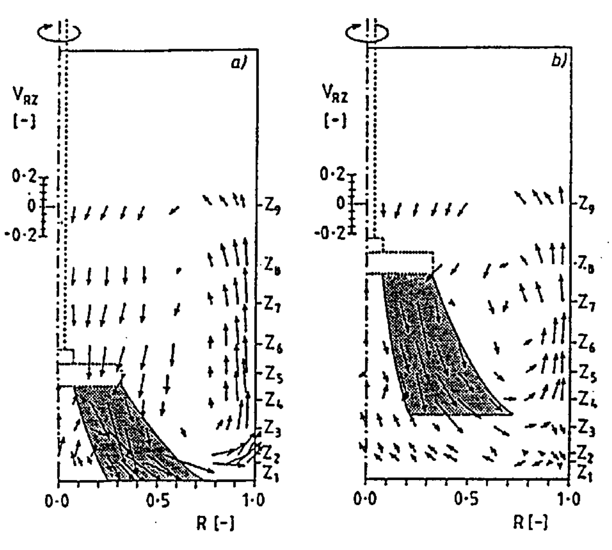

Fig. 1. Experimental results duplicated from Ref. 9. Upper impeller position on left and lower impeller position on right.

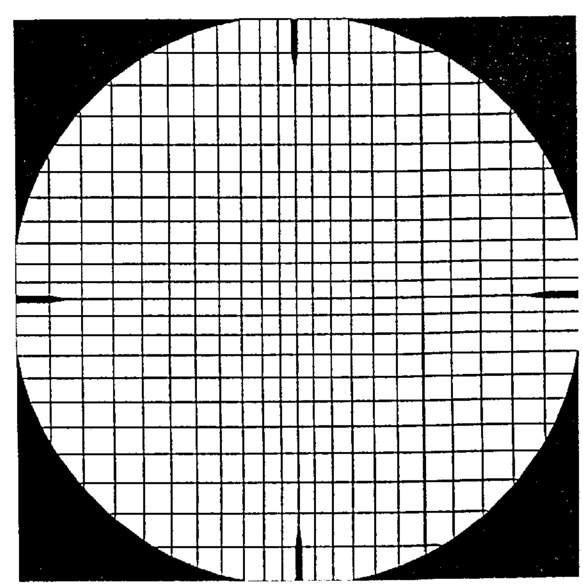

Fig. 2. Horizontal plane showing grid with tank and baffles shaded.

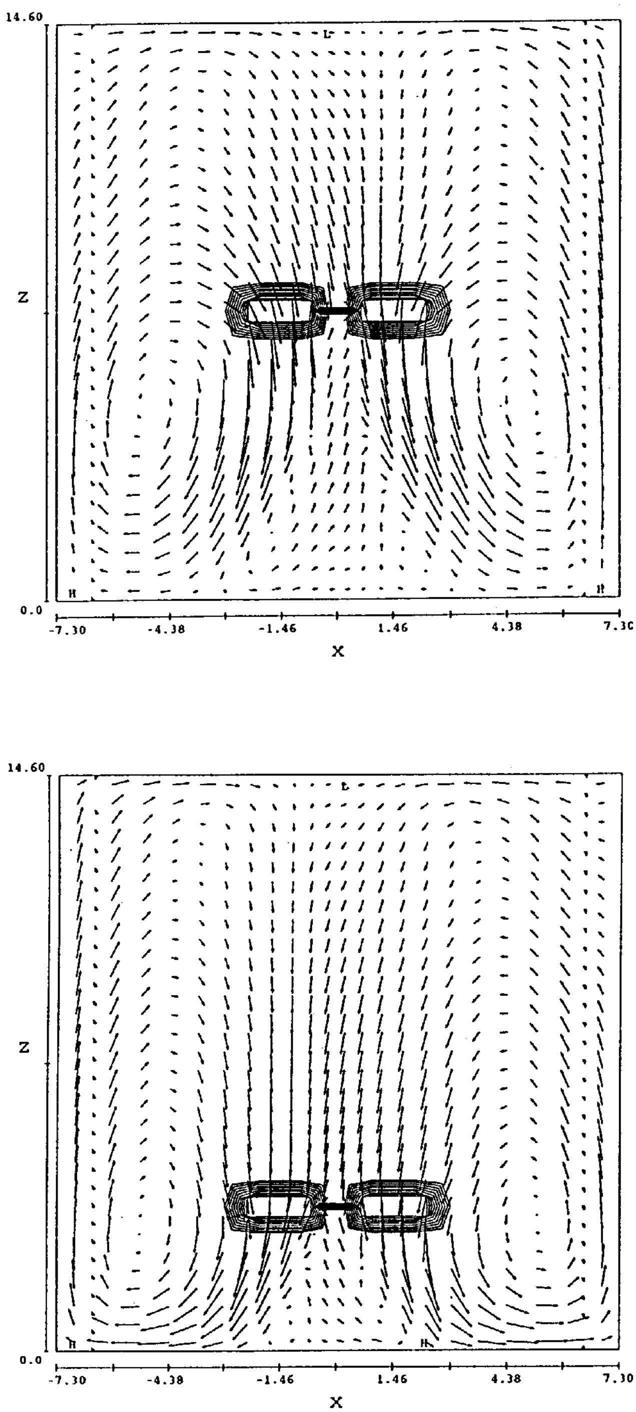

Fig. 3. Computed flow fields for upper impeller position (top) and lower impeller position (bottom). Impeller disk region is defined by contours of a function of the accommodation coefficient.

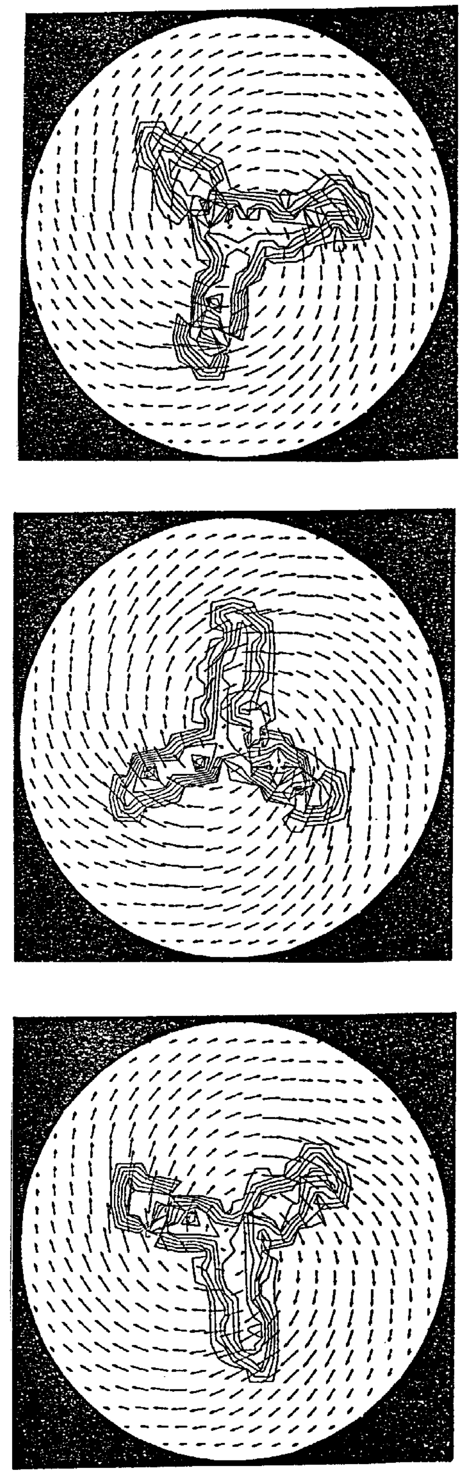

Fig. 4. Three plots of computed flow in plane of impeller showing the definition and rotation of the three blades. Times are 55.0 s (top), 55.4 s (middle) and 55.8 s (bottom).

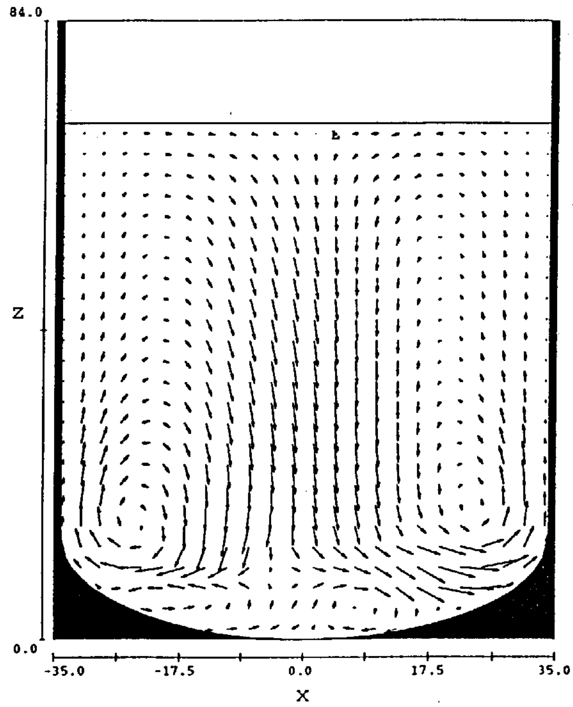

Fig. 5. Vertical plane near center of Phaudler-type tank at t=55.0 s. Free fluid surface at top remains nearly flat because of slow rotation.

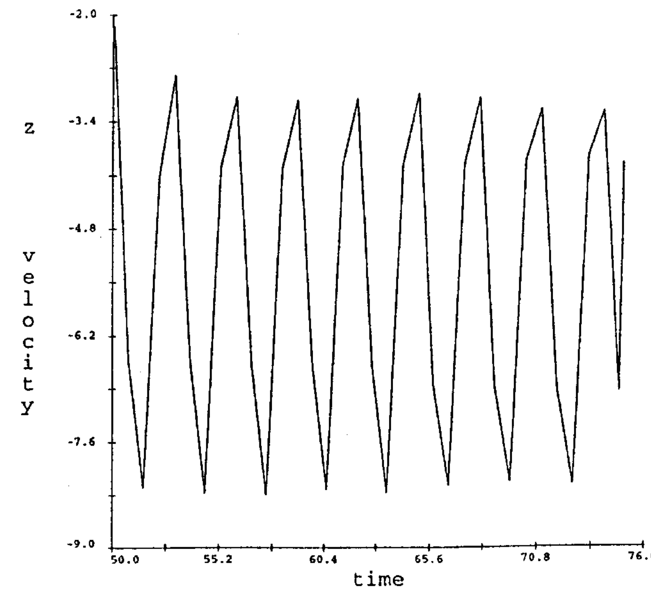

Fig. 6. Portion of time history of the vertical component of fluid velocity near the outer edge of the impeller showing periodic nature of the flow.

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