Can Theory Guide Experiments?

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1. The Problem

Blending or homogenisation of two or more miscible fluids is very widely encountered in a variety of physical and chemical processes. The blending process may be carried out in a batch or in a continuous mode of operation. The important process parameter for the blending process is the blending time, which is frequently termed as the mixing time. Figure 1 shows the geometry (stirred tanks) in which the blending process is commonly carried out.

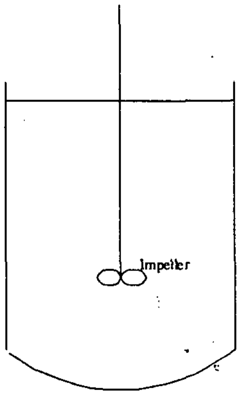


Fig. 1: Stirred Tank Reactor

It consists of a tank fitted with 4 baffles (to prevent the vortex formation) stirred with single or multiple impellers. The impeller(s) can be placed at any location and the tank can be filled to any desired height of liquid. In industrial practice, a wide variety of impellers are used. The blending time (mixing time) can be determined experimentally, by introduction of a tracer at some location in the vessel and measuring the tracer concentration as a function of time with the help of a sensor at one or more locations. The tracer input is usually in the form of a pulse. One of the most convenient techniques of measuring the mixing time is with the help of a tracer of sodium chloride solution and monitoring its concentration with the help of a conductivity probe. Typical concentration profile as measured by the tracer is shown in Figure 2. Mixing time is typically considered as the time required for the tracer concentration to reach within 95% of the completely mixed value.

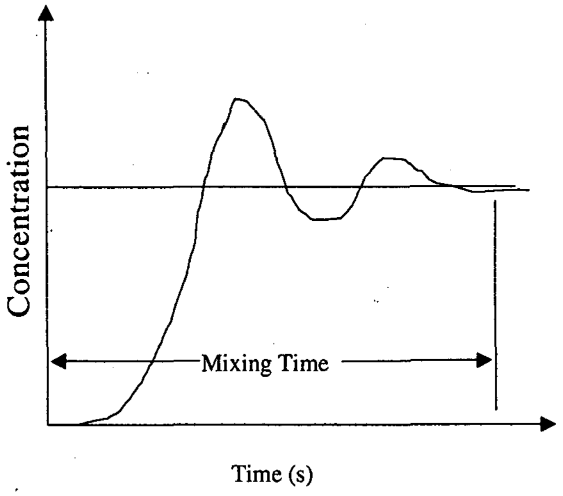


Fig. 2: Typical Concentration Profile with respect to Time in Stirred Tank Reactor

It has been observed in the past (previous published literature) that the geometry (tank size, liquid height, size, number and location of baffles, impeller design, impeller diameter, impeller location) and the operating conditions (impeller speed, physicochemical properties of the liquid phase) have a profound impact on the mixing time. The energy required for mixing is delivered by the impeller. This is measured in terms of the power consumed (power number of the impeller). The variables mentioned above also affect the power number of the impeller. The energy effectiveness of impeller - tank configuration for the mixing process can be compared in terms of the mixing time at a given level of energy consumption rate (power consumption). Thus, a configuration that produces faster mixing (lower mixing time) at a given level of power consumption is considered to be more energy efficient. From the above discussion it is clear that, there are a very large number of configurations (probably thousands) that need to be tested experimentally to determine their energy efficiency. Only when all these are tested, we can select the optimum out of the several thousands. It is also likely that there can exist a configuration that we have failed to consider while doing the experiments. A question naturally comes to mind is that, can we use theoretical reasoning to select the most energy efficient configuration? Or at least, can we use theory to reduce the number of experiments we need to carry out?

2. The Theory

The blending process occurs due to the transport at three levels: molecular, eddy and bulk (convection). Usually, the bulk motion (or bulk diffusion) is superimposed on either molecular or eddy diffusion or both. In industrial practice, many of the blending operations are carried out under turbulent conditions. In that case, the molecular diffusion can be neglected in comparison to the bulk diffusion (convection) and eddy diffusion. The convection occurs due to flow in the liquid phase. This is characterised by the mean velocity components in all the three directions in the liquid phase. The dispersion occurs because of turbulent motion. This is characterized by eddy diffusivity in the liquid phase. Thus, to predict the mixing characteristics and energy efficiency, one would need to know the mean velocity field and the eddy diffusivity levels throughout the tank. This can be done with the help of computational fluid dynamics (CFD) modeling.

Thus, CFD simulations were carried out to predict the mean velocity and eddy diffusivity levels throughout the tank. The CFD simulation involve solving the time averaged Reynolds transport equations along with a turbulence model. For this purpose, the transport equations (partial differential equations) are discretized over a set of grids in the entire flow domain. The resulting algebraic equations are solved iteratively. The numbers of grids are typically of the order 1,00,000. Computation time is about a couple of days on a PIII machine. The mean velocity and the eddy diffusivity predicted in this manner are used to predict the concentration profile and hence are used to calculate the mixing time. The CFD model is validated by comparison with experimental measurements. The results of this validation are shown in Tables 1 and 2.

Table 1 : Comparison of the Predicted Mixing Time with the Experimental Measurements

Impeller design	Tank dia (m)	Imp. dia (m)	Clearance	Blade width	$N\theta_{mix}$ measured	$N\theta_{mix}$ predicted
PBTD 45	0.57	T/3	T/3	0.3 D	42.8	42.80
PBTD 45	0.57	T/3	T/2	0.3 D	35.9	36.30
PBTD 45	1.5	T/3	T/3	0.3 D	40.1	42.80
PBTD 45	1.5	T/3	T/2	0.3 D	35.9	36.30
PBTD 45	1.5	T/5	T/3	0.3 D	146.0	139.17
PBTD 45	1.5	T/2	T/3	0.3 D	17.3	14.89
PBTD 30	0.57	T/3	T/3	0.3 D	61.4	55.32
PBTD 60	0.57	T/3	T/3	0.3 D	35.1	38.59
PBTU 45	1.5	T/3	T/3	0.3 D	41.0	30.04
PBTU 45	1.5	T/3	T/2	0.3 D	44.8	56.89

Table 2 : Comparison of the Predicted Mixing Time with the Experimental Measurements

P/M (W/kg)	θmix (s) T = 0.57m		θmix (s) T = 1.0 m		θmix (s) T = 1.5 m	
	measured	predicted	measured	predicted	measured	predicted
0.1	12.8	13.70	20.0	19.94	25.2	26.13
0.2	10.0	10.88	15.0	15.83	20.0	20.74
0.3	8.9	9.50	13.1	13.83	17.5	18.12
0.4	8.1	8.64	11.8	12.56	15.9	16.46
0.7	6.8	7.16	10.0	10.43	14.1	13.66
1.0	6.3	6.36	9.4	9.26	---	---

The data shows that the CFD model can accurately predict the mixing time. Hence the CFD model can be used to screen out various configurations / design more energy efficient mixing devices.

The validated model is used to study, the relative importance of the mean flow and eddy diffusivity levels. For this purpose, the predicted values of mean velocity and the turbulence fields were multiplied by a factor. In this manner, their values were modified independently of each other. These modified values were used to predict the mixing time. Figure 3 shows the sensitivity of these parameters.

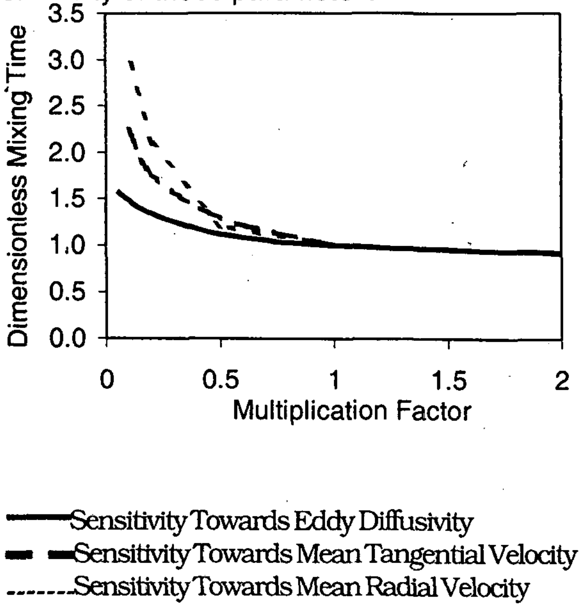


Fig. 3

From the figure it can be seen that the dimensionless mixing time increases by only about 50% even when the eddy diffusivity levels are reduced by twenty times. Conversely, when the eddy diffusivity levels are doubled the mixing time improves only marginally.The mixing time was also not very sensitive to the levels of radial and tangential velocity in the tank. A reduction in the mean radial velocity and mean tangential velocity by 10 times causes the mixing time to go up only by 3 times and 2.2 times respectively. The mixing time is, at least, more sensitive to these components of mean velocity than the eddy diffusivity levels.

3. The Experiment

The above result suggests that the mixing process can be made more energy efficient by reducing the eddy diffusivity levels substantially and reducing the mean velocity in the radial and tangential directions partly. Thus, instead of screening all possible impeller types and all geometries, it was thought desirable to look for a device that will reduce the level of radial and tangential mean velocity and eddy diffusivity levels.One simple device that does this is a pipe.In a pipe flow, the mean flow is predominantly in one direction and the eddy diffusivity levels are substantially lower.

Thus, further experiments were carried out in a 0.5m diameter tank filled to height of 0.5m. A pump was used to circulate the liquid in the tank with the help of a 40 mm diameter pipe. The set-up is shown in Figure 4. A pulse of sodium chloride solution was put in as a tracer and the conductivity was monitored at four locations (indicated as 1 - 4) with the help of a conductivity probe and a chart recorder. The mixing time was considered as the time required for the conductivity to reach 95% of the fully mixed value. Each mixing time experiment was repeated at least 3 times. This device is called as a jet mixer.

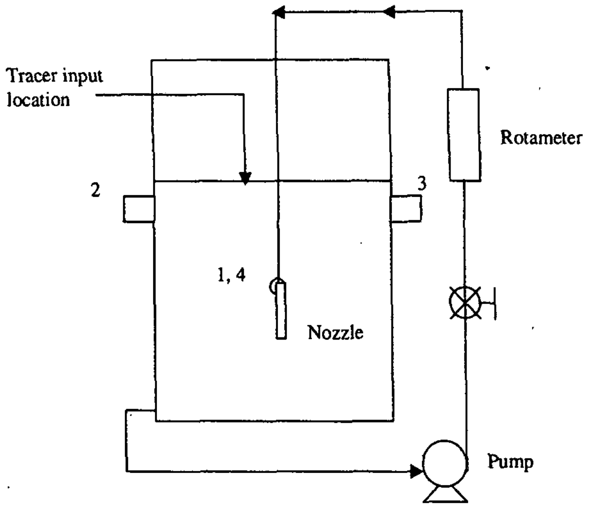
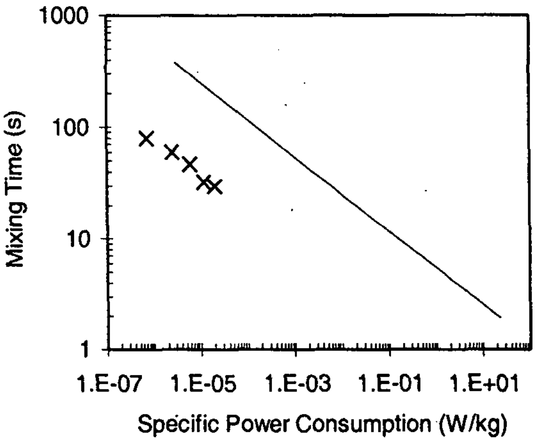


Fig.4: The experimental Set-up

The energy efficiency of the mixing process in jet mixers is compared with that of stirred tanks in Figure 5. From the figure it can be seen that the mixing time for jet mixers is substantially lower than impeller stirred tanks for the same level of power input per unit volume. Thus, the energy efficiency increases substantially. In this manner, the theory has been able to pave a way for directing experiments and designing better mixing systems.



--- Impeller Stirred Tank
X Jet Mixers with 40 mm dia. Nozzle

Fig.5 : The energy efficiency of the mixing process in jet mixers compered to that of stirred tank.

Dr. A W. Patwardhan is a lecturer in Chemical Engineering at the UDCT, Mumbai. He has worked as a consultant to Emmellen Biotech Pharmaceuticals and is a consultant to Reliance Industries. His research areas include mathematical modeling, computational fluid dynamics, stirred reactor and rotating biological contactors.