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Application of simulation tool for estimation of impeller power requirement in bioreactor

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Abstract
Simulation tool was applied to determine various bioreactor design parameters *viz* impeller Reynolds's number and impeller power requirement. Estimation of impeller power helps to design and select rotor drive assembly. Bioreactor with vertical cylindrical design and 10 litre capacity was used as initial design framework. Different ratios of height and diameter (H/D = 0.75, 0.9, 1.05, 1.20, 1.35 and 1.5) was considered in the simulation program. Power requirement was estimated for four different impeller designs (1, 2, 3 and 4) for a wide range of rotational speed (25, 50, 75, 100, 125, and 150 rpm). Impeller Reynolds's number was found in transitional region for all the impeller 1, 2, 3 and 4 operating between 25 to 150 rpm. Impeller Reynolds's number was in the range of 22 to 858 and estimated power requirement was in the range of 14 to 83.10 W for impeller speed 25-150 rpm.

Keywords: agitation, bioreactor, impeller Reynolds's number, simulation, power

1. Introduction
Computational simulation is being widely used in research and development process in the engineering, biological, and social sciences. It enables to conduct study of at the macro, micro and molecular levels, increasing understanding of different factors and analyze their interaction. It enables us to study properties of different components in complex systems. Simulation tool has become important in the design, testing, and production process reducing total cost in product development. It helps to save time to establish a product in the market and ensure the success of the product. The rapid pace in which the computational power has increased, researchers can transform complex mathematical formulas into computer codes and program enabling simulation of mathematical functions (Gordon and Guilfoos, 2017) [1]. Simulation studies helps to generate data under controlled conditions by pseudo-random sampling and does not require detailed experimentation. Various statistical methods and tools form the backbone of simulation studies, strengthen the generated information and aids data validation (Morris *et al*., 2019) [2]. The process of generating the data depends on the problem to be solved and sometimes requires to develop specific program for the simulation study. Simulation modelling can deliver specific solutions across sectors and disciplines by providing clear insights into complicated systems.
Simulation modelling allows to evaluate many "what-if" possibilities in a given environment. It is possible to see the impact of various process variables on output variables. Before making any real-world decisions, a prior visualization of the results can be made in advance. Virtual investigations using simulation models are less expensive and time consuming than real-world experiments.
Bioreactors are widely in the food and beverage processing, production of pharmaceutical products and for industrial waste treatment. Bioreactors provide suitable environment for cells and enzymes for carrying various biochemical processes. Agriculture, food and healthcare, resource recovery, and fine chemicals are all examples of biochemical engineering applications. Biological processes are extremely diverse. As a result, the designer should optimise both the reaction mechanism and the actual reactor. Choosing which biological system to utilise is always the initial step in design (McDuffie *et al*., 1991) [3].
In the present study simulation tool was applied for designing bioreactor suitable for anaerobic digestion of cattle manure slurry and to estimate power requirement for operating the impeller.

2. Materials and Methods
2.1 Simulation platform
The simulation computing system was based on 64 bit Intel i7 3.5 GHz processor with 4GB DDR4 memory (Lenovo, India).

The programming for simulation and visualization was done in Python 3.8 software. Python is a general-purpose, versatile and popular programming language. The language is currently being used in diverse application domains. These include software development, web development, Desktop GUI development, education, and scientific applications. So, it spans almost all the facets of development. Its popularity is primarily owing to its simplicity and robustness. Python also finds its applications in scientific analysis. SciPy is used for Engineering and Mathematics, and IPython is used for parallel computing. Those of you working in statistics and machine learning would find some of these libraries extremely useful and easy to use. SciPy provides MATLAB like features and can be used for processing multidimensional arrays.

The simulation program was developed to automatically calculate the rheological properties of cattle manure slurry at different temperature and total solids. The information was stored as data set 1 and became input for calculating secondary parameters like impeller Reynolds's number and power requirement.

2.2. Impeller design

Four different impeller were considered for simulation studies:

a. Impeller 1 (Da = 0.3Dt) (1)

b. Impeller 2 (Da = 0.4Dt) (2)

c. Impeller 3 (Da = 0.5Dt) (3)

d. Impeller 4 (Da = 0.6Dt) (4)

Where,

Da = Impeller diameter (m)

Dt = Bioreactor diameter (m)

2.3. Power requirement

The power requirement of the agitator motor, P in watts was obtained from the expression.

$$P = N_p \rho D_a^5 N^3 \quad (5)$$

Where,

Np is the power number, which depends on the Reynolds number and was obtained from Nomographs.

Da the impeller diameter,

N the rotational speed, ρ the fluid density.

The degree of laminarity or turbulence within the reactor was defined by the impeller Reynolds number, given by the expression

$$N_{Re} = \frac{D_a^2 N \rho}{\mu} \quad (6)$$

Where, N_{Re} is the Reynolds number and μ is the fluid viscosity (Anyanwu *et al*., 2012) [4].

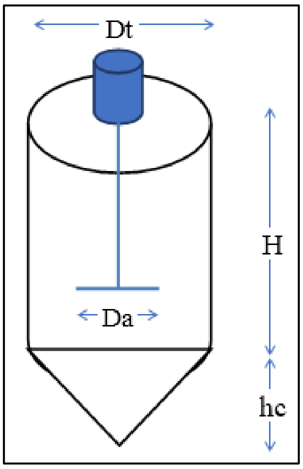


Fig 1: Bioreactor design

3. Results and Discussion

3.1 Impeller Reynold's number

Impeller Reynolds's number (Re) was calculated on the basis of four different diameter of impellers: a. Impeller 1 (da1 = 0.3Dt), b. Impeller 2 (da1 = 0.4Dt), c. Impeller 3 (da1 = 0.5Dt) and d. Impeller 4 (da1 = 0.6Dt). The Impeller Reynolds's number for different impellers 1, 2, 3 and 4 were calculated and stored as variable I_{Re1}, I_{Re2}, I_{Re3} and I_{Re4}, respectively. Impeller speed was varied in the range of 25-150 rpm as it is an important factor which controls energy input and Reynolds number (Lawson. *et al*., 2022)[5]. The impeller Reynolds number I_{Re1}, I_{Re2}, I_{Re3} and I_{Re4} was in the range of 22.53 to 35.76, 40.05 to 63.58, 62.58 to 99.35 and 90.12 to 143.06, respectively for 25 rpm impeller speed. The impeller Reynolds number (I_{Re1}, I_{Re2}, I_{Re3} and I_{Re4}) for different designs at 50 rpm impeller speed was in the range of 45.06 to 286.13 (Fig. 2).

Impeller Reynolds number gives an idea if the flow in stirred tanks is laminar or turbulent. The value of I_{Re} decides the transition and depends on the tank and impeller geometry. The standard values for laminar flow is I_{Re} <10 and while turbulent I_{Re} >10^4 (Doran, 2013) [6]. At 75 rpm impeller speed, values of impeller Reynolds number for I_{Re1}, I_{Re2}, I_{Re3} and I_{Re4} was 67.59 to 107.30, 120.17 to 190.75, 187.76 to 298.06 and 270.38 to 429.20, respectively (Fig. 3a).

Close observation of data helped to study the linear and exponential trend in I_{Re} increase for different impeller design and speed. The simulation tool helped to visualize range of impeller Reynolds number at 100 rpm with it values in the range of 90.12 to 143.06, 160.22 to 254.34, 250.35 to 397.41 and 360.51 to 572.27 for impeller design 1, 2, 3 and 4 respectively (Fig 3b). Reynolds number is a metric for comparing the overall energy dissipation rate necessary for system mixing (Jo *et al*., 2021) [7].

The impeller Reynolds number I_{Re1}, I_{Re2}, I_{Re3} and I_{Re4} were 112.65 to 178.83, 200.28 to 317.93, 312.94 to 496.76 and 450.63 to 715.34, respectively at 125 rpm impeller speed. Maximum values of impeller Reynolds number for impeller 1, 2, 3 and 4 at 150 rpm were 214.60, 381.51, 596.12 and 858.41, respectively (Fig 4). The impeller Reynolds number was quite low considering impeller speed in the range of 25-150 rpm. When $H:D_t$ ratio increased from 0.75 to 1.5, impeller Reynolds number showed decreasing trend for all four impeller designs. In bioreactor processing, higher Reynolds numbers higher power consumption (Ghotli. *et al*., 2020) [8].

For the 10-litre bioreactor capacity, impeller Reynolds's number was found in transitional region (<10^4 for many impellers) for all the impeller 1, 2, 3 and 4 operating at 25-150 rpm.

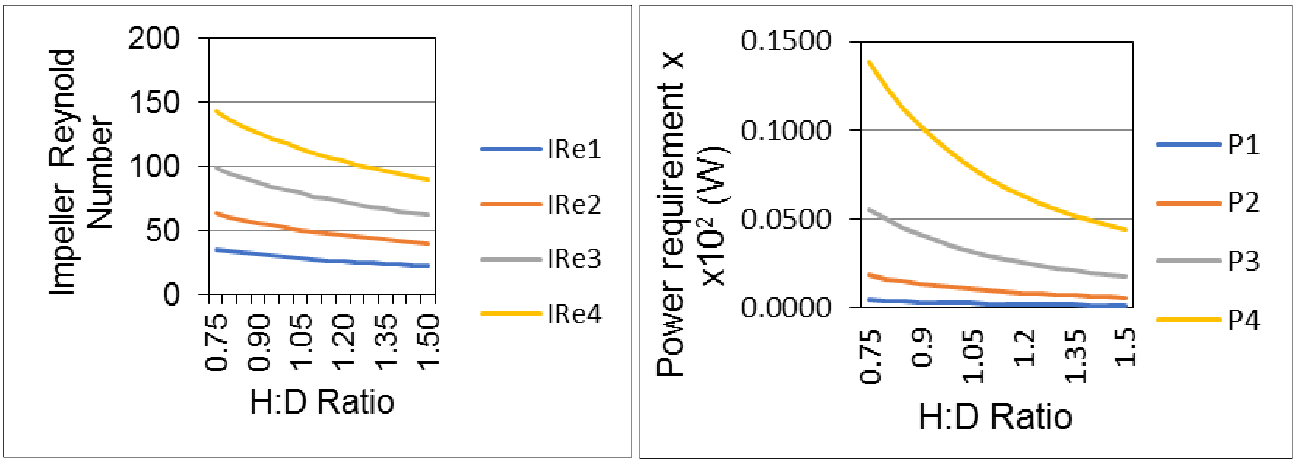
3.2 Power requirement

The power requirement for different impellers 1, 2, 3 and 4 were estimated as P1, P2, P3 and P4, respectively. The The power requirement ranges for P1, P2, P3 and P4 from 0.14 to 0.43, 0.57 to 1.82, 1.75 to 5.57 and 4.36 to 13.85 W respectively at 25 rpm impeller speed (Fig. 2a).

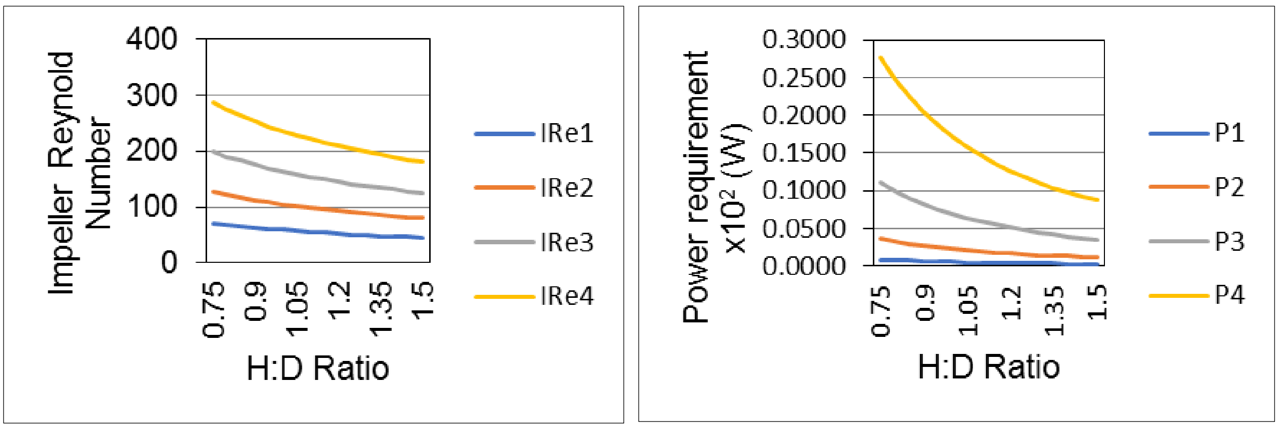
In case of impeller 1 and 2 there was linear decrease in the power when H/D ratio increased from 0.75 to 1.5. While for impeller 3 and 4 exponential decreasing trend was observed with increase in H/D ratio. The power requirement ranges for P1, P2, P3 and P4 from 0.27 to 0.87, 1.15 to 3.65, 3.51 to 11.13 and 8.73 to 27.70 W respectively for 50 rpm (fig. 2b). In a similar study, numerical topology optimization of impeller blades in baffled stirred tanks was demonstrated. Brinkman penalization method was used to alter the impeller blade geometry without having to adapt the computational grid (Munz and Schäfer, 2020) [9]. In the present study four different impellers were considered by changing the ratio of Dt.

The power requirement ranges for P1, P2, P3 and P4 from 0.41 to 1.30, 1.72 to 5.47, 5.26 to 16.70 and 13.09 to 41.55 W respectively for 75 rpm. The power requirement ranges for P1, P2, P3 and P4 from 0.55 to 1.73, 2.30 to 7.30, 7.01 to 22.26 and 17.45 to 55.40 W respectively for 100 rpm (Fig. 3). The study allows for the estimation of power requirement for a wide range of bioreactor design considerations. It has been established that simulations help in prediction of the flow, impeller power consumption and the geometrical dimensions of the impeller (John *et al*., 2022) [10].

The power requirement ranges for P1, P2, P3 and P4 from 0.68 to 2.16, 2.87 to 9.12, 8.77 to 27.83 and 21.81 to 69.25 W respectively for 125 rpm. The power requirement ranges for P1, P2, P3 and P4 from 0.82 to 2.60, 3.45 to 10.94, 10.52 to 33.40 and 26.18 to 83.10 W respectively for 150 rpm (Fig. 4). Impeller Reynolds's number was in the range of 22 to 858 and estimated power requirement was in the range of 0.14 to 83.10 W for impeller speed 25-150 rpm. The power consumption of a rotating impeller in stirred tanks is an important factor to consider when determining its efficiency (Ameur. *et al*., 2017) [11].



(a) Impeller operated at 25 rpm

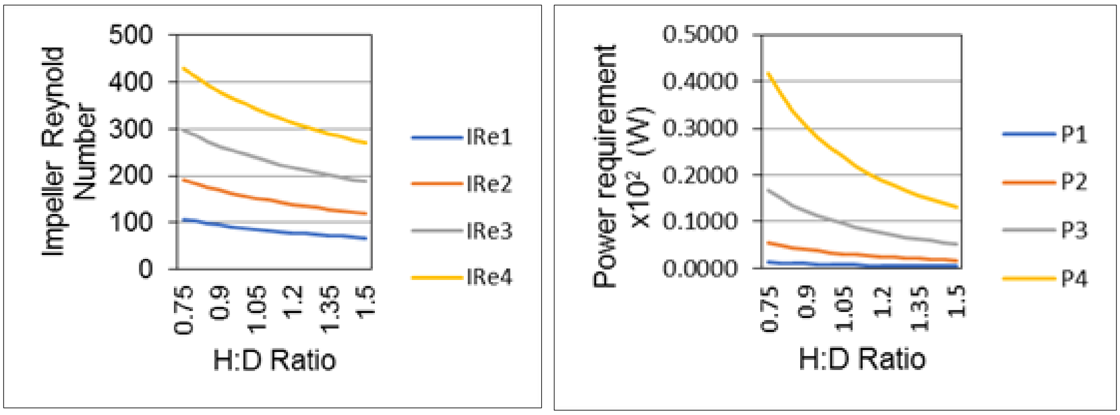


(b) Impeller operated at 50 rpm

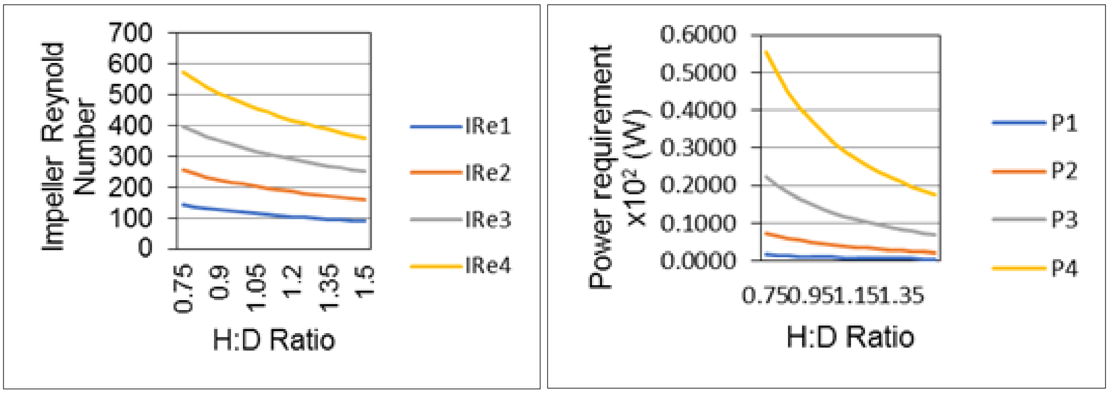
Fig 2: Impeller Reynolds's number and power requirement for 10 litre bioreactor operated at impeller speed 25-50 rpm

Table 1: Simulation results for H:D Ratio 0.75-1.5 to determine bioreactor geometric dimensions (Capacity: 10 litre)

H:D Ratio	Rcp	Vbt	H	Dt	hc	Vc	Dt outlet
0.75	10	0.001	0.089	0.119	0.060	0.067	0.015
0.8	10	0.001	0.093	0.117	0.058	0.065	0.015
0.85	10	0.001	0.097	0.114	0.057	0.064	0.014
0.9	10	0.001	0.101	0.112	0.056	0.062	0.014
0.95	10	0.001	0.105	0.110	0.055	0.061	0.014
1	10	0.001	0.108	0.108	0.054	0.060	0.014
1.05	10	0.001	0.112	0.107	0.053	0.059	0.013
1.1	10	0.001	0.115	0.105	0.052	0.058	0.013
1.15	10	0.001	0.119	0.103	0.052	0.057	0.013
1.2	10	0.001	0.122	0.102	0.051	0.056	0.013
1.25	10	0.001	0.126	0.101	0.050	0.056	0.013
1.3	10	0.001	0.129	0.099	0.050	0.055	0.012
1.35	10	0.001	0.132	0.098	0.049	0.054	0.012
1.4	10	0.001	0.136	0.097	0.048	0.053	0.012
1.45	10	0.001	0.139	0.096	0.048	0.053	0.012
1.5	10	0.001	0.142	0.095	0.047	0.052	0.012



(a) Impeller operated at 75 rpm



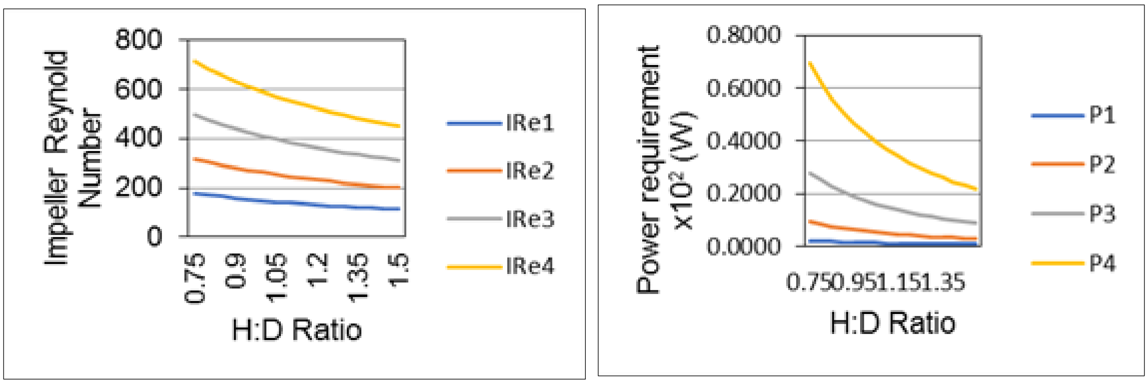
(b) Impeller operated at 100 rpm

Fig. 3: Impeller Reynolds's number and power requirement for 10 litre bioreactor operated at impeller speed 75-100 rpm

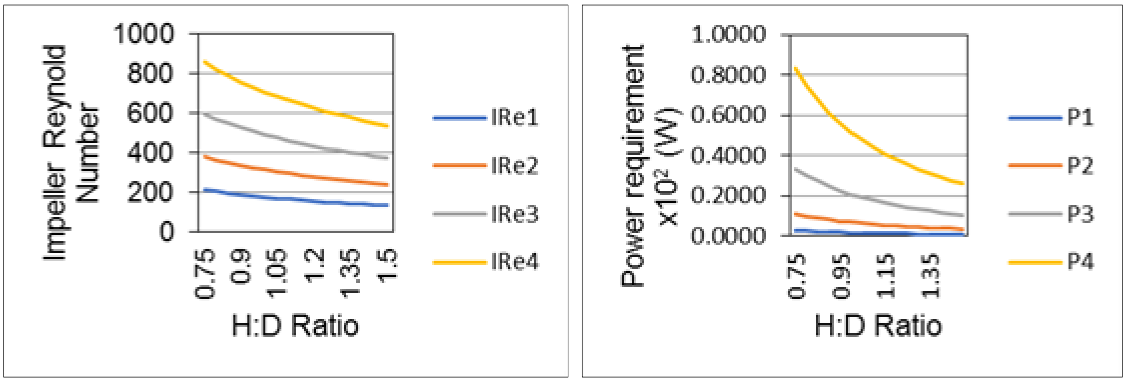
Table 2: Simulation results for H:D Ratio 0.75-1.5 to determine impeller dimensions for 10 litre bioreactor

H:D Ratio	Length of propeller (m)	Impeller diameter (m)			
		Impeller 1	Impeller 2	Impeller 3	Impeller 4
		Da1	Da2	Da3	Da4
0.75	0.137	0.036	0.048	0.060	0.072
0.8	0.141	0.035	0.047	0.058	0.070
0.85	0.145	0.034	0.046	0.057	0.069
0.9	0.149	0.034	0.045	0.056	0.067
0.95	0.153	0.033	0.044	0.055	0.066
1	0.157	0.033	0.043	0.054	0.065
1.05	0.161	0.032	0.043	0.053	0.064
1.1	0.165	0.031	0.042	0.052	0.063
1.15	0.169	0.031	0.041	0.052	0.062
1.2	0.172	0.031	0.041	0.051	0.061

1.25	0.176	0.030	0.040	0.050	0.060
1.3	0.180	0.030	0.040	0.050	0.060
1.35	0.183	0.029	0.039	0.049	0.059
1.4	0.187	0.029	0.039	0.048	0.058
1.45	0.191	0.029	0.038	0.048	0.057
1.5	0.194	0.028	0.038	0.047	0.057



(a) Impeller operated at 125 rpm



(b) Impeller operated at 150 rpm

Fig 4: Impeller Reynolds's number and power requirement for 10 litre bioreactor operated at impeller speed 125-150 rpm

4. Conclusions

The simulation method based on Python platform was found suitable for estimation of impeller power requirement in a bioreactor. Impeller Reynolds's number and power requirement followed a decreasing trend with the increment of H:Dt ratio (0.75 to 1.5). Linearity of impeller Reynolds's number with proportional power consumption was observed during the analysis and visualization of data. Simulation helped to determine power requirement for a wide range of impeller design operating at varying speed (25-150 rpm).

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