CZECH TECHNICAL UNIVERSITY IN PRAGUE

FACULTY OF MECHANICAL ENGINEERING

Department of Process Engineering

CFD simulation of heat transfer in an agitated vessel with a pitched six - blade turbine impeller

Master thesis

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MASTER'S THESIS ASSIGNMENT

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Guidelines:

- Make a literature research concerning the heat transfer in agitated vessels.
- Create a model for the given geometry in ANSYS CFD.
- Perform numerical simulations of heat transfer in the agitated vessel for different rotation speeds and evaluate heat transfer coefficients at the bottom and vertical wall.
- Evaluate the impact of the impeller distance from the bottom.
- Summarize the methodology used in the thesis and propose possible improvements of the solution procedure.

Bibliography / sources:

Name and workplace of master's thesis supervisor:

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Assignment valid until: __________

Ing. Karel Petera, Ph.D. Supervisor's signature	prof. Ing. Tomáš Jirout, Ph.D. Head of department's signature	prof. Ing. Michael Valášek, DrSc. Dean's signature

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Finally, I would like to dedicate this thesis to my father Jagan Mohan Rao, I know he would be proud of me.

ABSTRACT

Heat Transfer to a Newtonian fluid in jacketed vessel equipped with a pitched blade turbine (PBT) has been numerically investigated. The turbine has six blades at 45^{o} angle and it is placed in a cylindrically baffled vessel with a flat top and bottom. The cylindrical walls and bottom of the vessel are maintained at constant heat flux q = 3000 W/m^2 boundary condition. Numerical simulations of heat transfer in the agitated vessel for different rotational speeds from 300 to 900 rpms were performed evaluating heat transfer coefficients at the bottom and vertical walls by varying Off-bottom clearance h/d =1, 2/3, 1/3 (impeller distance from the bottom of agitated vessel). To study the flow field and transient heat transfer in agitated vessel a commercial software ANSYS Fluent 15.0 has been employed. The sliding mesh technique available in ANSYS Fluent was used to model flow around the rotating impeller and k-ω based Shear -Stress-Transport (SST) turbulence model was chosen to model turbulence. An internal source(sink)of heat was used to eliminate the fluid temperature increase which might influence the evaluation of the heat transfer coefficients. By performing the transient simulations and calculated the Nusselt numbers at bottom, wall, (Bottom +wall), the heat transfer correlation was developed and compared with experimental data in the literature.

Keywords: CFD, transient heat transfer simulation, PBT, Sink, Off-bottom clearance, sliding mesh, Nusselt number.

Table of Contents

List of Figures

List of Tables

NOTATIONS

Dimensionless number

Re	Reynolds number [-]
Pr	Prandtl number [-]
Nu	Nusselt number [-]
Po	Power number [-]

Turbulence modelling

k	Turbulent kinetic energy [m^2 / s^2]
ε	Kinetic energy dissipation rate [m^2/s^3]
ω	Specific dissipation [s^{-1}]
u'	Fluctuating velocity [m/s]
U	Mean velocities [m/s]
μ_t	Turbulent viscosity [m^2/s]

Parameter of Agitated vessel

D	Vessel diameter [m]
H	Vessel height /Liquid height [m]
d	Impeller diameter [m]
w	Width of impeller blade [m]
h	Height of impeller [m]
h/d	Off -Bottom clearance [m]
t	Blade thickness [m]
N	No. of Blades
θ	Blade angle [degree]
b	Blade width [m]
B	Number of baffles
$\mathrm{b_t}$	Baffle thickness [m]
n	Impeller rotation speed [rpm]

Parameters of Impeller

α	Pitch Angle [θ]

χ	Blade Thickness [m]
D	Impeller diameter [m]
H_{od}	Outer side diameter [m]
W_h	Hud Height [m]
W	Blade width [m]
W_p	Projected blade width [m]
P	Power [W]

Fluid properties

ρ	Density of fluid [Kg/m^3]
μ	Dynamic viscosity of the fluid [Pa s]
Cp	Specific heat of fluid [J/Kg/K]
λ	Thermal conductivity [W/m K]
ν	Kinematic viscosity [m^2/s]
a	Thermal diffusivity [m^2/s

Heat transfer analysis

q	Heat Flux [W/m^2]
Q	Heat transfer rate [m^2]
α	Heat transfer coefficient [W/m^2 K]
$\Delta \overline{T}$	Mean temperature difference [K]
T_h	Temperature of the heating medium [K]
T_b	Temperature of batch liquid [K]
m	Mass of batch liquid [Kg]
Δt	Heating time [s]
Vi	Viscosity ratio [-]
U	Overall heat transfer coefficient [W/m^2 K]
τ	Moment [N.m]
ω	Angular velocity of impeller [rad s^{-1}]
t_m	mixing time [s]

CHAPTER 1 INTRODUCTION AND OBJECTIVES OF THIS WORK

1.1 Introduction

In many chemical industries and processing operation units mixing plays an important role to mixing up the liquids, solid to liquid suspensions, gas to liquid dispersions etc. For this application agitated vessels are used in industries like food, pharmaceutical, water treatment plants, manufacture of paints and cosmetics etc. In fact, this two-words agitation and mixing are sounds different meaning, but Agitation refers to forcing a fluid by mechanical equipment to flow in a circulatory or other pattern inside a closed container. Mixing is a random distribution of two different or same phases of fluids. The real time application of agitated vessel is used in detergent industries to mix perfumed fragrance with the washing liquid. [Brodkey et al.1998]

In process industries agitation promotes an excellent example of occurring homogenizing of temperature, physical properties, chemical reactions, heat transfer, mass transfer of the properties of components. Mixing leads to good quality of products and homogeneity of materials.

Agitation vessel furnished with tank, impeller mounted on an overhung shaft, baffles in contact with the process fluid. Accessories such as inlet, outlet lines and drain valve and coils, jackets providing heating system. The design of agitated vessel varies widely depending on the application in industrial scale model or experimental work in laboratory scale up. In following chapters about agitated vessel parameters and theory are briefly explained.

Heat transfer in agitated vessel is one of the most important factor to be consider for maintaining the quality of product. Usually, agitated vessel has heat transfer surface in form of jacketed or internal coil, for supply heating or cooling the vessel, a recirculation loop with an external heat exchanger also be used. Depending on the fluid in agitated vessel heat transfer rate is set. Dimensionless groups are used to calculate in present work.

Process engineering mainly focuses on design, operations, and maintenance of chemical and manufacturing industries. Process engineer job role is to fill the gap in between recovery of raw material and manufacturing of finish products. Process engineer must apply the key concepts of mechanical and fluid dynamics principles to conversion of matter by effect of mechanical action. Process engineering benefits significantly from modelling and simulation as a mean to optimize existing processes and to new once and to overcome the drawback of old models. Where computational fluid dynamics (CFD) help to analyse the design and modelling of fluid flows in the geometry. Due to complexity of the fluid flows CFD helps to visualization of fluid interaction, heat transfer, velocity profiles of the design. In recent years there is vast change in technology which helps to design the model and test it with real time conditions to save the investment cost and production cost. In market there many number of software to test the simulations of fluid flow and heat transfer like open FOAM, ANSYS Fluent, SIM SCALE, ANSYS CFX, Autodesk simulations etc. In this master thesis work is about CFD simulation of heat transfer in an agitated vessel.

1.2 Objectives of this work

1. Study and design a model of agitated vessel geometry in computational fluid dynamics (CFD). Using simulation software ANSYS 15.0 version.
2. Performing numerical simulations of heat transfer in an agitated vessel for different rotation speeds (300 – 900 rpm) and giving the constant heat flux source of q= 3000 and 30000 W/m^2 (500 rpm) at the bottom and walls of vessel.
3. By varying the impeller distance from the bottom of vessel ratios of h/d = 1, 2/3 and 1/3.
4. Using CFD sliding mesh technique of heat transfer in a jacketed cylindrical agitated vessel mounted with a 45° angle pitched six -blade turbine impeller (PBT).
5. Compare the obtained results with the available literature and propose further improvements of this work.

2.1 Introduction

Mixing is a physical operation carried out to reduces nonuniformities in the fluid by eliminating gradients of concentration and temperature. Mixing produces a homogeneity of two different or same components to be perfectly mixed. Mixing can be achieved in chemical industries by machinal agitation using impeller. This chapter deals with agitated vessels and their types.

2.2 Agitated Vessel Geometry

The shape of the base for agitated tanks effects the efficiency of mixing. Depending on application profiles are chosen, like a) flat b) dished c) round d) conical. In industries applications mostly utilize cylindrical agitated vessel equipped with baffles. A standardized mechanical stirred agitated vessel shown in Figure 2.1 and parts are described below.

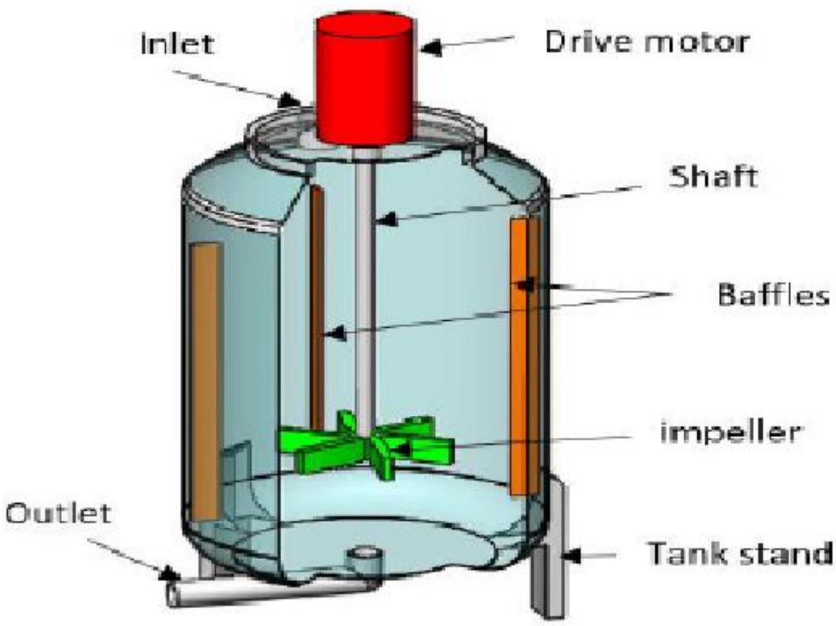


Figure 2.1 Typical configuration of agitated vessel [Torotwa et. al.,2018]

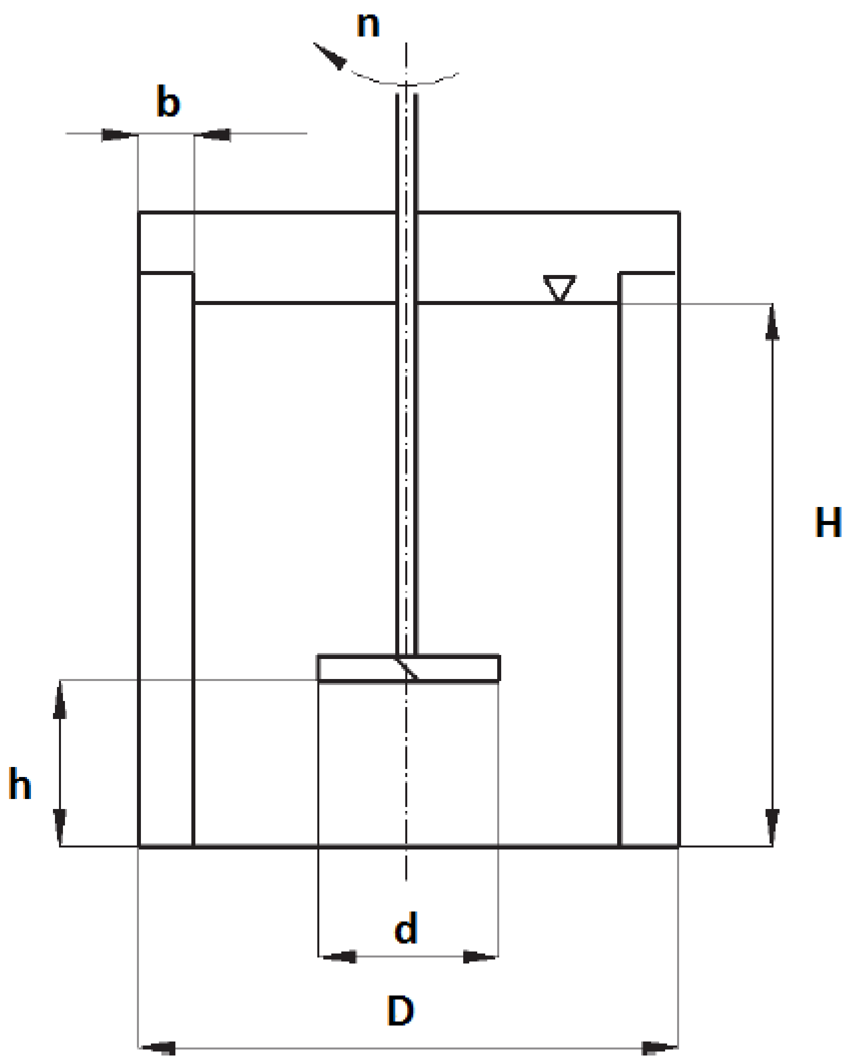


Figure 2.2 Geometric specifications for a stirred tank. [Beshay, K. R et. al., 2001]

In standard vessel configuration, the impeller diameter is denoted by d is 1/3 of the vessel diameter D. Impeller height, h from the bottom of the tank is 1/3 of the vessels diameter. The liquid level is indicated by letter H. the four baffles have a width, b of 1/12 of vessels diameter. [Brodkey, R. S et. al., 1998].

Agitated vessels are useful for liquids of any viscosity up to 750 Pa.s, but although not more than 0.1 Pa.s are rarely encountered through on contacting two liquids for reaction or extraction purposes. In many examples, the contents of agitated vessels are to be heated or cooled. and often heating and cooling are required at different portions of the production cycle. Heat transfer is an important factor influencing the design of agitated vessels and determine the quality of product outcome. The impeller speed and the agitator selection determine the heat transfer in the system, but other conditions such as the flow characteristics of the fluid and processing conditions determine the power characteristics of the fluid and prepare the power requirements of the agitator selection primarily in most cases. Heat transfer equations used once agitator has been specified rather than to selection of the selection of the most suitable agitator and vessel geometry. [Warren L. et. al.,1993 and Chisholm, D et al., 1998]

The main objectives of agitation in solid- liquid systems can be divided in four categories:

a) To avoid solid accumulation in stirred tank.
b) Maximise contacting area between solid and liquids.
c) Dispersing a second liquid, immiscible with the first, to form an emulsion or suspension.
d) Raise heat transfer between the liquid and a coil or jacketed vessel.

The main components of an agitated vessel are

1. Drive System
2. Shaft
3. Baffles
4. Impeller Types
5. Draft Tubes
6. Inlet and Outlet Ports

Drive System: It constitute of motor and gearbox of the mixer. The motor can operate by electric DC motor, driven by pressure, hydraulic fluid, steam turbine or diesel and gas engine. Standard motor power will be 2984 to 671400 W and above depends of application of mixing agitator. Gear box is used to obtain the desired mixer shaft speed from the motor speed. A gear box can have two or three gear reduction and can fabricated to provide any gear ratio required.

Shaft: Shaft are connected between impeller and drive system. Multiple impeller is mounted on same shaft. During the process, liquid vapours or gases should not leak thought shaft nozzle and should not exchange external or internal agents of environment. Most common technique used sealing shaft is with stuffing box.

Baffles: are vertical strips of metal mounted on walls of the agitated tank, are installed to eliminate vortexing and swirling and to increase the fluid velocity by diverting the flow across the cylindrical vessel. Generally, number of baffles used in agitated vessel are three four and six. A standard configuration of baffle width T, 1/10 and 1/12 of vessel diameter.

Baffles helps to change the flow of fluid tangential to vertical flows, provide top to bottom mixing and increase the drag and power draw of impeller. Baffles are not used for laminar mixing of viscous fluids.

Impeller Types: A basic classification of fluid flows patterns and impeller types are listed in below table 2.1. Impeller are used in transitional and turbulent mixing depending on application shape and geometries are specified in figure 3.3 four blade pitch blade turbine explained. For liquid blending and solid suspension axial flow impeller are suitable for efficient mixing. while radial flow impellers are best used for gas dispersion. Impeller type and operation conditions are describing by Reynolds number and power number as well as individual characteristics of impeller type. Ratio of impeller diameter $1/3^{rd}$ of vessel diameter. Standard impeller speeds are 37, 56, 68, 100, 155,250, 320rpms. The impeller is placed at 1/3, 2/3, and 1 distances from the bottom of agitated vessel, ratio is chosen on the viscosity of the liquid and liquid level off the bottom. For mixing in flat tank location of impeller also changes like side entering mixer for large product storage, bottom entering, and angular top entering mixer are placed. The propeller, paddles, turbines, flat-blade turbine, pitched-blade turbine, and disk flat blade turbine are called Nonproximity impellers. Nonproximity impellers are the impellers blade rotates some distance from the vessel wall.

Axial Flow	Propeller, Pitch Blade Turbine, Hydrofoils
Radial Flow	Flat-Blade impeller, Disk Turbine (Rushton), Hollow-Blade Turbine
High Shear	Cowles, Disk, Bar, Pointed Blade Impeller
Specialty	Retreat Curve Impeller, Sweptback Impeller, Spring Impeller, Glass- Lined Turbine
Up/Down	Disks, Plate, Circles

Table 2.1 Types of Impellers and their Flow classification [Edward L et al.,2003].

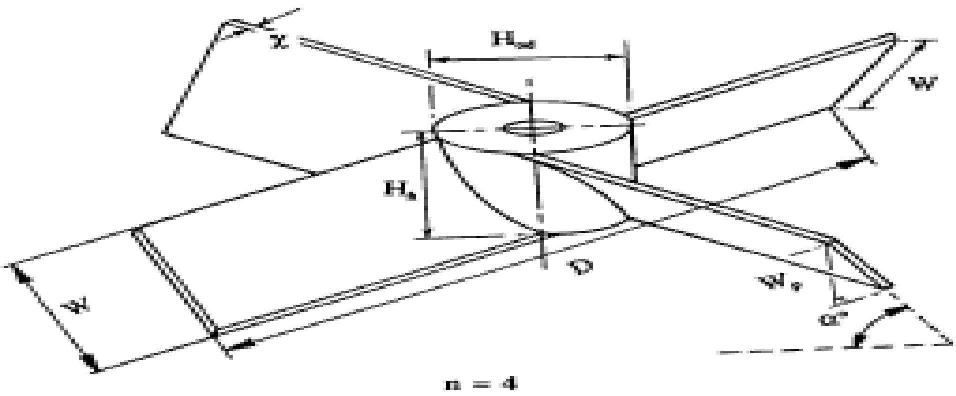


Figure 2.3 A four blade Pitched Blade Turbine with (PBT) with nomenclature. [Andrew Tsz ,1992].

D - Impeller Diameter

H_{od} - Outside Diameter

H_h - Hub Height

n - Number of Blades

W - Blade Width

W_p - Projected Blade width

α - Pitch Angle

χ - Blade Thickness.

Draft Tubes: A draft tube is cylindrically mounted around and slightly larger in diameter than the impeller. Usually, draft tubes are used with axial impellers to direct suction and discharge streams. An impeller – draft tube system behaves as an axial flow pump with low efficiency. it's a "top to bottom" circulation pattern.

Inlet and Outlet port: The design of inlet and outlets are based on the process and the type of feed and rate of feed dispersion. For the slow batch processes, the inlet can be from the top and quick dispersion rate of the feed, the inlet nozzle should be located at highest of the vessel where a turbulent region can be formed by inlet flow rate. The outlet nozzle can be placed at the bottom head of the vessel so that fluid can completely be exuded.

2.3 Heat Transfer Surfaces

The process mixing/agitation operation are also involved with heat transfer. Heat transfer in agitated vessel equipped with jackets, an internal helical pipe coil, tube baffles and plate coil baffles and heat exchanger as shown in Figure 2.4.

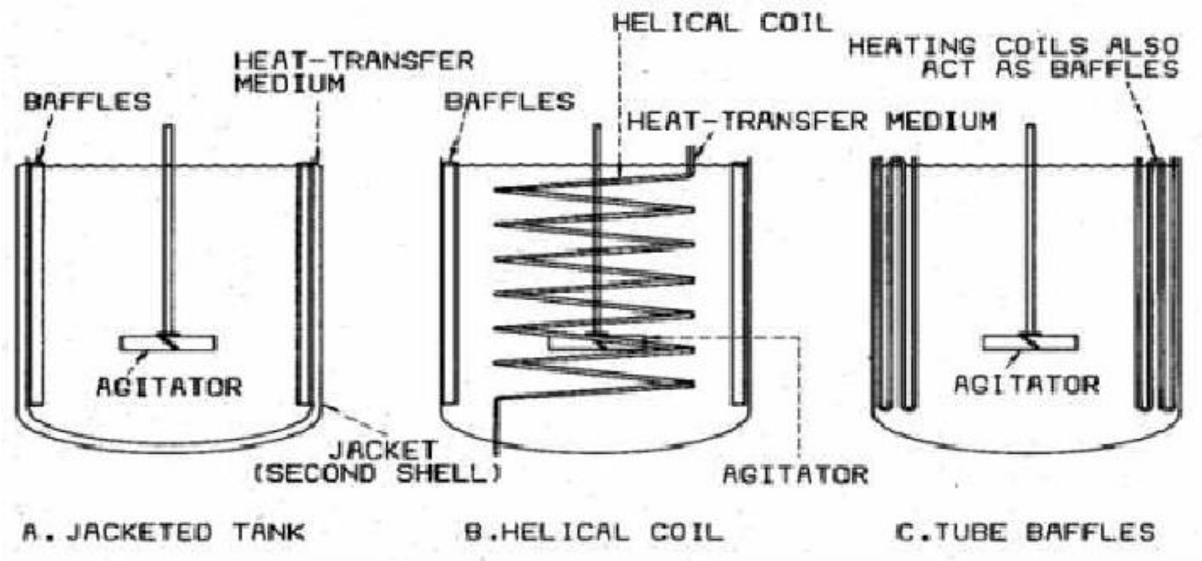


Figure 2.4 Different type of heat transfer equipment for mixing [Harwinder 2014].

Selection criteria for most efficient geometry for heat transfer surface are

a) Type of surface

b) the number of coils, plates etc.

c) The location of a surface in the vessel

d) The gap between a coil and banks spacing of harps.

e) Spacing between tubes in harps and helical.

For example, a typical requirement in industrial mixing is the blending of components to get a stable concentration in fluids for this purpose no need for heat transfer surfaces. In one of the application, mixing of the fluid requires a cycle of cooling or heating for an agitated liquid for this approach is to transfer the necessary heat transfer is provided by jacketed vessel.

e.g. In the fermenter, for the large area heat transfer requirement the jacked vessel is not enough so, that a combination of jacket and tube baffles are handled. The heat transfer in an agitated vessel and its equations are exposed in more particular in the coming chapters. [Dostál M el al., 2010].

CHAPTER 3 HEAT TRANSFER IN AGITATED VESSEL

3.1 Heat Transfer in Agitated Vessel

An agitated vessel is used for heating or cooling of agitated fluid. The fundamental heat transfer rate equation can have expressed as

$$Q = \alpha S \Delta \overline{T} \qquad [3.1]$$

Heat transfer rate Q between the agitated liquid and the jacked vessel. Where α heat transfer coefficient, S is the heat transfer area and $\Delta \overline{T}$ mean temperature difference.

3.2 Dimensionless Numbers

Dimensionless parameters are helpful to find out the heat transfer coefficients and their relations with other parameters in an agitated vessel. It reduces the number of dependent variables. Basic dimensionless parameters are explained below

Reynolds Numbers

Reynolds number characterize the regime of flow i.e. whether the flow is laminar or turbulent. It is a ratio of inertia forces to viscous forces.

$$Re = \frac{N\, D^2 \rho}{\mu} \qquad [3.2]$$

Where,

N - Rotational speed of the impeller

D- Impeller diameter

ρ - Density of fluid

μ - Dynamic viscosity of fluid

Reynolds number

Re < 50 Laminar flow

50 < Re <5000 Transitional flow

Re > 5000 Fully Turbulent flow.

Nusselt Number

For calculation of heat transfer in an agitated vessel for wall side or bottom side Nusselt number is used. Nusselt number is one of important parameters to calculate the heat transfer rate between the fluid and the vessel.

$$Nu = \frac{\alpha\, D}{\lambda} \qquad [3.3]$$

Where

α - Heat transfer coefficient of the process

D - Diameter of the agitated vessel

λ – Thermal conductivity of fluid

Prandtl Number

Prandtl number is the ratio between kinematic viscosity by thermal diffusivity. Terms are explained below.

$$Pr = \frac{v}{a} = \frac{uc_P}{\lambda} \qquad [3.4]$$

μ - Dynamic viscosity of the fluid

c_p - Specific heat capacity

λ - Thermal conductivity of fluid properties

3.3 Heat Transfer Correlations for Agitated vessel

Agitated vessels in real time operation where heat addition or removal from the process fluid is required, vessel is supplied with heat transfer surfaces. Mixing operation increases heat transfer intensity in general. As we know heat transfer in agitated vessel is equipped by jackets, internal helical coils, and internal baffles coils. A general relation using all dimensionless numbers is usually written as

Nu = f (Re, Pr, Geometry parameters) [3.5]

Correlation for the process of the heat transfer coefficient in agitated vessel are formed form experiments performed on small scale model industrial tanks with the geometrically scaled down.

$$Nu = C\ Re^{a}\ \mathrm{Pr}^{\mathrm{b}}\ \mathrm{V_I}\ G_d \qquad [3.6]$$

Where

$$Vi = {}^{\mu_b}/_{\mu_w} \qquad [3.7]$$

Nu is Nusselt number, Re is Reynolds number, Pr is Prandtl number and Vi is the wall viscosity correction factor and $\mathrm{G_d}$ is a geometric correction factors. The exponents a, b, c is varied with the parameter constant C with the system. For Jacketed vessel with baffles and different impeller is shown in Table 3.1 taken from book, [Chisholm et al.,1989.]

Impeller	N_B**(Blades)**	**Baffles**	**C**	**Exponents of**			**Recommended geometric**
				Re^a	Pr^b	Vi^c	**Corrections** G_d
Paddle	2	Yes	0.415	2/3	1/3	0.24	
		No	0.112	3/4	0.44	0.25	$\left(\frac{Dv}{Di}\right)^{0.40} \left(\frac{L_i}{D_i}\right)^{0.13}$
Various							
Turbines:		No	0.54	2/3	1/3	0.14	$\left(\frac{L_i/Di}{1/5}\right)^{0\cdot15} \left(\frac{N_{bl}}{6}\right)^{0.15}$
Disk, flat 6							$[sin(\theta)]^{0.5}$
Pitched blades		Yes	0.74	2/3	1/3	0.14	$\left(\frac{S_{bl}/D_i}{1/5}\right)^{0.2} \left(\frac{N_{bl}}{6}\right)^{0.2}$
							$[sin(\theta)]^{0.5}$
		No	0.37	2/3	1/3	0.14	$\left(\frac{D_v/Dj}{3}\right)^{0.25} \left(\frac{H_i}{H_i}\right)^{0.15}$
Propeller	3						
		Yes	0.5	2/3	1/3	0.14	$\left(\frac{1.29\ P/D_i}{0\cdot29+P/D_i}\right)$

Table 3.1 Heat Transfer Correlation for Jacket Vessel with Different Impellers.

a Baffled and unbaffled.

b Relatively low range of Reynolds numbers 20,4000. And other correlations presented in this table were developed for range Re_a reaching 10^5.

Dittus – Boelter's correlation generally used in the case of flow in pipe, in agitated vessel it is used as reference draft tube around the impellers.

$$Nu = 0.023\, Re^{0.8}\, \mathrm{Pr}^{0.33} \qquad [3.8]$$

Petera et al., 2017 measured the heat transfer at the bottom of a cylindrical vessel impinged by a swirling flow from impeller in a draft tube using the electro diffusion experimental method by axial flow impeller in draft tube. A new correlation was proposed from this paper

$$Nu = 0.041\, Re^{0.826}\, Pr^{\frac{1}{3}}\, S^{0.609} \qquad [3.9]$$

Petera et al., 2008 transient measurement of heat transfer coefficient in agitated vessel

$$Nu = 0.823\, R\, \mathrm{Re}^{\frac{2}{3}}\, Pr^{\frac{1}{3}}\ Vi^{0.14} \qquad [3.10]$$

3.4 Time Estimation for Heating or Cooling of Batch of Liquid

In industries agitated vessel is used for batch or continuous rectors. In this case we are simulating the agitated vessel in batch mode. In practical applications, function of time is one of the parameter to operate the batch rector. The mean temperature difference the batch liquid and heating or cooling depends upon function of time. The overall heat transfer coefficient U and time for heating or cooling in a batch liquid in an agitated vessel can be estimated by some correlations.

The heat transfer rate can be calculated from the equation:

$$Q = m\, c_p\, \frac{dT_b}{dt} = UA(T_h - T_b) \qquad [3.11]$$

Where

T_h - Temperature of the heating medium

T_b - Temperature of the batch liquid

m – Mass of batch liquid

c_p – Specific heat capacity of the batch liquid

Equation (3.8) can rearranged in the form

By integrated over the time interval Δt required to heat the agitated liquid from temperature T_{b1}toT_{b2}

$$\int_{Tb1}^{Tb2} \frac{dT}{T_b - T_b} = \frac{U\ A}{W\ C_p} \int_0^{\Delta t} dt \qquad [3.12]$$

Which results into:

$$ln \frac{T_h - T_{b1}}{T_h - T_{b1}} = \frac{U\ A}{m\ C_p}\ \Delta t \qquad [3.13]$$

From equation (3.11) the heating time Δt, can be calculated, supposing that we know the overall heat transfer coefficient U. This coefficient considers heat transfer coefficients on the both sides of the heat transfer surface.

$$\frac{1}{U} = \frac{1}{\alpha_1} + \frac{1}{\alpha_2} \qquad [3.14]$$

CHAPTER 4 POWER CHARACTERISTICS OF IMPELLER

4.1 Power Characteristics of Impeller

One of the most important parameter in the industrial mixing is selection of impeller type. For rotation of the impeller inside the agitated vessel electric motor are required with power consumptions. one of the factor for the cost of equipment is agitated drive system. To determine the power characteristics of the impeller Dimensionless group of power number is used to calculate.

4.2 Power Number - Dimensionless Group

The power required was calculated from equation [4.1] the values of torque and angular velocity of the impeller are measured numerically as a monitored quantity in ANSYS Fluent. In experimental setup torque values are measured by using strain gauges etc.

$$P = \tau * \omega \qquad [4.1]$$

τ - Moment

ω – Angular velocity

Power number is calculated from equation

$$P_o = \frac{P}{\rho * N^3 * D^5} \qquad [4.2]$$

Where

P_o - Power number

P - Power

ρ - Density of fluid

N - Number of rotations

D – Diameter of impeller

4.3 Calculation of power Number for 6 Blade PBT Impeller

In this present work, the input power required for the 6 blade PBT impeller was calculated for the different rotational speeds ranging between 300-900 rpm for the distance of impeller from bottom of vessel h/d = 1, 2/3 and 1/3 of impeller diameter (66.66 mm). The results for power number are tabulated in Table 4.1

Off-Bottom Clearance	Rotational Speed, N (rpm)	Re [-]	Po [-]
h/d = 1	300	22116	1.62
	500	36860	1.61
	700	51604	1.79
	900	66348	2.01
h/d=2/3	300	22116	1.76
	400	29488	1.66
	500	36860	1.88
	600	44232	1.88
	700	51604	1.88
	800	58976	1.83
	900	66348	1.87
h/d=1/3	300	22116	2.11
	500	36860	2.04
	700	51604	2.00
	900	66348	2.29

Table 4.1 Calculation of Power number.

The below graph represents power characteristics of high - speed impellers operated with baffle vessel, 1 – six-blade turbine with disk(Rushton turbine) (CVS 69 1021),2- six-blade open turbine, 3 – pitched six-blade turbine with pitch angle 45° (CVS 69 1020), 4 – pitched three- blade turbine with pitch angle 45° (CVS 69 1025.3), 5- propeller (CVS 60 1019), 6a,b – high shear stress impeller (CVS 69 10381.2).In this present work we are dealing with pitch blade turbine pitch angle with 45 ° observer the number **3** in Figure 4.1.

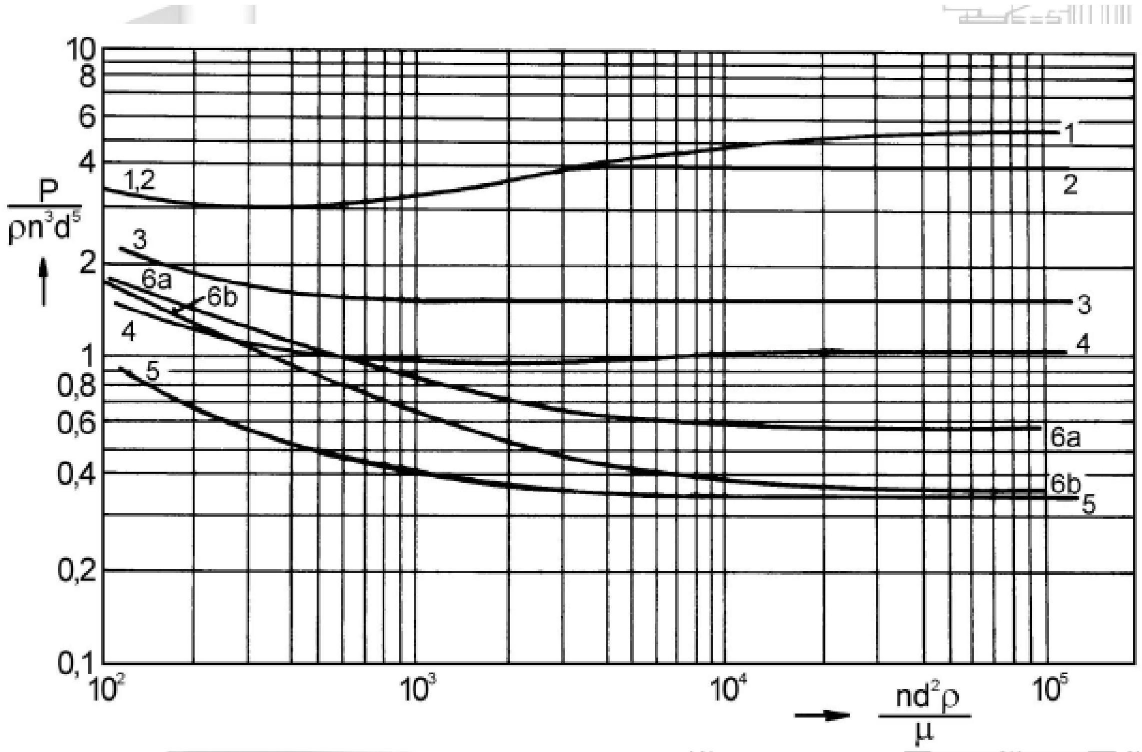


Figure 4.1 Power number vs Reynolds number (log – log scale).

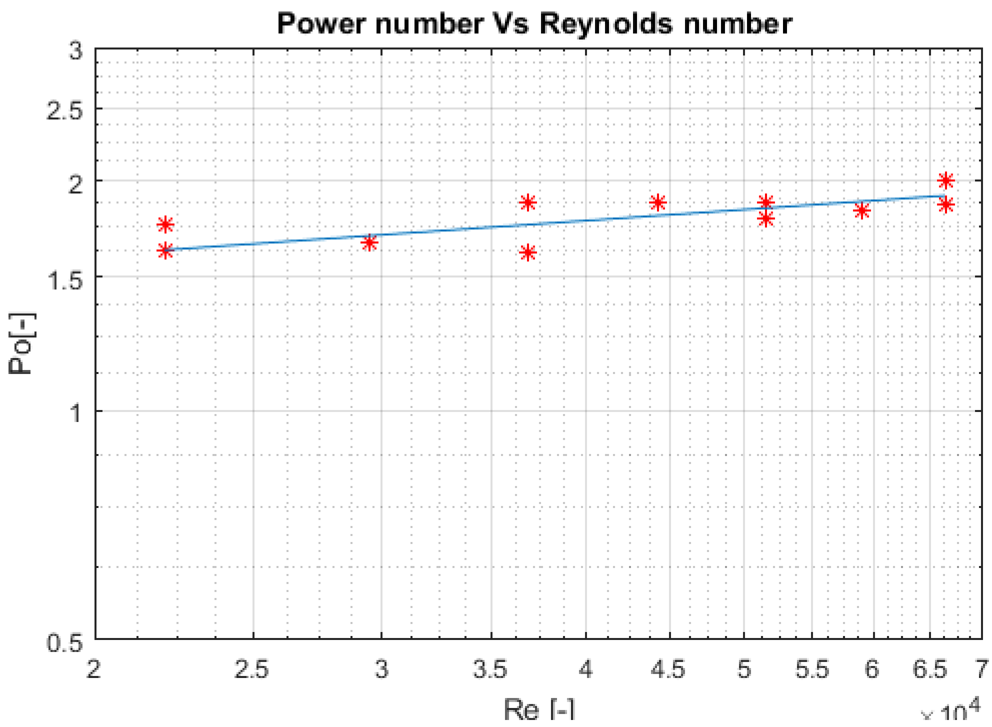


Figure 4.2 Power vs Reynolds number obtained power characteristics of 6 blade PBT impeller, Off bottom clearance h/d – 1, 2/3, 1/3.

It can be observed from the Figure 4.2 power characteristics of PBT impeller. The power model can describe the non-linear relationship between the Reynolds number and Power number as:

$$Po = a\,Re^b \qquad [4.3]$$

$$Po = a \qquad [4.4]$$

Where a and b in Eq. (4.3) are model parameters. The null hypothesis is simple model compared to power model. The power model gives more accurate description of functional relationship between the Power number and the Reynolds number. The MATLAB script written for performing non-linear regression function and the 'nlinlfit2' procedure shown in Appendix A [Project – I Course 2016 and Chakravarty ,2017]. It was found that the power number predicted by the null-hypothesis was 1.78 ± 0.07 (4.30%) which was compared with average value obtained in experimental work performed by [Beshay,K .R el at., 2001]. In my calculation of power (τ, ω) I took values from Fluent. OUT file which is last rotational speed of impeller which is not average valve.

4.4 Estimation of Mixing Time

To express the degree of homogeneity in agitated vessel containing a batch of liquid to be mixed, important parameter required is mixing time, t_m. The mixing time depends on different factors such as size of the tank, impeller size and type of impeller in agitated vessel, fluid properties and impeller rotational speed. The equation used to calculate mixing time expressed as: [Hydromechanical process course by Prof. Ing. Tomás Jirout 2017]

$$nt_m = f\left(\frac{n\,d^2\rho}{\mu}\right) = f(Re) \qquad [4.5]$$

Where nt_m is speed of the impeller, n is the impeller rotational speed in rev/s. For low Reynolds number, the dimensionless rotational speed,nt_m is a function of Reynolds number. If higher values of Reynolds number mixing time reaches constant homogenize of the fluid will be reached.

In present work, the rotational speeds of impeller are ranging 300 to 900 rpm. The simulation run-time was based on the theoretically evaluated mixing time, t_m .in agitated vessel. The transient simulations were performed in ANSYS Fluent for seven different rotational speeds of the impeller rang 300,400,500,600,700,800,900 rpms and different Off bottom clearance 1, 2/3 and 1/3 cases. The run-time for transient analysis was taken on basic of the mixing time t_m from equation 5.3 for different Reynolds number corresponding to rotational speed. Run time for simulation based on different rotational speeds can be shown in Table 4.2.

Rotational speed, N (rpm)	**Simulation run-time t_m**
300	20
400	15
500	10
600	10
700	10
800	10
900	10

Table4.2 Run-time for simulation.

CHAPTER 5 COMPUTATIONAL FLUID DYNAMICS

5.1 Introduction

The abbreviation CFD stands for computational fluid dynamics. It deals with area of numerical analysis in the field of fluid's flow phenomena. As sophisticated computer techniques have been developed in recent decades, CFD method is a useful and powerful solving tool for the industrial and non-industrial problems like heat and mass transfer, chemical reaction and predicting fluid flow (laminar, turbulent regime). Some of applications like

- Aerodynamic of aircraft and vehicle: lift and drag
- Hydrodynamics of ships
- Power plant: combustion in internal and gas turbine.
- Chemical process engineering: mixing and separation, polymer moulding external and internal environment of buildings: wind loading and heating/ventilation.
- A lot of other fields where CFD involves marine, meteorology, biomedical, environment, hydrology, and oceanography engineering.

How does CFD works

CFD contains three main elements

PRE-PROCESSOR

- Geometry creation
- Geometry clean up
- Mesh generation
- Boundary conditions

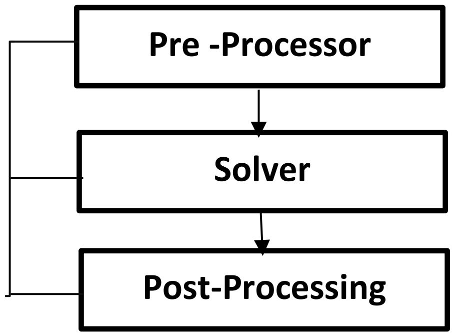
SOLVER

- Problem specification
- Additional model
- Numerical computation

POST – PROCESSING

- Understanding flow with colour contour etc
- Vector plots
- Particle tracking

- ➢ Average values (drag, lift, heat transfer, velocity's)
- ➢ Report generation



A common CFD solver is mostly based on finite volume method and finite element method used as well. This means that domain is discretized into finite set of control volumes and general conservation (transport) equations for mass, momentum, energy, species, etc. are solved on this set of control volumes. A finite control volume can be expressed as, ϕ e.g. a velocity component or enthalpy. [Versteeg H K el at,.2007].

Rate of change of ϕ in the control Volume with respect To time	=	Net rate of increase of ϕ due to convection into the control volume	+	Net rate of increase of ϕ due to diffusion into control volume	+	Net rate of creation of ϕ inside the control volume

5.2 Governing equations of fluid and heat transfer

CFD is based on the fundamental governing equations of fluid dynamics-the continuity, momentum, and energy equations which speak about physics. But they are mathematical statements of three fundamental physical principle upon which all of fluid dynamics is depends on

1. Mass is conserved
2. Newton's second law F=ma.
3. Energy is conserved.

These governing equations in conservation form for unsteady, three-dimensional, compressible, viscous flows are discussed in subsequent sections.

5.2.1 Continuity equation

Continuity equation in conservation form is obtained by applying the principle of conversation of mass on a control volume fixed in space and described in differential form is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \qquad [5.1]$$

Where $\vec{u}$ is the flow velocity at a point on the control volume surface $\vec{u} = f(x, x, z, t)$

and ρ is density of fluid.

For incompressible flow equation [5.1] written as simplified manner

$$\nabla . \vec{u} = 0 \qquad [5.2]$$

5.2.2 Momentum Equation

Conservation form of momentum equation by the application of Newton's second law of motion to a fixed fluid element is described by three scalar equations X, Y and Z directions for viscous flows it is called Naiver- Stokes equation.

Conservation form is described as:

$$\rho \left[\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} \right] = -\nabla p + \nabla . \vec{\vec{\tau}} + \rho \vec{f} \qquad [5.3]$$

Where $\nabla \cdot \vec{\vec{\tau}}$ is the viscous tensor and $\vec{f}$ is body force per unit mass.

Navier- Stokes equation in teams of X, Y and Z components as:

X- component of momentum equation:

$$\frac{\partial (\rho u_x)}{\partial t} + \nabla \cdot (\rho u_x \vec{u}) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x \qquad [5.4]$$

Y-component of momentum equation:

$$\frac{\partial (\rho u_y)}{\partial t} + \nabla \cdot (\rho u_y \vec{u}) = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + \rho f_y \qquad [5.5]$$

Z-component of momentum equation:

$$\frac{\partial(\rho u_z)}{\partial t} + \nabla \cdot (\rho u_z \vec{u}) = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho f_z \qquad [5.6]$$

The equation [5.4,5.5 and 5.6] are Navier -Strokes equations in conservation form.

5.2.3 Fourier -Kirchhoff equation [Energy equation]

Primary aim of the energy transport equations is calculation of temperature field given velocity's, pressures, and boundary conditions. Temperatures can be derived from the calculated enthalpy (or internal energy) using thermodynamics relationship

$$\frac{Dh}{Dt} = C_P \frac{DT}{Dt} + \left(v - T \left(\frac{\partial v}{\partial T} \right)_p \right) \frac{DP}{Dt} \qquad [5.7]$$

Giving the transport equation for temperature

$$\rho c_P \left[\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T \right] = \lambda \nabla^2 T + \vec{\vec{\tau}} : \vec{\Delta} + \dot{q}^{(g)} \qquad [5.8]$$

Where C_p is specific heat at constant pressure, T is absolute temperature , $\vec{\vec{\tau}}$ is dynamic stress tensor , $\vec{\Delta}$ is symmetric part of the velocity gradient tensor and $\dot{q}^{(g)}$ is internal heat sources or sink (it is necessary to include also reaction and phase changes enthalpies and electric heat).[Momentum and Heat transfer course by Rudolf Zitny, 2017].

5.3 What is Turbulence

Everyone at one time or another has been encountered with the nature of turbulence flow .in real world most of engineering problem are related to turbulence. For example, travelling in flight due to high turbulence effect the air craft will be vibrating to escape from the turbulent effect pilot change the altitude of aircraft. However, it is very difficult to give precise definition of turbulence. Some of characteristics of turbulent flow: [ANSYS 15.0 Training material]

- Enhanced Diffusivity
- Enhanced dissipation
- Large Reynolds number
- Three- Dimensionality
- Vorticity fluctuation
- Fractalization Mechanisms

Overview of Computational Approaches

There are three basic approaches can be used to calculate a turbulent flow:

Direct Numerical Simulation (DNS)

- It is technical possible to resolve every fluctuating motion in flow.
- Meshing of grid should be very fine and number of timestep very small.
- Demands increase with Reynolds number.
- This DNS is only a research tool for lower Reynolds number flow.
- Restricted to supercomputer applications.

Large Eddy simulation (LES)

- In terms of computational demand LES lies in between DNS and RANS.
- Like DNS, a 3D simulation is preformed over many timesteps.
- Only the large 'eddies' are resolved.
- The grid can be coarser and timesteps larger than DNS because the smaller fluid motion is represented by a sub-grid-scale (SGS) model.

Reynolds Averaged Naiver Stokes Simulation (RANS)

- Many different models are available.
- Main tool used by engineers.
- Equations are solved for time-averaged flow behaviour and the magnitude of turbulent fluctuations.
- All turbulent motion is modelled.

5.3.1 RANS Turbulence Modelling

A turbulence model is defined as a set of algebraic or differential equations which determine the turbulence transport terms in the mean flow equations and close to the system of equations. In fluids, all turbulent flows characterized by random fluctuations of transport quantities such as flow velocity, pressure, temperature etc.

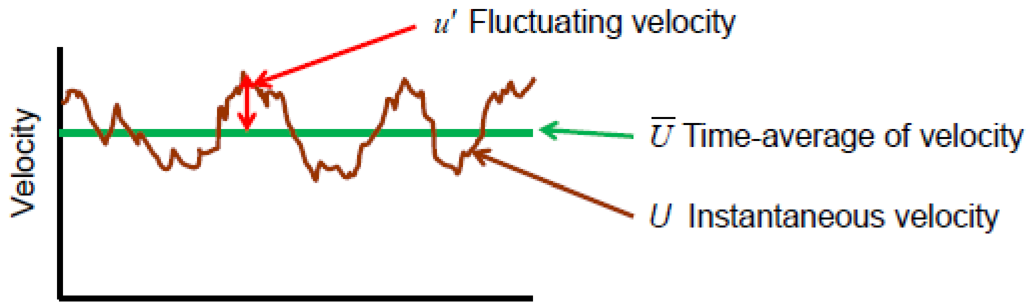


Figure 5.1 Instant velocity in turbulent flow.[ANSYS Fluent training material, 2017]

Any point in time:

$$U = \bar{U} + u' \qquad [5.9]$$

where

U – Mean velocities

$\bar{U}$ – Time average of velocity

u' − Fluctuating velocity

In Navier -Stokes equation which governs the velocity and pressure of fluid flow, the time dependent velocity fluctuations are separated from the mean flow velocity by the averaging of the Navier stokes equation and the resulting equation obtained is called Reynolds averaged Naiver-Stokes (RANS) equation can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho \pi_i)}{\partial x_i} = 0 \qquad [5.10]$$

$$\frac{\partial(\rho\bar{u}_i)}{\partial t} + \frac{\partial(\rho\bar{u}_i\bar{u}_i)}{\partial x_j} = -\frac{\partial\bar{P}}{\partial x_i} t \frac{\partial}{\partial x_j}\left[u\left(\frac{\partial\bar{u}_\iota}{\partial x_j}+\frac{\partial\bar{u}_j}{\partial x_j}-\frac{2}{3}\delta_{ij}\frac{\partial\bar{u}m}{\partial x_m}\right)\right]+\frac{\partial}{\partial x_j}-\rho\bar{u}_i\cdot\overline{u_j'} [5.11]$$

where

$\rho\bar{u}_\iota\bar{u}_j$ − Reynolds stress tensor, R_{ij}

RANS model falls into one of two categories. The difference in these is how the Reynolds stress $\bar{u}_\iota\bar{u}_J$ term on the previous equation [5.11]. By introducing the concept of eddy turbulent viscosity(EVM).

$$-\rho\bar{u}_i \cdot \bar{u}_J = \mu_t\left(\frac{\partial\bar{u}_i}{\partial x_j}+\frac{\partial\bar{u}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\rho_k + \mu_t\frac{\partial\bar{u}_m}{\partial x_m}\right) \qquad [5.12]$$

Where

$\mu_t -$ Turbulent viscosity

$$u_t = \rho c_u \frac{k^2}{\varepsilon} \qquad [5.13]$$

In equation [5.13], k represents the turbulent kinetic energy, ε represents kinetic energy dissipation rate and c_u is empirical constant.

5.3.2 Turbulence Models Available in Fluent

One-Equation model Spalart-Allmaras
Two-Equation Models Standard k -ε RNG k- ε Realizable k-ε
Standard k-ω SST k-ω
Reynolds Stress Model
k-kl-ω Transition Model

Table 5.1 Turbulence Model in ANSYS Fluent.

Two equations models are under Reynolds Averaged Navier stokes based models. Once model by model come down the increase of computational cost per iteration increase.

5.4 k – ω SST Turbulence Model

In present work k – ω Shear – Stress – Transport (SST) turbulence model is chosen to turbulence simulation in an agitated vessel. Its hybrid of two models which is k- ω model near the wall and k- ε model in the free stream. Where k represents the turbulent kinetic energy ε is explained in equation [5.13] and ω is specific dissipation rate. k-ω is most widely adopted in the aerospace, turbo-machinery, and heat transfer applications. For more accurate predictions and robust for wide range of boundary layer flows with pressure gradient by including the transport effects into the formulation of eddy- viscosity. [ANSYS Training Material]

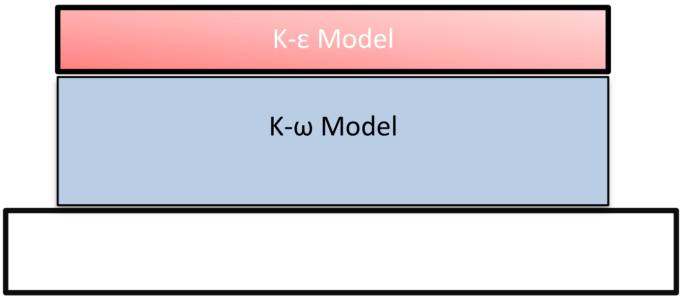


Figure 5.2 k-ω SST Turbulence model blends with k- ω & k-ε.

The transport equations for k-ω SST model are (ANSYS Fluent 17.0, User's Guide,2016):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} = \left(\Gamma_k \frac{\partial k}{\partial x_j}\right) + \tilde{G}_k - Y_k + S_k \qquad [5.14]$$

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho_\omega u_i) = \frac{\partial}{\partial x_j}\left(\Gamma_w \frac{\partial \omega}{\partial x_j}\right) + G_\omega - y_\omega + D_\omega + S_\omega \qquad [5.15]$$

In these equations [5.14] and [5.15] the terms $\tilde{G}_k$ represents generation of turbulent kinetic energy it is same as in standard k-ω model. G_ω represents generation of ω, Γ_k and Γ_ω represent effective diffusivity of k and ω. Y_k and Y_ω represents dissipation of k and ω due to turbulence, $D\omega$ represents cross diffusion, s_k and s_ω are the user defined source terms.[ANSYS 17 Fluent Theory guide 2017].

5.4.1 Turbulent Boundary Layers

A turbulent boundary layer consists of distinct regions. For CFD, the most important are the viscous sublayer, immediately adjacent to the wall and slightly further away the log layer and away from the wall.

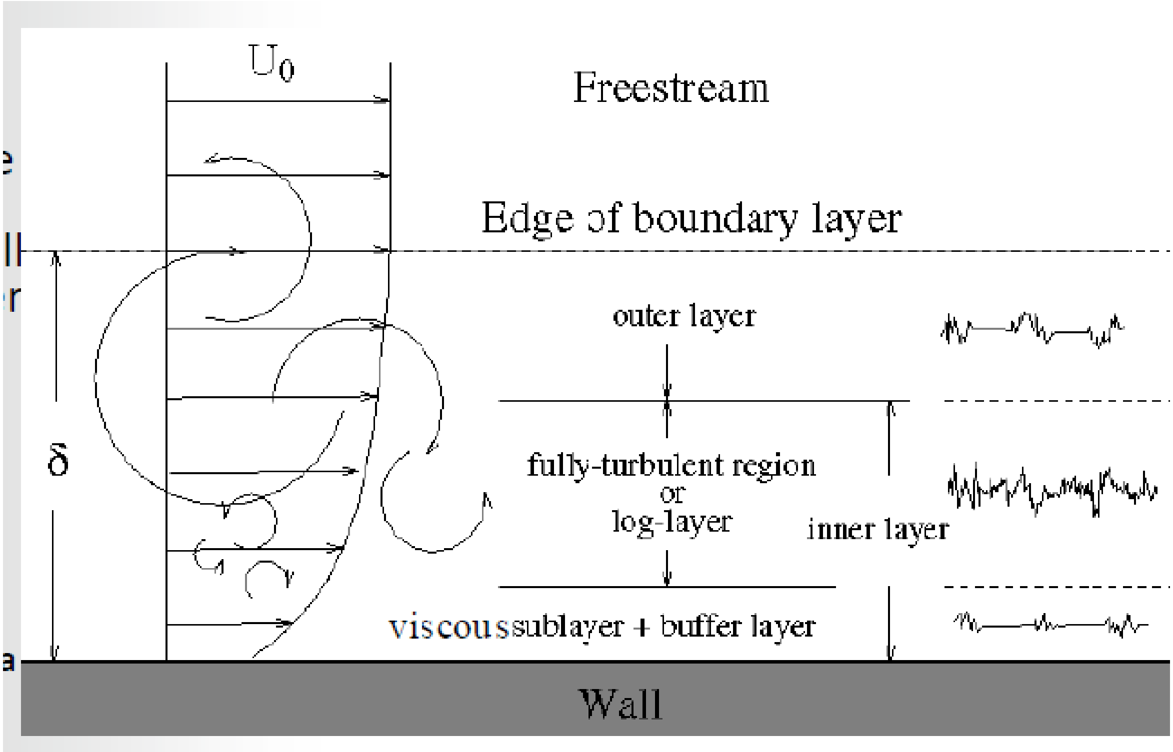


Figure 5.3 Describing turbulence boundary layers [ANSYS Training Material,2017]

Near to a wall, the velocity changes rapidly. The velocity is made dimensionless, defined as:

$$u^t = \frac{u}{u_t}; u_t = \sqrt{\frac{\tau_{wall}}{\rho}} \qquad [5.16]$$

Where

u - velocity of the flow,

τ_{wall} -wall shear stress

ρ – Density of fluid

The distance is made dimensionless:

$$Y^+ = \frac{Yu_\tau}{\nu} \qquad [5.17]$$

Where Y is the distance from wall, we can create a plot in logarithmic scale, which represents the dimensionless boundary layer profiles. The size of your grid cell nearest to the wall value of Y^+ is very important. In the near -wall region, the solution gradients are very high, but accurate calculations in the near -wall region for best solution of your simulations. First grid cell need to be at about $Y^+ = 1$ and a prism layer mesh with growth rate no higher than = 1.2 is best value to maintain near the wall this will add a significantly results to mesh count.

This is approach you will take and recommended turbulence model for SST k- ω. Using a wall fall function first gird to be 30 < Y^+ = 300 values and for Reynolds number Y^+ can be higher. [ANSYS training material 15.0] .

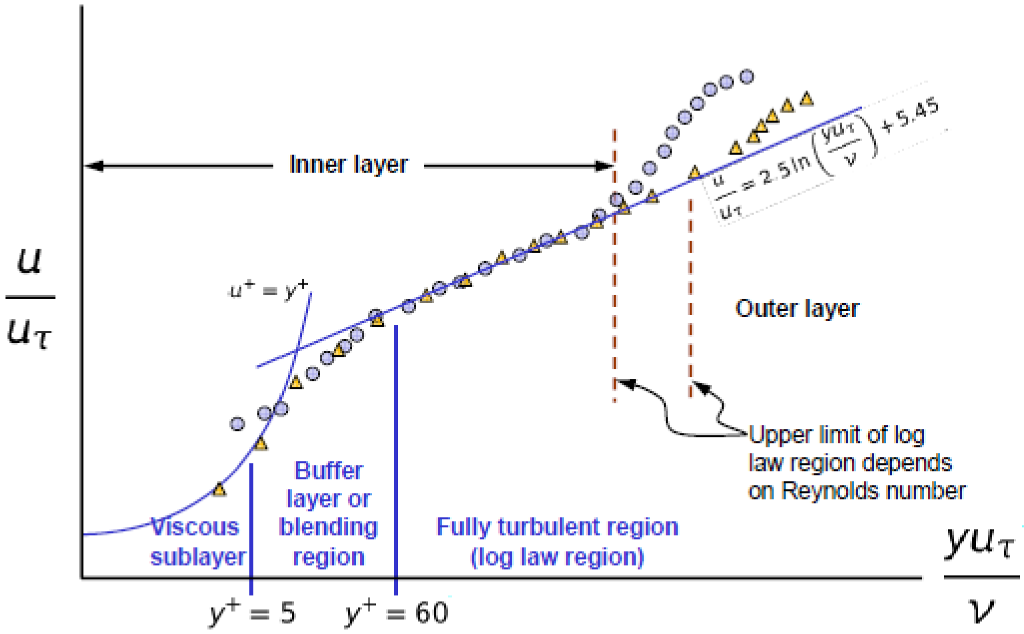


Figure 5.4 The universal law of wall model [ANSYS Training materials,2017].

5.5 Meshing

Meshing is a pre-processing step for the computational field simulation. The whole geometry domain space of interest is divided into a large number of small cells known as 'the grid', computational cell or control volume is called mesh. ANSYS CFD uses Finite Volume Methods (FVM). The grid can be in many shapes and sizes. For example, the elements are either quadrilaterals, triangles, tetrahedral, prisms, pyramids, and hexahedra these shapes are for 2D and 3D geometry. Each series of line or planar faces connecting the boundaries of domain are used to make the elements.

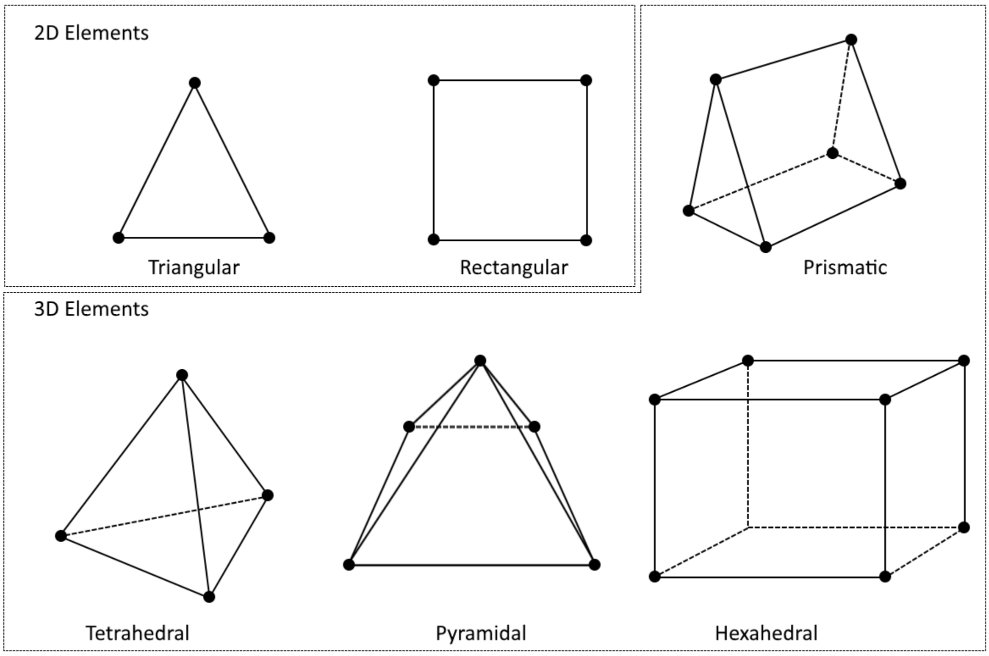


Figure 5.5 Mesh elements [ANSYS Training Material,2017]

5.5.1 Meshing Methods

Meshing methods available for 3D in ANSYS Meshing software.

- Automatics
- Tetrahedrons
  - Patch Conforming
  - Patch Independent
- Multizone
  - Mainly Hexahedral elements
- Hex dominant
- Sweep
- Cut cell

5.5.2 Meshing process in ANSYS

- Set physical and Meshing method
- Specify global mesh settings
- Insert Local mesh settings
- Preview and generate mesh
- Check mesh quality

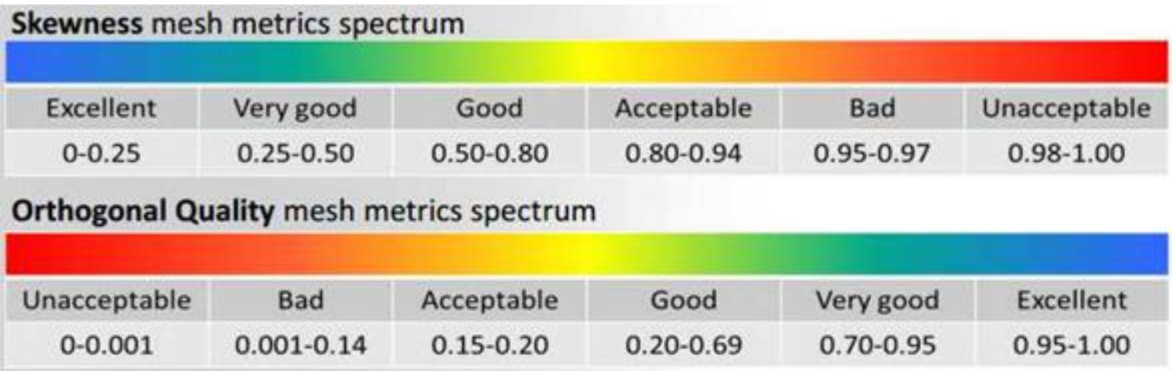
5.5.3 Mesh Quality Metrics

A good meshing is required for best simulation and minimize the error in solvers. Good mesh has three components good resolution, appropriate distribution, and good mesh quality. To decide the mesh quality ANSYS provide the tool to check the mesh size.

1.Orthogonal Quality (OQ)

2.Skewness

Low orthogonal quality or high skewness values are not recommended. Generally, try to keep minimum orthogonal quality >0.1, or maximum skewness <0.95, these values may be different on the physics and location on the cell. Fluent can display the metric spectrum of skewness and orthogonal mesh metrics spectrum. [ANSYS 15.0 training material]



Skewness mesh metrics spectrum

Excellent	Very good	Good	Acceptable	Bad	Unacceptable
0-0.25	0.25-0.50	0.50-0.80	0.80-0.94	0.95-0.97	0.98-1.00

Orthogonal Quality mesh metrics spectrum

Unacceptable	Bad	Acceptable	Good	Very good	Excellent
0-0.001	0.001-0.14	0.15-0.20	0.20-0.69	0.70-0.95	0.95-1.00

Figure 5.6 Skewness and Orthogonal mesh quality. [ANSYS Training Material,2017]

5.6 Modelling the Flow Around Impeller

ANSYS Fluent tool provides solution to the rotation of parts in a fluid like impeller, rotating blades and moving walls. Due to motion of impeller in agitated vessel, there is presence of rotation parts and surrounding non- stationary parts in agitated vessel like wall boundaries (e.g. baffles). To consider the effect of rotation parts in geometry, there are different techniques avail in ANSYS fluent. The techniques are explained below.

5.6.1 Moving Reference Frame

One of the concept called Moving Reference Frame (MRF) approach is used. Moving reference approach is a steady-state method most of industrial problems it is used. In stirred tanks the impeller moving with some angular velocity ω, the underlaying physics behind this model is robust and elegant. Agitated vessel is divided in two region of mesh cells is created at pre- processing. the mesh around the impeller is MRF zone and stationary zone near the wall of agitated vessel (baffles and tank wall). During the simulation phase the MRF zone is rotated about the axis of coordinates of body and other part of vessel will be non-moving zone. MRF is also known as the ‘Frozen rotor approach’ and its most applied with the incompressible, steady-state RANS solve with multiple MRF with k – ε turbulence model.

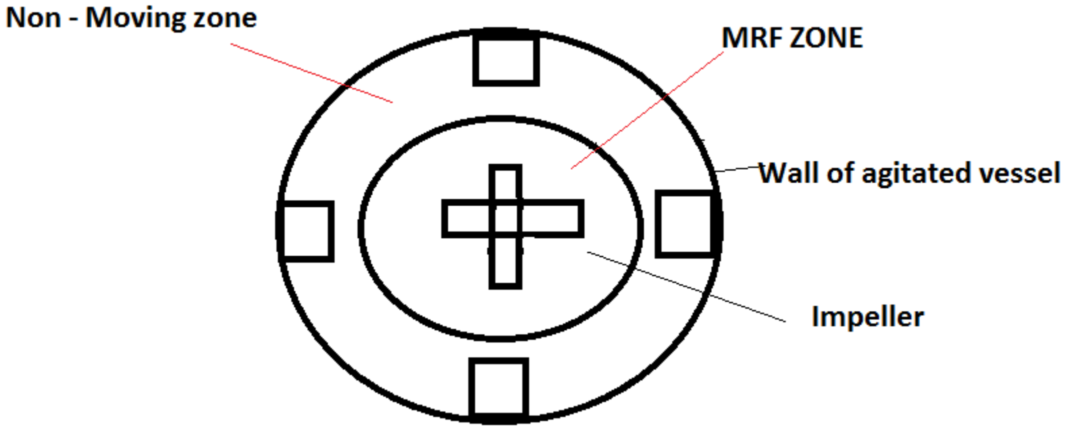


Figure 5.7 MRF Model

5.6.2 Sliding Mesh Technique

In the present work simulation are carried out by using sliding mesh technique. Around the impeller the flow of fluid is unsteady inside the baffled agitated vessel. Therefore, to take account of baffles and their interaction with the rotating impeller. Sliding mesh technique is a time – dependent solution approach in which grid surrounding the rotation components moves during each time step and fluxes are modelled at sliding /moving interface. In order to rotate one mesh relative to another, the boundary between the meshes needs to be a surface of revolution. The sliding mesh model is the most rigorous and informative solution method for agitated vessel simulations. Transient simulations using this model can result from the periodic impeller – baffle interaction. The sliding mesh technique is similar to the MRF model in both modelling techniques a separate fluid region for the impeller is defined. In sliding mesh impeller mesh region is disconnected from the mesh of the agitated vessel by using the in ANSYS Design modeler tool and ANSYS meshing. In the tank region the standard conservation equations for mass and momentum are solved and rotating impeller region a modified set of balance equations is solved [5.18] modified continuity equation and [5.19] modified momentum balance: [A. Bakker et. al, and Edward Paul et.al].

$$\frac{\partial}{\partial x_j}\left(u_j - v_j\right) = 0 \qquad [5.18]$$

$$\frac{\partial}{\partial t}\rho u_i + \frac{\partial}{\partial x_j}\rho(u_j - v_j)u_i = \frac{-\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \qquad [5.19]$$

Where

$u_j -$ Liquid velocity in stationary reference frame

$v_j -$ Velocity component arising from mesh motion

$p -$ Pressure

$\tau_{ij} -$ stress tensor

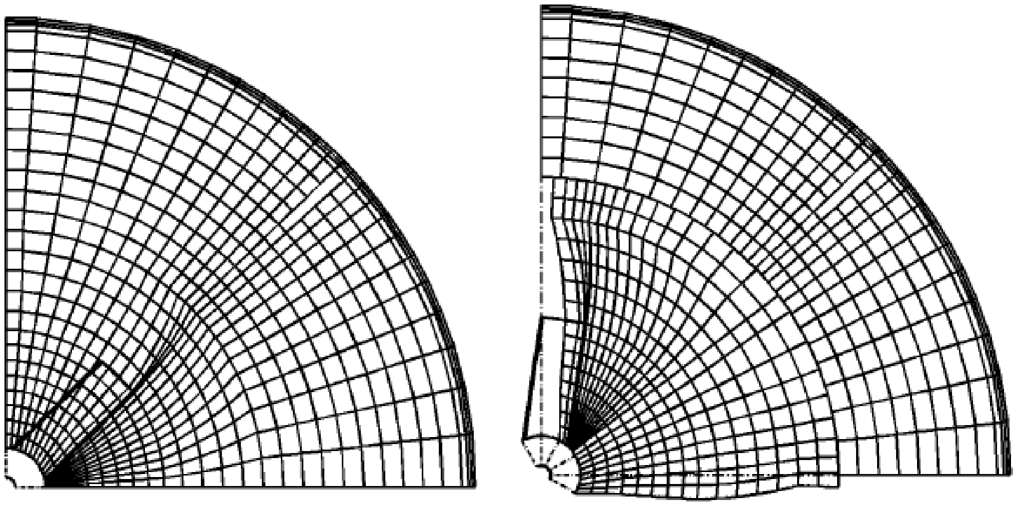


Figure 5.7 Grid used in the sliding mesh method. In figure it shown the grid at two different time steps. Mesh is moving with impeller region and slides with the stationary region for the rest of agitated vessel. [Edward L. Paul et al, 2003].

CHAPTER 6 NUMERICAL METHODOLOGY AND MODEL DESCRIPTION

Introduction 6.1

This chapter presents description of the problem statement, geometrical configurations and performing CFD simulation with appropriate boundaries conditions of the agitated vessel. The geometry is scaled model of the actual vessel used in plant equipment. The following section describes the geometrical parameter of the agitated vessel used for CFD analysis.

6.2 Problem Statement

In present work , CFD simulation of heat transfer in an agitated vessel for single phase Newtonian liquid under unsteady state condition in baffled, jacked agitated vessel equipped with Pitched Blade Turbine (PBT) having six blade at 45° and supplying q = 3000 W/m^2 constant heat flux for different rotation speeds of 300 to 900 rpm and evaluating heat transfer coefficients at bottom and vertical wall with varying distance from the bottom of vessel 1/3,2/3, 1 scaled model of industrial agitated vessel (batch reactor), have been performed using ANSYS Fluent.

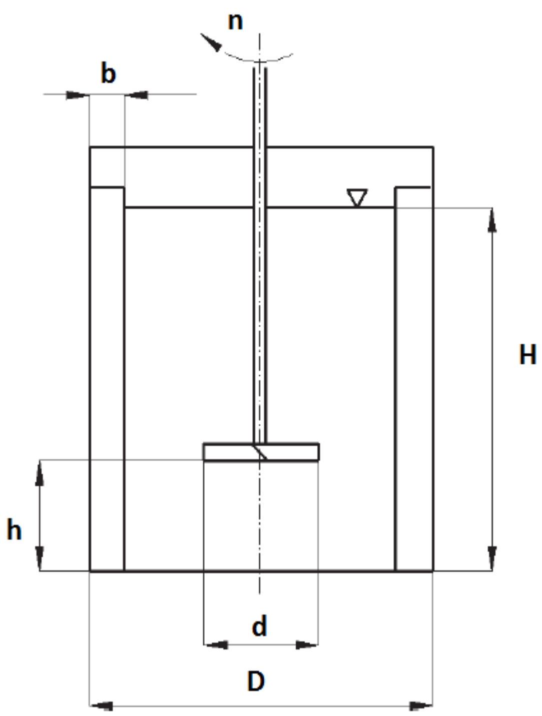


Figure 6.1 Schematic diagram of the agitated vessel with nomenclature. [Beshy, K. R el, at.,2001].

6.3 Geometrical configuration

The system under investigation in present work is the flat-bottom, baffled cylindrical agitated vessel equipped with six- blade 45° Pitched blade turbine(PBT). The agitated vessel filled with water up to the level D=H. A schematic diagram of agitated vessel is shown in Figure 6.1. Water was chosen as the liquid medium in this primary study. Fluid properties are chosen by ANSYS Fluent default values for simulation. The dimensional date of the agitated vessel and impeller and fluid properties is shown in tables 6.1 and 6.2.

Item	Symbol	Dimension
Vessel diameter	D	0.2 m
Vessel height/liquid height	H	0.2 m
Impeller diameter	d = D/3	0.0666667 m
Width of impeller blade	w	0.02
Off- Bottom clearance	h =d $(1, \frac{2}{3}, \frac{1}{3})$	0.066667, 0.04444, 0.02222 m
Blade thickness	t	0.001 m
No. of Blades	N	6
Blade angle	θ	45°
Baffle width	b	0.02 m
Number of baffles	B	4
Baffle thickness	b_t	0.002 m

Table 6.1 Agitated vessel dimensions

Item	Symbol	Value
Density	$\boldsymbol{\rho}$	998.2 Kg / m^3
Dynamic viscosity	μ	0.001003 Pa. s
Specific heat	Cp	4182 J/Kg/ K
Thermal conductivity	λ	0.6 W/m K

Table 6.2 Fluid properties **ANSYS** Fluent values.

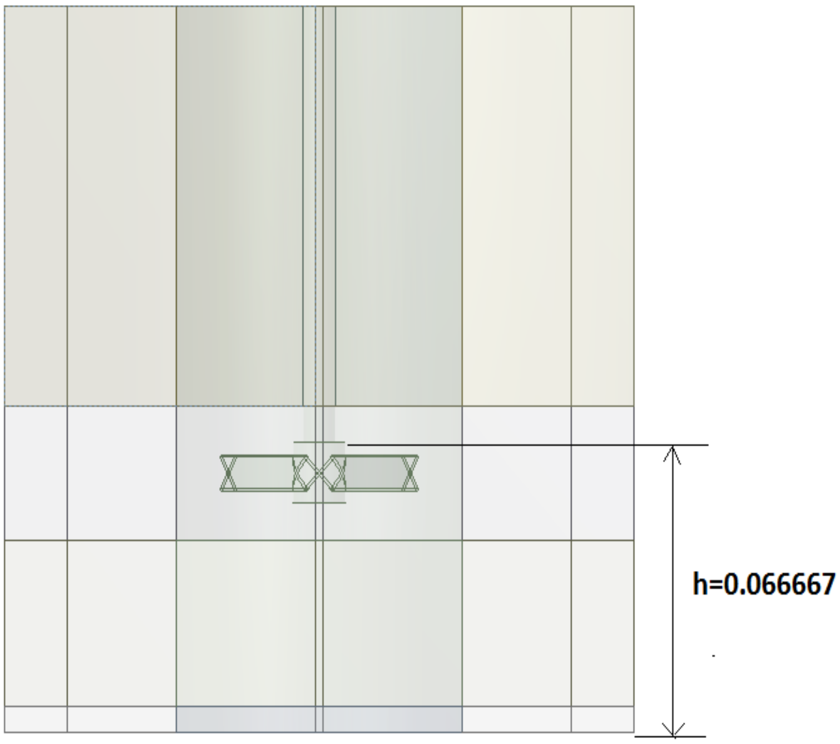
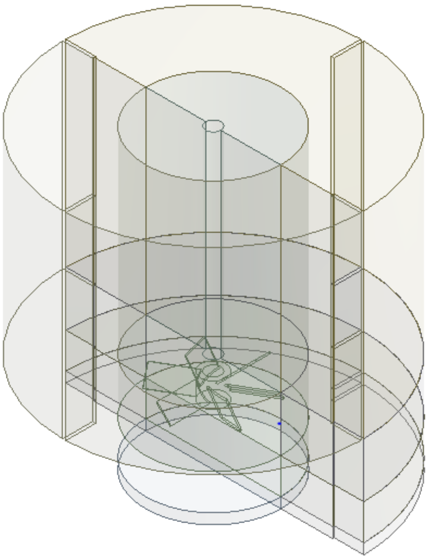


Figure 6. 2 Agitated vessels Off -Bottom clearance with 1, 2/3, 1/3 h = 0.066667 m, h = 0.04444, h= 0.02222m.

6.4 Computational Grid

The modelled geometry was discretized using tetrahedral, hexahedral, and polyhedral mesh elements in ANSYS meshing. For simulation of 2/3 Off -bottom clearance tetrahedral mesh was generated around the impeller region and rest of domain was discretized is generated by hexahedral meshing. The total number of mesh elements generated was 2,167,821 more than 2 million. For simulation of h/d =1/3 and h/d = 1 Off bottom clearance mesh around impeller region improve the quality by changing the tetrahedral mesh elements into polyhedral mesh elements and now total number of elements decreased to 1706192. Polyhedral meshing gives better accuracy results and faster runtime solutions. Figures 6.3,6.4 and 6.5 showing vessel geometry in isometric view consisting of a cylindrical tank with impeller region and the baffles and mesh generated for agitated vessel with hexahedral, tetrahedral polyhedral around impeller.



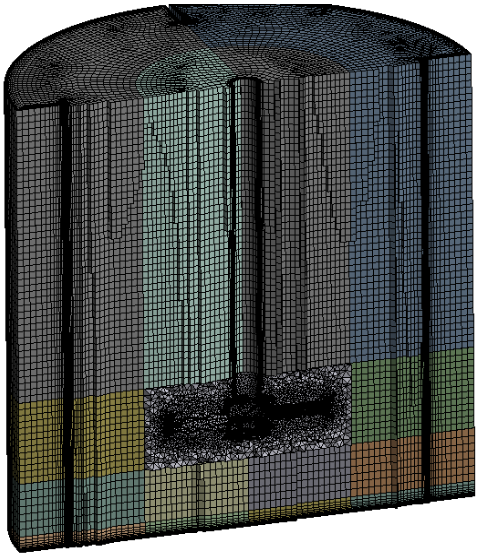


Figure 6. 3 and Figure 6. 4 Isometric view germetrical model and compyutational grid of agitated veseel.

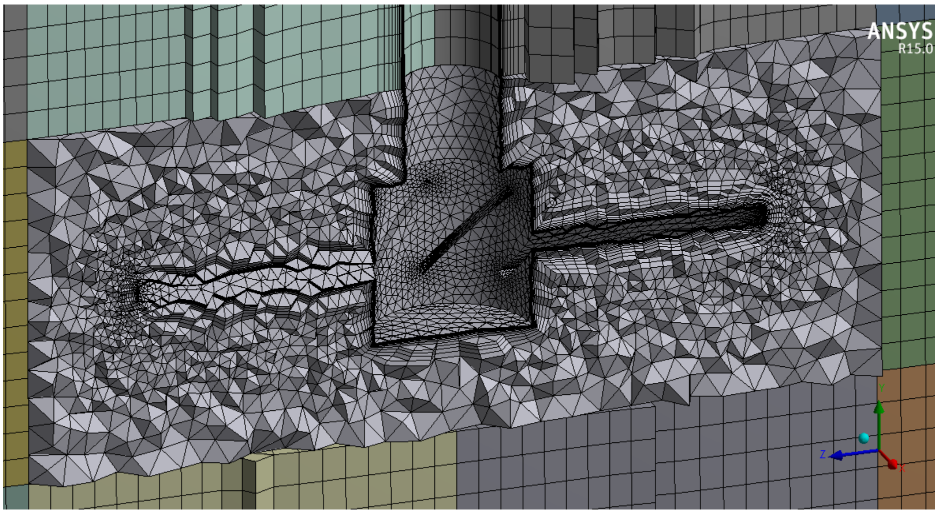


Figure 6. 5 Tetrahedral mesh elements around impeller region.

6.5 Mesh Quality

As it was discussed in chapter 5 [Figure 5.6] about mesh quality depends of size of mesh and number of mesh elements. The parameters like skewness, orthogonal quality, aspect ratio, etc. The values obtained of the mesh quality measures for the generated computational grid of agitated vessel are tabulated in Table 6.3.

Quality Measure	Value
Maximum Skewness	0.97
Minimum Orthogonal Quality	0.105089
Maximum Aspect Ratio	4.51293e+02

Table 6.3 Mesh quality measures for generated gird.

The mesh quality measures are satisfactory further steps to processed for ANSYS Fluent simulations.

The next chapter describes the solution procedure for the transient simulation performed in ANASYS Fluent (CFD) of heat transfer in an agitated vessel. Fluent settings, boundary conditions, solution methods and Results etc.

CHAPTER 7 CFD SIMULATION OF HEAT TRANSFER IN AGITATED VESSEL

7.1 Introduction

The section in this chapter explains the set-up of ANSYS Fluent 15.0 and boundary conditions to obtain the result to investigate the heat transfer in a baffled agitated vessel with a 6 blade PBT impeller and studying the effect of heat transfer at bottom and vertical walls for different off – bottom clearances from the impeller. The analysis of velocity flow fields at different rpms of impeller.

7.2 Solution Procedure

To set up the ANSYS Fluent software for the CFD simulation of discretized model of agitated vessel were performed. As the number of mesh elements generated was more than 2 million (2211235) simulations are performed at the facility servers (256 GB RAM) was provided by Czech Technical University computation servers. To save the simulation time parallel simulation were performed in personal computer with I5 Processer with 12 GB RAM. In university servers to complete the CFD simulation for 700 rpm, run time of 10 seconds 7-9 days and in personal computer more than 30 days for simulation time.

ANSYS Fluent .IN journal file is written with all the commands for execution by the solver of ANSYYS Fluent in batch mode were created for different rotational speeds and run time with heat flux q = 3000 and 30000 $\mathrm{W/m^2}$.

Example of journal file written for rotational speed of 300 rpm and simulation run time 20 seconds refer [Table 5.2] for different rpms and runtime. Journal file is shown below:

```
; fluent150t 3ddp -t 16 -g -i fluent.in
/file/read-case-data init-hs.cas.gz
;
; will overwrite files without a confirmation
/file/confirm-overwrite no
;
/mesh/reorder/reorder-domain
;
; rotation speed definition
/define/parameters/input-parameters edit "rotation-speed"
"rotation-speed" 300
;
```

```
; first - switch energy off and perform some steady-state
iterations
/define/models energy no
/define/models steady yes
/solve/iterate 2000
; save steady-state
/file/write-case-data steady.cas.gz
;
; switch to transient model
/define/models unsteady-1st-order yes
; switch energy on + dissipation: no, pressure work: no, kinetic
energy: no,
;   diffusion at inlets: yes
/define/models energy yes no no no yes
; switch to Sliding Mesh - we have SM activated
;;/define/boundary-conditions/modify-zones/mrf-to-sliding-mesh
fluid-inner ()
; switch to MRF
;;/define/boundary-conditions/modify-zones/copy-mesh-to-mrf-motion
fluid-inner ()
;
;
/solve/set time-step 0.001
/solve/set extrapolate-vars yes
; init statistics
/solve/init/init-flow-statistics
;
/define/boundary-conditions/wall tank-bottom 0 no 0 no yes heat-
flux no 3000 no no no no 0 no 0.5 no 1
/solve/patch fluid-inner fluid-outer () temperature 300
; heat source to eliminate heating by heat flux through the walls,
W/m3
; q = 3000
/define/parameters/input-parameters edit "heat-source" "heat-
source" -74746.70976
; q = 30000
/define/parameters/output-parameters/print-all-to-console
/define/parameters/output-parameters/write-all-to-file params0.out
```

```
;
; auto-save every 1 s
/file/auto-save/data-freq 1000
/file/auto-save/append-file-name-with flow-time 6
/file/auto-save/retain-most-recent-files yes
/file/auto-save/max-files 1
/file/auto-save/root-name "autosave.gz"
; perform first set of iterations corresponding to ~ 5s ?
/solve/dual-time-iterate 4000 20
;
; define mean heat transfer coefffients, they are not defined
before some statistics is collected
/define/parameters/output-parameters/create/surface-integral
"mean-alpha" area-weighted-avg mean-heat-transfer-coef tank-bottom
tank-wall ()
/define/parameters/output-parameters/create/surface-integral
"mean-alpha-bottom" area-weighted-avg mean-heat-transfer-coef
tank-bottom ()
/define/parameters/output-parameters/create/surface-integral
"mean-alpha-wall" area-weighted-avg mean-heat-transfer-coef tank-
wall ()
;
; print all parameters to console
/define/parameters/output-parameters/print-all-to-console
/define/parameters/output-parameters/write-all-to-file params1.out
/file/write-case-data trans1-%t.cas.gz
;
; init statistics for the next set of time steps
/solve/init/init-flow-statistics
; perform another set of iterations/time steps
;;/solve/dual-time-iterate 2 5
/solve/dual-time-iterate 16000 20
/exit yes.
```

7.2.1 Models

The $k-\omega$ based Shear-Stress-Transport (SST) turbulence model was choose for our simulation of heat transfer in an agitated vessel. In chapter 7 briefly explained about k-ω SST turbulence model with energy equation ON. In Figure 7.1 set up of different model options.

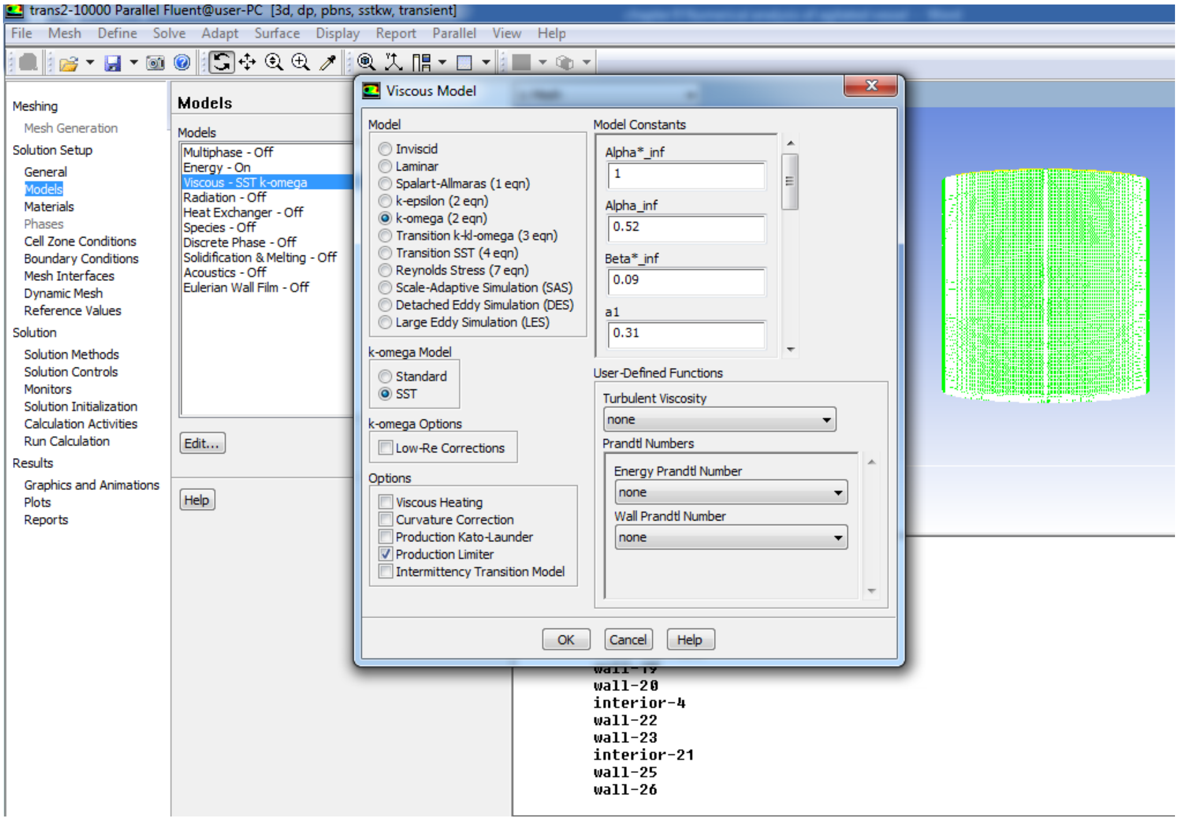


Figure 7.1 ANSYS Fluent 15.0 set up for models.

7.2.2 Material

The fluid for simulation in an agitated vessel is 'water' (material) with constant thermos-physical properties of ANSYS Fluent data base.

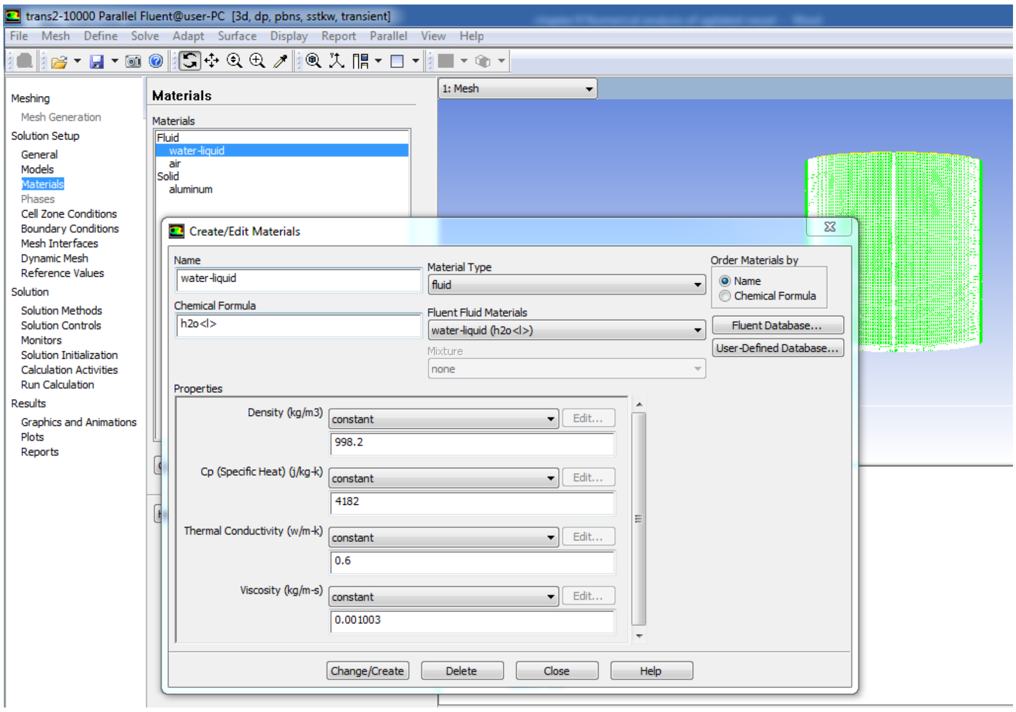


Figure 7.2 ANSYS Fluent 15.0 material properties set up with Fluent data base.

7.2.3 Cell Zone and Boundary Conditions

In cell zone conditions selection of you can define the parameter for fluid inner and fluid outer in our case inner fluid is around the impeller region domain with specific rotation speed, while the region outer fluid domain is agitated tank with baffles was kept stationary. In chapter 5 we discussed about moving reference frame (Frame motion) and sliding mesh technique (Mesh motion) available in ANSYS Fluent, in our simulation were performed using sliding mesh technique is used Figure 7.3 set up condition is shown:

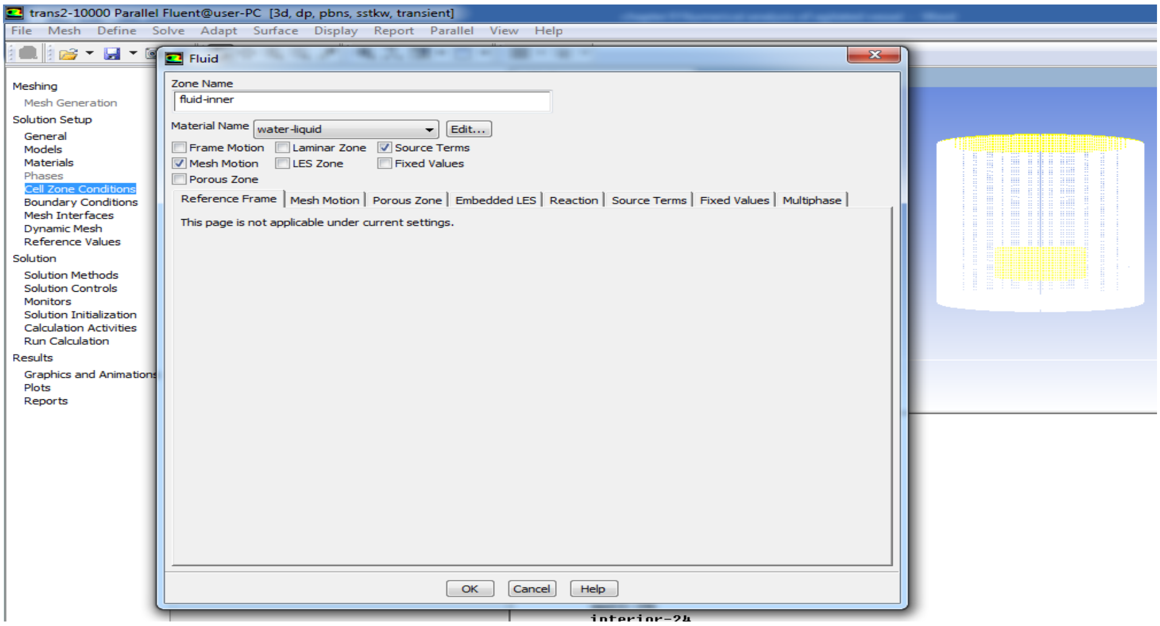


Figure 7.3 ANSYS fluent 15.0 Cell zone with sliding mesh technique set up.

In cell zone conditions for fluid-inner and fluid outer we are providing the source terms that acts like heat sink in agitated vessel. Heat source (sink) to eliminate heating by heat flux through the walls. The value of heat source used in simulations -74746.71 W/m^3. See the equation number [8.1] in chapter 8 more details.

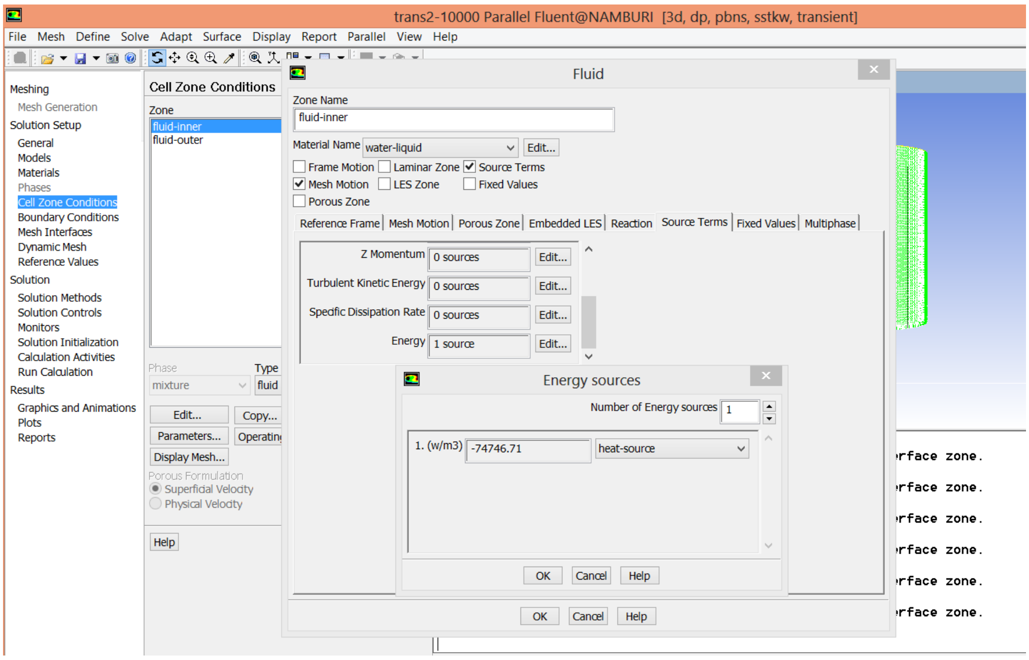


Figure 7.4 ANSYS Fluent 15.0 heat source set up.

Boundary Conditions

Boundary conditions are initial condition parameters for running the simulation selection of material, thermal conditions wall motion, shear conditions, wall roughness etc. In Figure 7.4 shown the ANSYS Fluent set up for boundary conditions. In thermal condition we kept constant heat flux with $q = 3000$ W/m^2 at tank-bottom and tank-wall acts as heat source. In the wall motion for impeller including shaft was set as ‘moving wall’, ‘no slip’ was applied as shear condition.

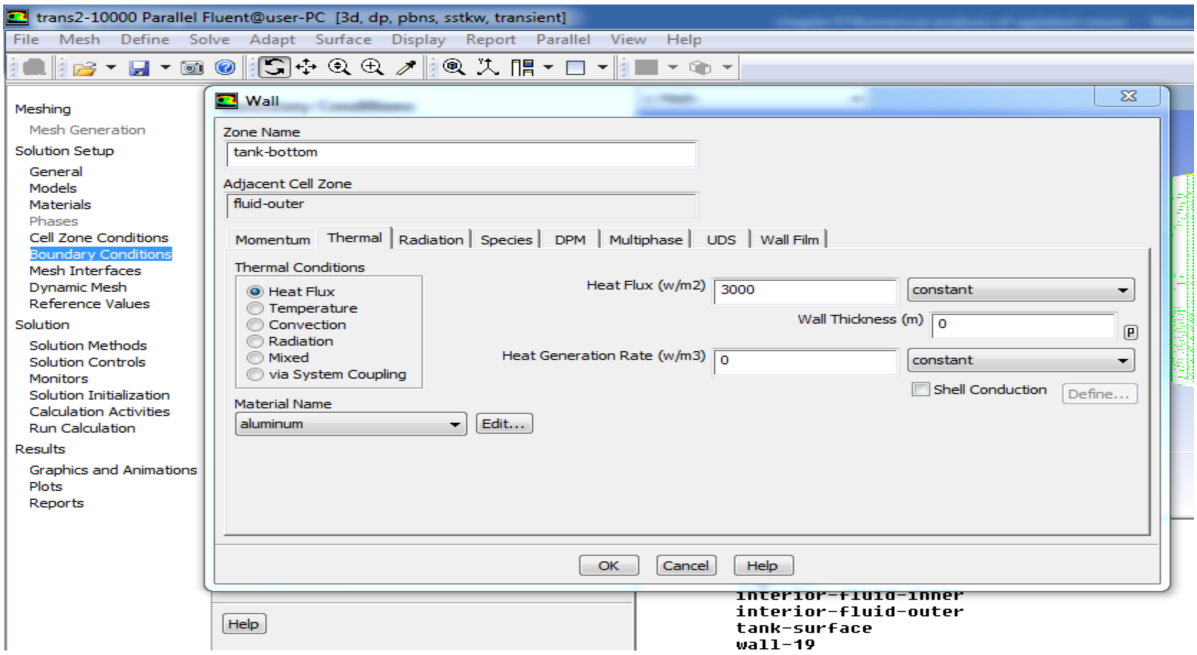


Figure 7.5 ANSYS Fluent 15.0 Boundary conditions set-up.

7.2.4 Solution Method

Solver Type: Pressure based solver was selected for simulations in ANSYS Fluent. The first 2000 iterations were performed for steady state case to fully developed flow profile in the tank than simulation switched to transient model with energy equation on.

Solutions Methods: pressure-velocity coupling SIMPLE algorithm was chosen. Spatial Discretization: For momentum, turbulent kinetic energy, specific dissipation rate and energy second-order accurate upwind scheme was selected. Pressure: Standard, Gradient: Green-Gauss node based.

Run Calculations: Time step size chosen 0.001 s, the maximum iterations per time step ware 20 for all the simulations. According to run-time for transient analysis was selected based on the mixing time t_m for different rotational speeds refer Table 5.2.

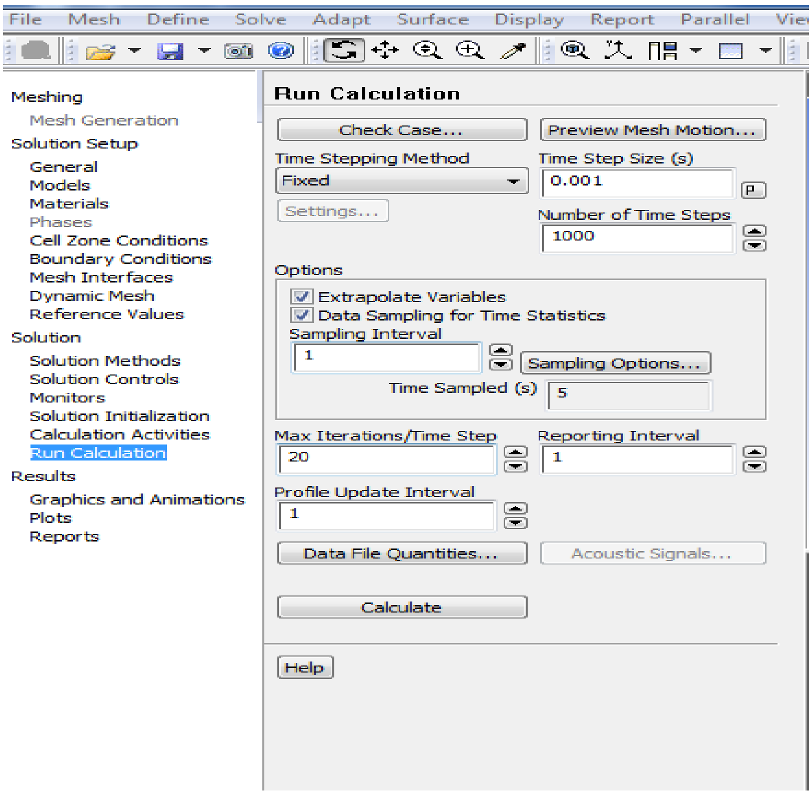


Figure 7.6 ANSYS Fluent 15.0 set up for solution methods.

7.3 Computational Results

The post -Processing results in ANSYS Fluent 15.0 for different rang 300- 900 rpms and Off-bottom clearances h/d = 1, 2/3 ,1/3 cases. Here some of velocity contours, temperature contours at bottom of agitated vessel and path lines are illustrated. The axial flow pattern was developed by the PBT impeller inside the agitated vessel. In velocity contours plots for the Off -bottom clearance 1,2/3, 1/3 obverse the light blue spot show dead zones of mixing.

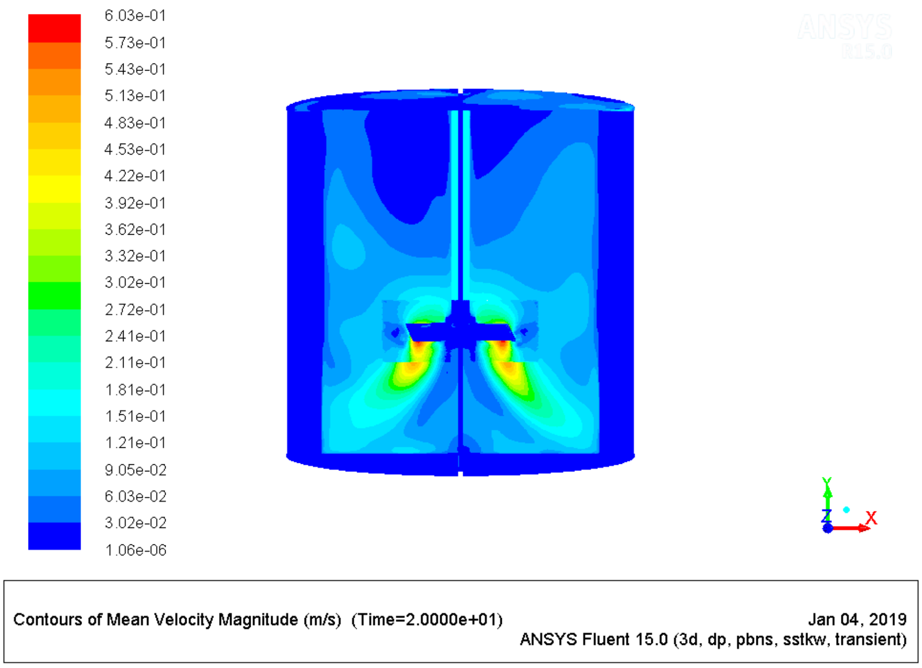


Figure 7.7 Velocity contours of agitated vessel Off-clearance 1, 500 rpm.

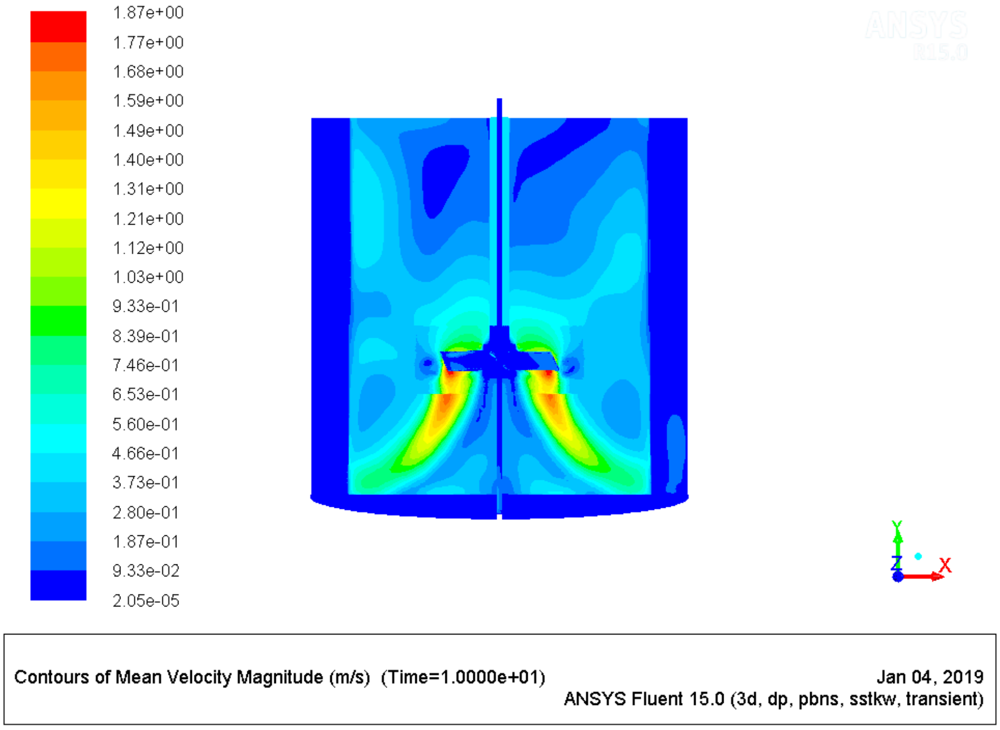


Figure 7.8 Velocity contours of agitated vessel Off-clearance 1, 900rpm.

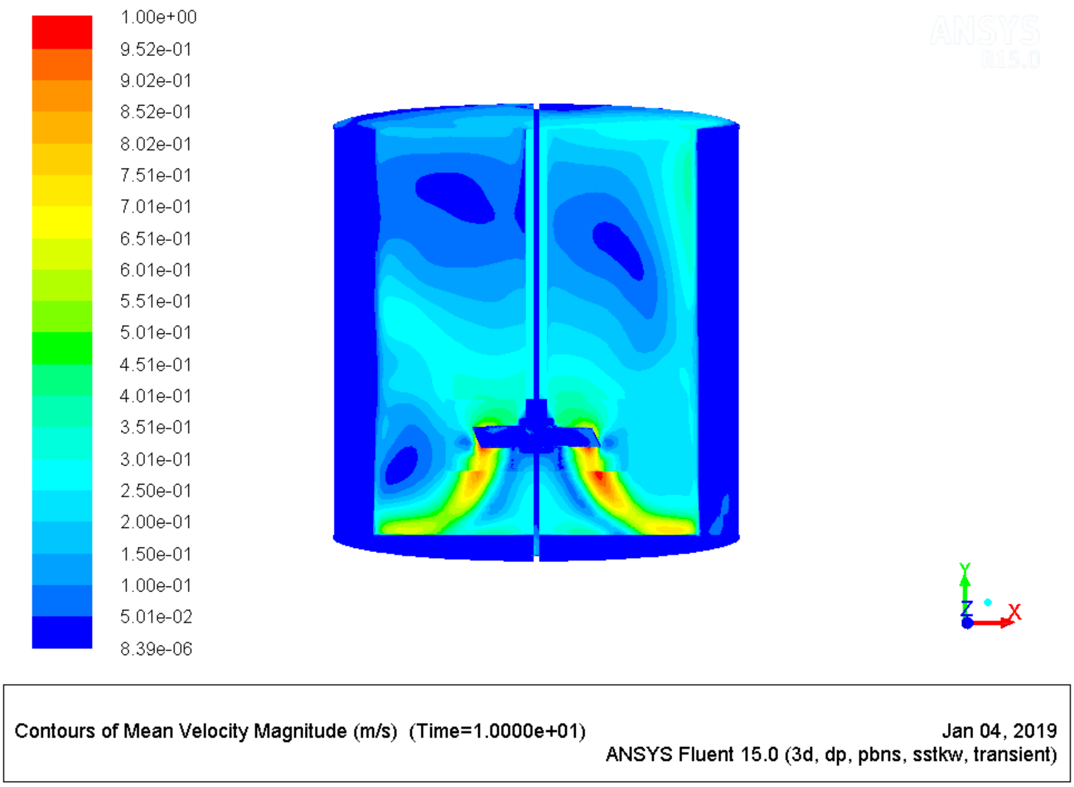


Figure 7. 9 Velocity contours of agitated vessel Off-clearance 2/3 ,500rpm.

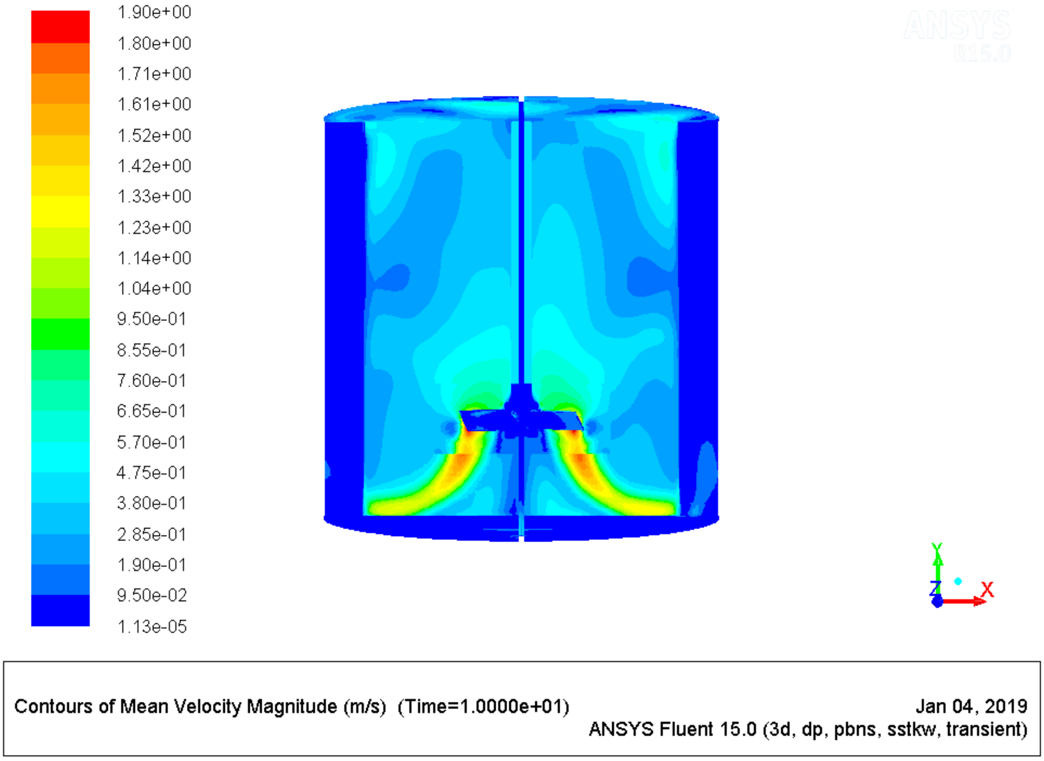


Figure 7.10 Velocity contours of agitated vessel Off-clearance 2/3,900 rpm.

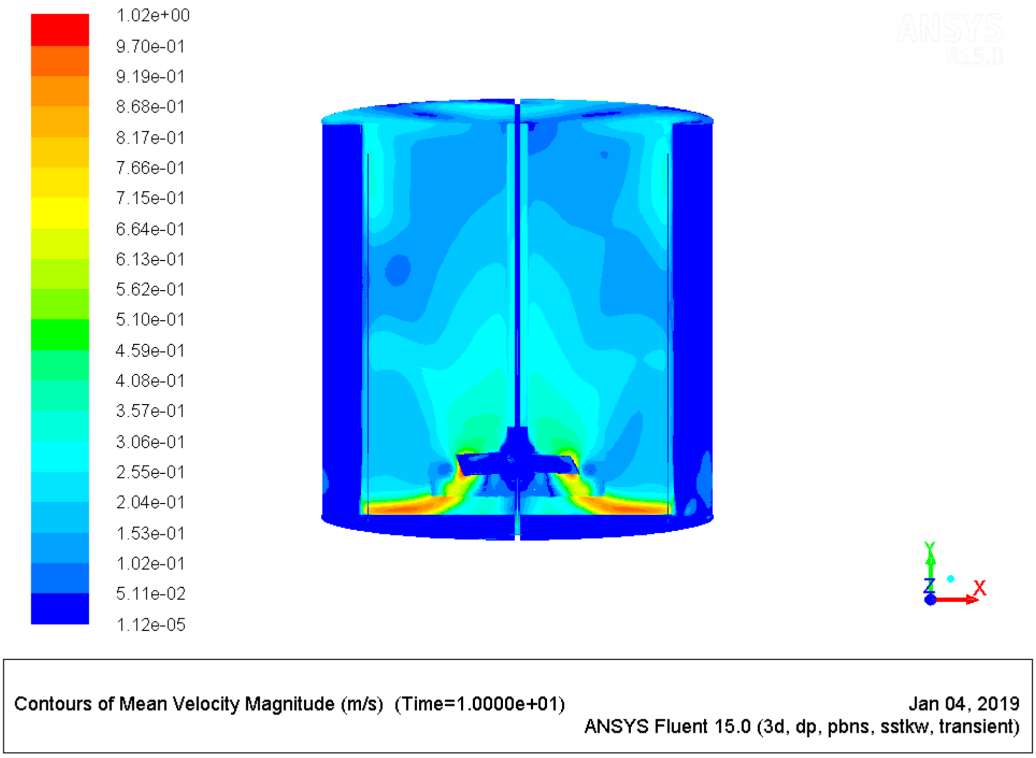


Figure 7.11 Velocity contours of agitated vessel Off-clearance 1/3 500 rpm.

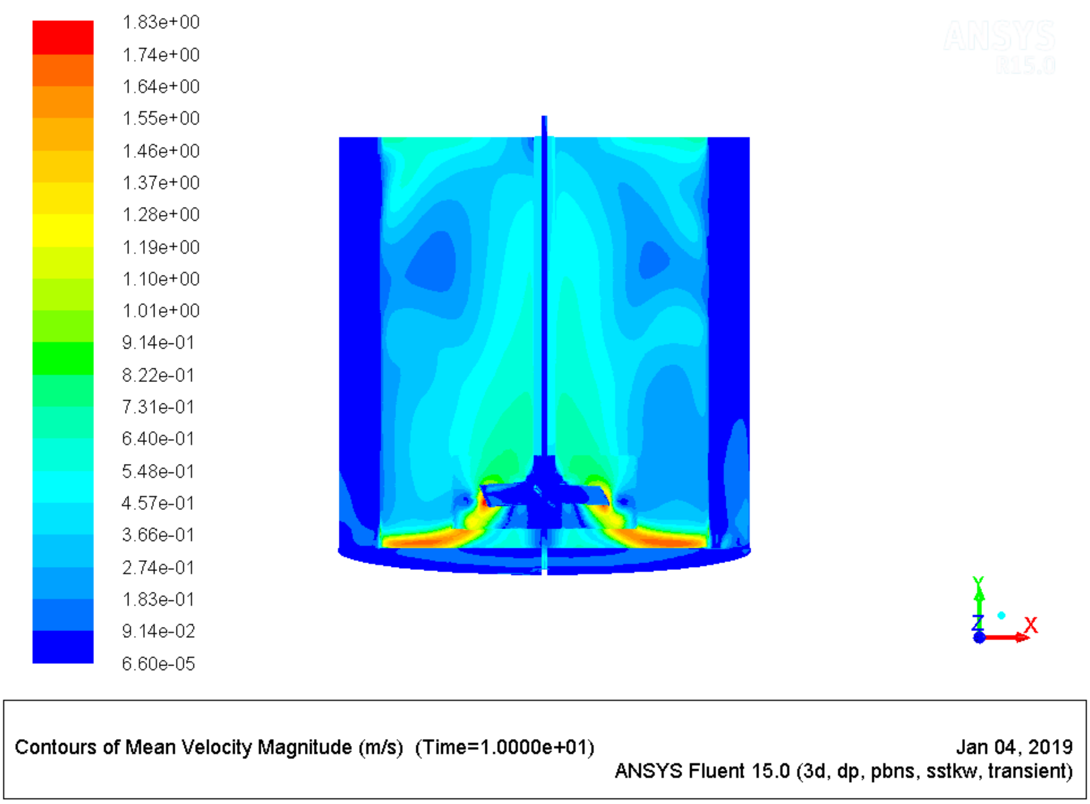


Figure 7.12 Velocity contours of agitated vessel Off-clearances1/3 ,900 rpm.

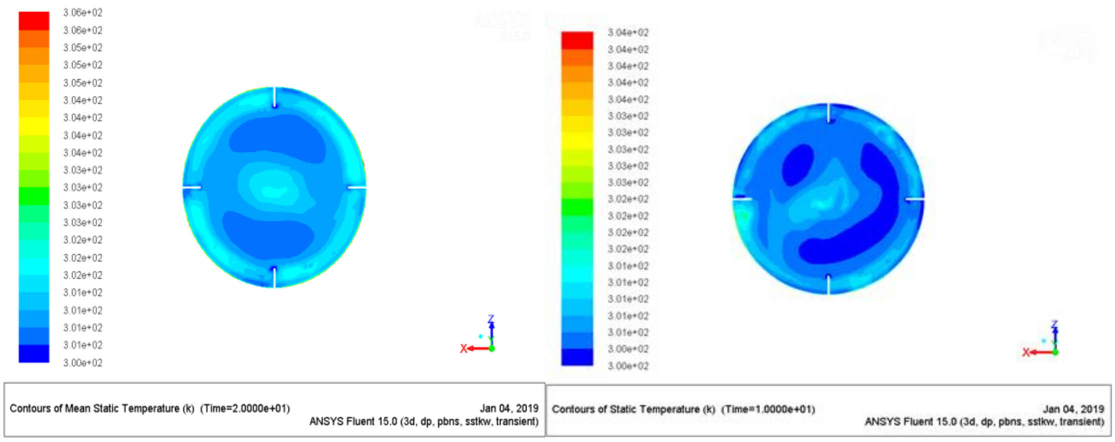


Figure 7.13 Contours of temperature, bottom of agitated vessel Off-clearance 1,500rpm and 900 rpm.

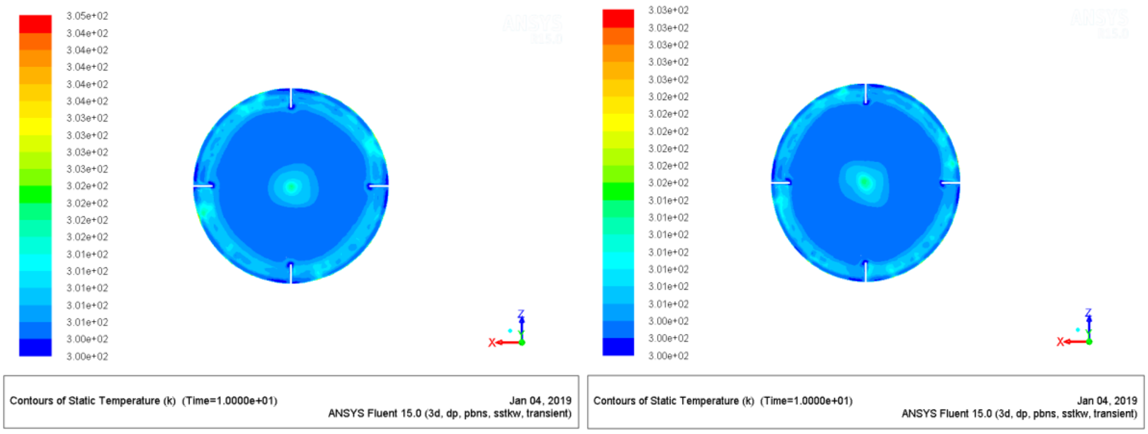


Figure 7.14 Contours of temperature, bottom of agitated vessel Off-clearance 1/3,500 and 900 rpm.

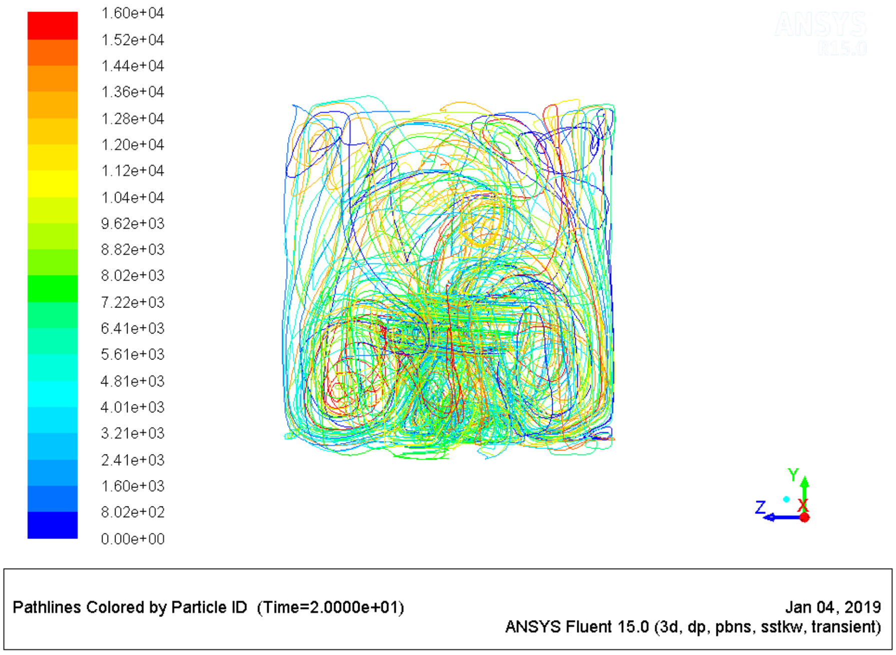


Figure 7.15 Impeller Path Lines Off-clearance1,500rpm.

CHAPTER 8 SIMULATION RESULTS CORRELATION

8.1 Introduction

The theory of agitated vessel and heat transfer in agitated vessel was explained in chapter 3 and 4. To find out heat transfer in agitated vessel helps to design and operation in industries for process of batch or continuous rector. Heat transfer rate and surface of agitated vessel should maintain perfectly for homogeneity and thermos-physical properties of fluid in agitated vessel. It was found by conducting a literature search heat transfer in agitated vessels with pitch blade turbine (PBT) most of the research concentrated on flow patterns of impeller and characteristics, power requirements different type of impeller velocity profiles. Little amount of research developed on numerical analysis of heat transfer in agitated using tube baffles and coils. One of the main objectives in this work elevate heat transfer of agitated vessel bottom side, wall side and overall heat transfer (bottom + wall) heat through the jacketed vessel. Analysis of impeller distance from bottom of vessel was accomplished. The following section provide a brief overview of comparing the obtained results with available Nusselt number correlations in literature.

8.2 Heat Transfer Surfaces

In a jacketed agitated vessel, the steady state heat transfer is reached when temperature of the jacket (wall +bottom) and batch reactor remains constant. It can be achieved when constant inlet (source) or outlet (sink) of system is balanced with the heat supplying or removing through the vessel jacket. The unsteady heat transfer of system occurs when the temperature of the batch changes during the agitation (exothermic or endothermic) from initial to final temperatures. In chapter 2 we have explained type of heating system is providing to agitated vessel in industries.

8.3 Solution Procedure

In present work, CFD simulation of transient (time -dependent) heat transfer in an agitated vessel was studied with a pitched six-blade turbine impeller with supplying constant source heat flux $\mathrm{q} = 3000\ \mathrm{W/m^2}$ at the wall and bottom of the vessel. Initial temperature set at 300 K at the wall of agitated vessel. During the agitation of fluid in tank, the temperature of the system would increase by supplying the heat flux to the system. To prevent the temperature change of the fluid in the agitated vessel, heat sink was used in the simulations. Its value $\dot{Q}^{(g)}$ was based on the following equation.

$$q\,S = \dot{Q}^{(g)}\,V \quad [8.1]$$

$$\dot{Q}^{(g)} = \frac{-q * S}{V} \quad [8.2]$$

Where $\dot{Q}^{(g)}$is heat sink in this case. q = 3000 W/m^2 ,surface area S = 0.157, volume of the tank.by subsisting the values in equation 8.1 $\dot{Q}^{(g)}$ = -74746.71 W/m^3.Using the heat sink will help to avoid the necessity of a correction for the fluid temperature see [Chakravarty, 2017 for more details].

In one of the case the CFD simulation of agitated vessel at 500rpm simulated by the constant heat flux $q = 3000\ \mathrm{W/m^2}$and it was compared with10 time greater value $q = 30000\mathrm{W/m^2}$. The Fluent results of mean alpha α did not vary the value its almost same value with heat flux $q = 3000\ \mathrm{W/m^2}$, All consequent simulations were performed with q = 3000 W/m^2. Table 8.1 shows values of ANSYS Fluent output. Simulations were done for 500 rpm and different heat flux $q = 3000\ \mathrm{W/m^2}$ and $q = 30000\ \mathrm{W/m^2}$.

Output Parameter	Value units
Temperature	3.0000000890e+02 K
Mean -Alpha	3.4041022949e+03 $\mathrm{W/m^2}$K
Mean -Alpha- Bottom	5.1015629883e+03 $\mathrm{W/m^2}$K
Mean -Alpha- Wall	2.9764870605e+03 $\mathrm{W/m^2}$K

Table 8.1 Heat flux $q = 3000\ \mathrm{W/m^2}$, 500 rpm output values.

Output Parameter	Value units
Temperature	3.0000008934e+02 K
Mean -Alpha	3.4040815430e+03 $\mathrm{W/m^2}$K
Mean -Alpha- Bottom	5.1015004883e+03 $\mathrm{W/m^2}$K
Mean -Alpha- Wall	2.9764768066e+03 $\mathrm{W/m^2}$K

Table 8.2 Heat flux $q = 30000\ \mathrm{W/m^2}$, 500 rpm output values.

8.4 Correlations for the Nusselt Number

After ANSYS Fluent simulation for 15 different rotational speeds ranging from 300 rpm to 900 rpm and varying off -bottom clearance of h/d =1, 2/3,1/3 of impeller were performed. The values obtained of Nusselt number of mean alpha (Nu α Bottom +wall), Nusselt number mean alpha bottom (Nu α bottom), Nusselt number mean alpha wall (Nu α wall). Table 8.3 shows the mean values of Nusselt number with Reynolds number, which was calculated from the equations [3.2 and 3.3]. For the all the parameters calculation data can refer Appendix B.

CASE 1: Distance h/d = 1 Off Bottom – Clearance of Impeller.

Impeller Rotational speed (rpm)	**Reynolds Number, Re**	**Nusselt Number**		
		Nu Mean α	**Nu α Bottom**	**Nu α Wall**
300	22116	660.711	908.063	598.399
500	36860	952.525	1349.346	852.560
700	51604	1310.961	1824.793	1181.519
900	66348	1687.206	2267.020	1541.142

Table 8.3 Values Nusselt and Reynolds number according to the rotational speeds

CASE 2: Distance h/d= 2/3 Off Bottom – Clearance of Impeller.

Impeller Rotational speed (rpm)	**Reynolds Number, Re**	**Nusselt Number**		
		Nu Mean α	**Nu α Bottom**	**Nu α Wall**
300	22116	735.966	1127.500	637.333
400	29488	9532.660	1408.892	812.690
500	36860	1134.701	1700.521	992.162
500 ($q = 3000\ \mathrm{W/m^2}$)	36860	1134.694	1700.500	992.159
600	44232	1309.172	1934.040	1151.758
700	51604	1548.293	2213.601	1380.692
800	58976	1716.432	2463.305	1528.284
900	66348	1953.621	2722.939	1759.819

Table 8.4 Values **Nusselt** and Reynolds number according to the rotational speeds.

CASE 3: Distance h/d =1/3 Off Bottom – Clearance of Impeller.

Impeller Rotational speed (rpm)	**Reynolds Number, Re**	**Nusselt Number**		
		Nu Mean α	**Nu α Bottom**	**Nu α Wall**
300	22116	860.955	1279.885	755.421
500	36860	1298.673	1921.520	1141.769
700	51604	1718.972	2489.763	1524.799
900	66348	2245.243	3027.882	2048.085

Table 8.5 Values Nusselt and Reynolds number according to the rotational speeds.

Heat transfer correlation of Nusselt number Nu on different parameters is usually expressed as a combination of dimensionless groups in the form of heat transfer described in detailed in chapter 4.

Our aim was to present a correlation for the Nusselt number as follows:

$$Nu = C\ Re^{a}\ Pr^{c}\ Vi^{c}\ G_{c} \qquad [8.3]$$

Using MATLAB function a nonlinear regression was preformed using nlinfit to calculate the coeffects leading constant C and a.

From literature correlations found to compare our Fluent results of heat transfer in an agitated vessel are valid for a fluid of constant Prandtl number equal to 7.021 temperature - dependence of thermos physical properties of process fluid was neglected, and Reynolds number range$7\ X\ 10^{4} < Re < 7\ X\ 10^{5}$. The experimentally obtained heat transfer correlation for pitched blade turbine PBT impeller in baffled vessels developed by Chapman et al. 1964 described by :

$$Nu = 0.74\ \mathrm{Re}^{\frac{2}{3}} Pr^{\frac{1}{3}}\ Vi^{0.14} \left(\frac{S_{bl}/Di}{1/5}\right)^{0.2} \left(\frac{N_{bL}}{\sigma}\right)^{0\cdot 2} [\sin(\theta)]^{0.5} \qquad [8.4]$$

Where S_{bl} is width of the blade, D_i is impeller dimeter, N_{bl} is number of blades and θ is pitch angle of blade. For our geometrical specification, i.e. S_{bl} = 0.02, N_{bl}= 6 and θ = 45°.This chapman correlation is compared with our results for Off-bottom clearance of 2/3 impeller distance from the bottom of vessel.

According to Nagata et al. 1972. The following equations give the Nusselt number for stirred vessel fitted with the Pitch blade impeller for baffled vessel:

$$Nu = 1.4\ \left(\frac{d_R}{d_B}\right)^{0.3} \left(\frac{h}{d_B}\right)^{0.45} \left(\frac{h_R}{h_L}\right)^{0\cdot 2} \left(\frac{h_L}{d_B}\right)^{-0.6} \sin(\gamma)^{0.5}\ Z^{0.2}\ Re^{\frac{2}{3}}\ \mathrm{Pr}^{\frac{1}{3}} \left(\frac{\eta}{\eta_{\omega}}\right)^{0.14} \qquad [8.5]$$

Where impeller diameter to vessel diameter $\frac{d_R}{d_B} = \frac{1}{3}$, ratio of liquid height to vessel diameter $\frac{h_L}{d_B} = 1$, ratio of height of impeller above bottom to liquid height of liquid $\frac{h_R}{h_L} = \frac{1}{3}$, ratio of baffles width to vessel diameter $\frac{b_s}{d_B} = \frac{1}{10}$, number of baffles n_s = 4 . In our case we are comparing the results of Off-bottom clearance 1 and 1/3 impeller from bottom of vessel.

Table 8.6 shows the value of the coefficients C and a their confidence intervals regions where best fit values of parameters of Nusselt number at Nu mean- α (Bottom +Wall), Nu – α bottom, Nu α wall. For case h/d= 2/3 off -bottom clearance.

Nusselt Number	**C**	**Confidence interval of C**	**Percentage %**	$\boldsymbol{a}$	**Confidence interval of $\boldsymbol{a}$**	**Percentage %**
Nu- Mean α (bottom + wall)	0.037	±0.021	56%	0.90	±0.052	5.79%
Nu α bottom	0.151	±0.034	22.8%	0.80	± 0.021	2.62%
Nu α wall	0.021	± 0.015	72%	0.94	±0.066	7%

Table 8.6 Values of the coefficients for the correlation of Nusselt number, Off-bottom h/d=2/3.

The resulting correlations can be summarized as follows:

$$Nu_{mean} = 0.037\, Re^{0.90} Pr^{0.33} \qquad [8.6]$$

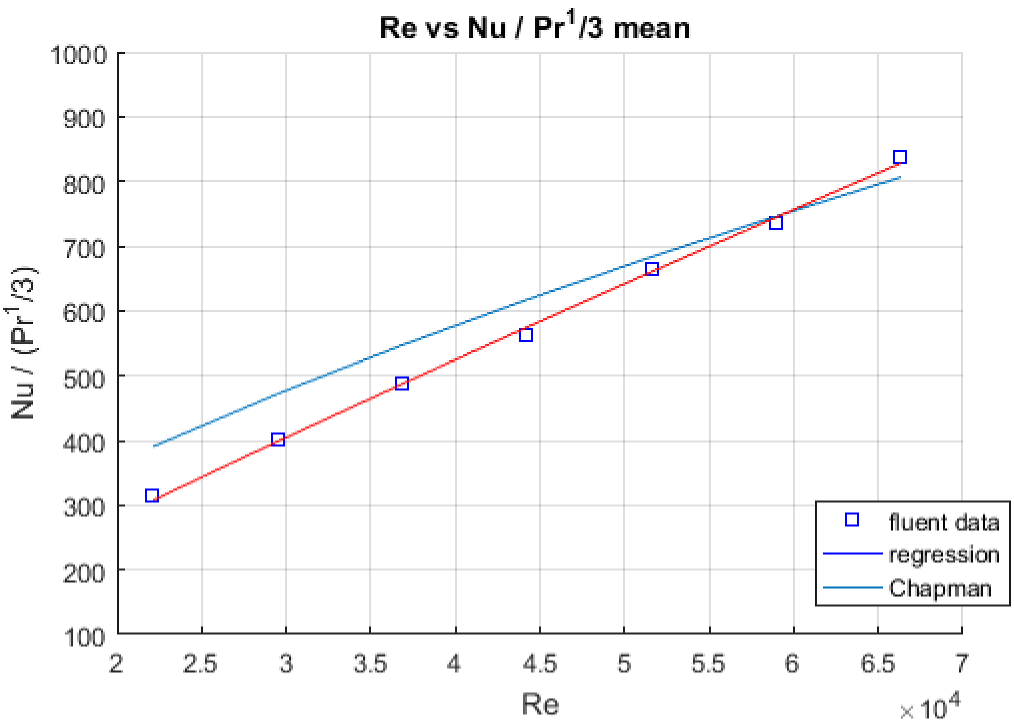
$$Nu_{bottom} = 0.151\, Re^{0.80}\, Pr^{0.33} \qquad [8.7]$$

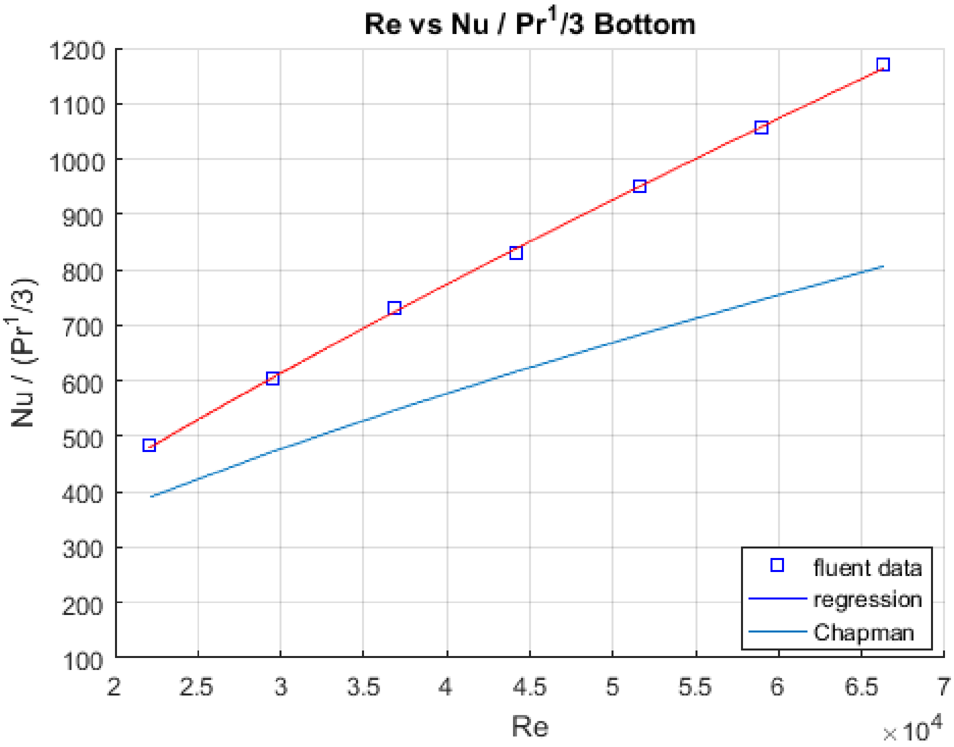
$$Nu_{wall} = 0.021\, Re^{0.02}\, Pr^{0.33} \qquad [8.8]$$

Equations 8.6, 8.7, 8.8 represents the heat transfer correlations obtained by the ANSYS Fluent evaluation of unsteady heat transfer with flat bottom agitated vessel mounted with 6 blade PBT impeller. Exponent ‘b’ of Pr was kept as 0.33 and Vi was completely neglected. Considering the geometry of agitated vessel impeller distance from bottom of vessel. The MATLAB script to calculate the regression parameters of ‘C’ and ‘a’ with confidence intervals for Fluent data of heat transfer Re vs $Re/\, Pr^{0.33}$.

```
data = load('data_all.csv')
% only h/d = 2/3
disp('--- h/d = 2/3 ---');
Xi = data(1:7,2);
Yi = data(1:7,4);
fmodel = @(b,x) b(1)*x.^b(2);
[b,resid,J] = nlinfit2(Xi,Yi,fmodel,[1 1]);
x = linspace(min(Xi),max(Xi),30);
y = fmodel(b,x);
% Chapman correlation
Xi_1 = Xi;
Yi_1 = 0.53*Xi_1.^0.66;
```

```
figure(1);
hold on
loglog(Xi,Yi,'bsq', x,y,'b-')
loglog(Xi_1,Yi_1,x,y,'r-')
xlabel('Re')
ylabel('Nu / (Pr^1/3)')
legend('fluent data','regression','Chapman')
title('Re vs Nu / Pr^1/3')
hold off
axis([20000 70000 100 1000]);
% table
disp('values form fluent')
t1=table(Xi,Yi)
disp('values calculated from chapman')
t2=table(Xi_1,Yi_1)
```





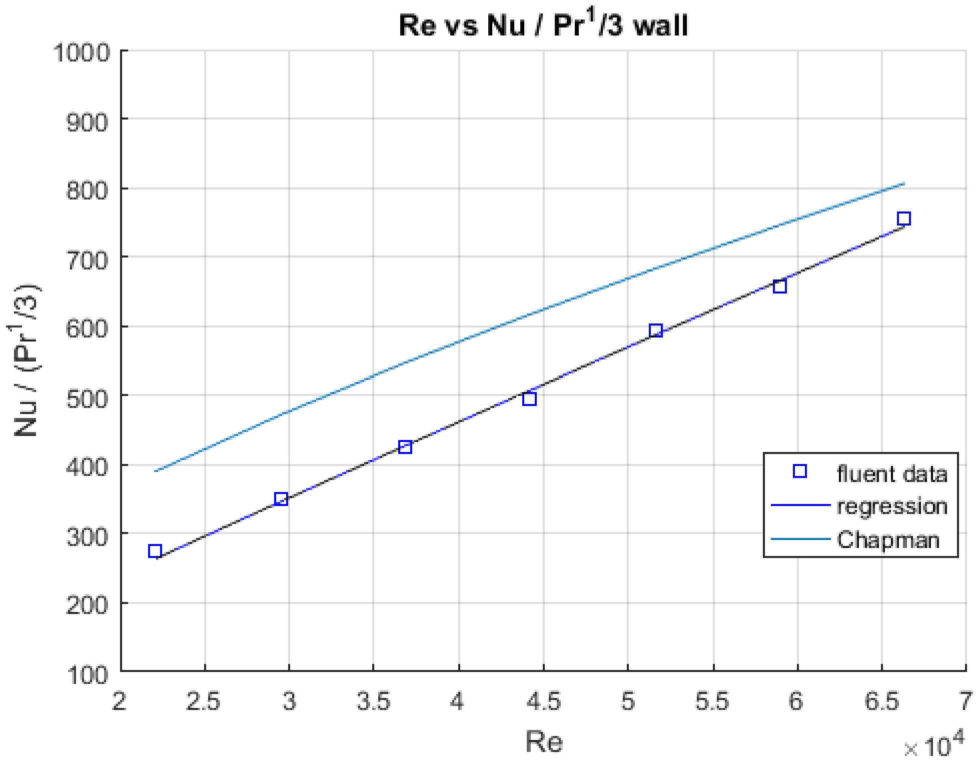


Figure 8.1 ,8.2, 8.3 Obtained data and fitted correlations compared Nu (bottom + wall), Nu bottom, Nu α wall with the experiment work of chapman et al. (1964).

The obtained heat transfer correlations were compared with the experimental work of Chapmen et al. (1964) equation 8.4. Where over all heat transfer Nu (bottom, wall) we got C = 0.058 with confidence interval and Chapman value of C = 0.74. It is observed results are relatively fine with the experimental data. There will be uncertainty of results will be there in any experiments, but we can identify further why we are getting leading constant C (parameter of Nusselt number) lower value.

In present work we are varying Off – bottom clearance of impeller 1 and 1/3 from bottom of tank. From the literature found that Nagata et al 1972 correlation Eq. [8.5] experimental work for impeller distance 1 and 1/3. Table 8.7 shows the value of the coefficients C and a their confidence intervals regions where best fit values of parameters of Nusselt number at Nu mean- α (Bottom +Wall), Nu – α bottom, Nu α wall for Off -bottom clearance h/d =1 shows the values. Table 8.8 shows for Off -bottom clearance h/d = 1/3.

Nusselt Number	**C**	**Confidence interval of C**	$\boldsymbol{a}$	**Confidence interval of** $\boldsymbol{a}$
Nu- Mean α (bottom+ wall)	0.034	±0.087…. (250%)	0.89	±0.23…. (25%)
Nu α bottom	0.077	±0.074…. (95%)	0.84	±0.87…. (%10.35)
Nu α wall	0.025	±0.081… (300%)	0.90	0.28 …. (31 %)

Table 8.7 Values of the coefficients for the correlation of Nusselt number, case Off- bottom h/d = 1.

The correlation can be summarized as follows:

$$Nu_{mean} = 0.034\ Re^{0.89} Pr^{0.33} \qquad [8.7]$$

$$Nu_{bottom} = 0.077\ Re^{0.84}\ Pr^{0.33} \qquad [8.8]$$

$$Nu_{wall} = 0.025\ Re^{0.90} Pr^{0.33} \qquad [8.9]$$

Nusselt Number	**C**	**Confidence interval of C**	$\boldsymbol{a}$	**Confidence interval of** $\boldsymbol{a}$
Nu- Mean α (bottom + wall)	0.046	±0.104 …. (223%)	0.89	± 0.205 …. (23%)
Nu α bottom	0.223	± 0.043 … (19%)	0.78	± 0.017… (2.30%)
Nu α wall	0.024	± 0.079 …. (318%)	0.94	±0.292 … (31 %)

Table 8.8 Values of the coefficients for the correlation of Nusselt number, case Off-bottom h/d =1/3.

The correlation can be summarized as follows:

$$Nu_{mean} = 0.046\, Re^{0.89} Pr^{0.33} \quad [8.10]$$

$$Nu_{bottom} = 0.223\, Re^{0.78} Pr^{0.33} \quad [8.11]$$

$$Nu_{wall} = 0.034\, Re^{0.89} Pr^{0.33} \quad [8.12]$$

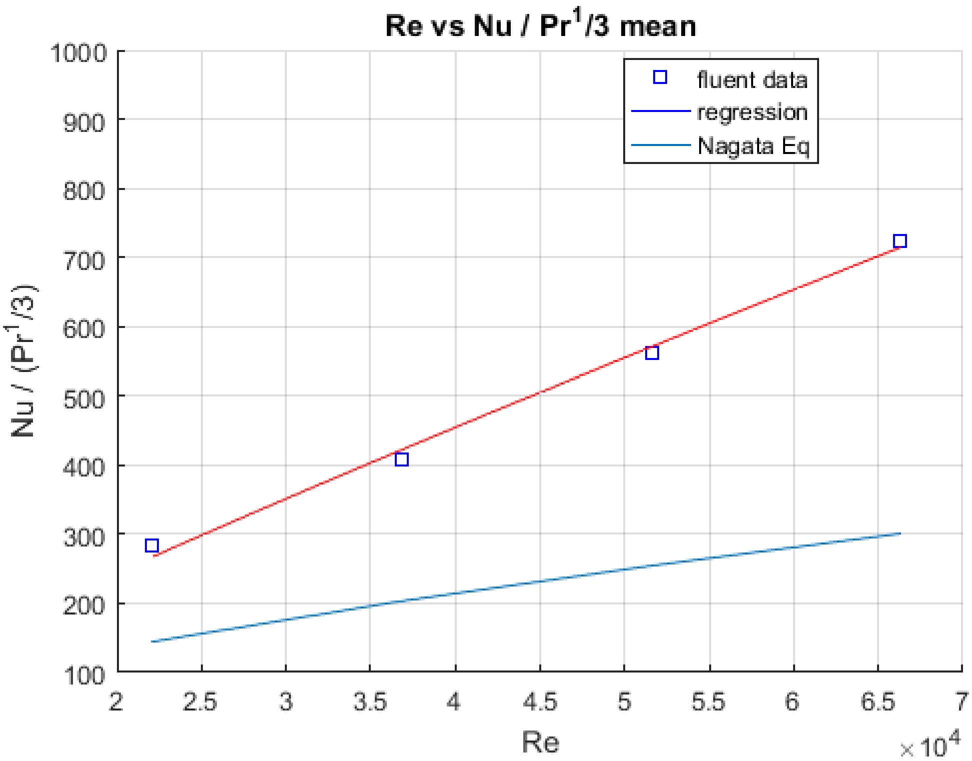


Figure 8.4 Obtained data and fitted correlations compared Nu α (bottom + wall), with the experiment work of Nagata et al. (1972), Off-bottom clearance h/d = 1.

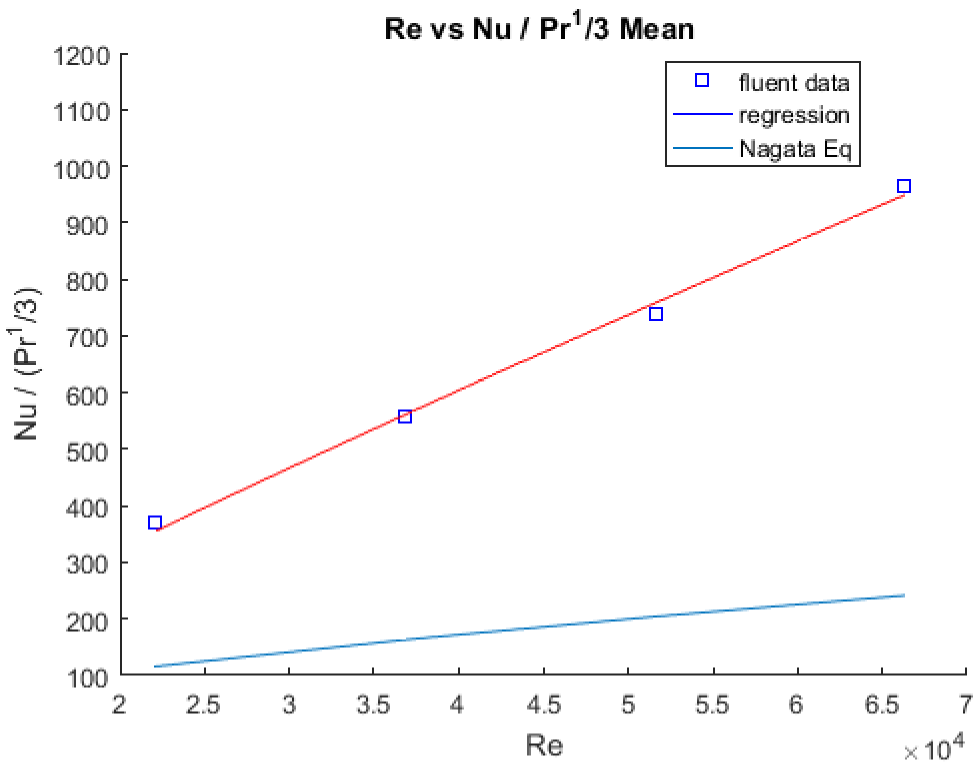


Figure 8.5 Obtained data and fitted correlations compared Nu α (bottom + wall), with the experiment work of Nagata et al. (1972), Off-bottom clearance/d = 1/3.

Mainly the value of C leading constant depends upon geometry of the system (standard or nonstandard geometry) and the type of impeller, number of blades and angle of blade and geometry of agitated vessel with round or flat bottom head. In our results the values of C and 'a' of Re got confidences intervals varying high where the value of C = 1.4 in Nagata et al. (1972). It would be better to run more simulations for different rpm to obtain the data for the off- bottom clearance 1 and 1/3. One of the other reason may be boundary conditions of system and to get better values increasing the run-time simulation Δt, reducing the time step size (s).

The influence of impeller distance from bottom for vessel for all h/d = 1, 2/3 and 1/3 cases were evaluated in MATLAB regression. See Appendix

The correlation can be summarized as follows h/d = 1, 2/3, 1/3

$$Nu_{mean} = 0.035\, Re^{0.89}\, Pr^{0.33} \left(\frac{h}{d}\right)^{-0.24} \qquad [8.13]$$

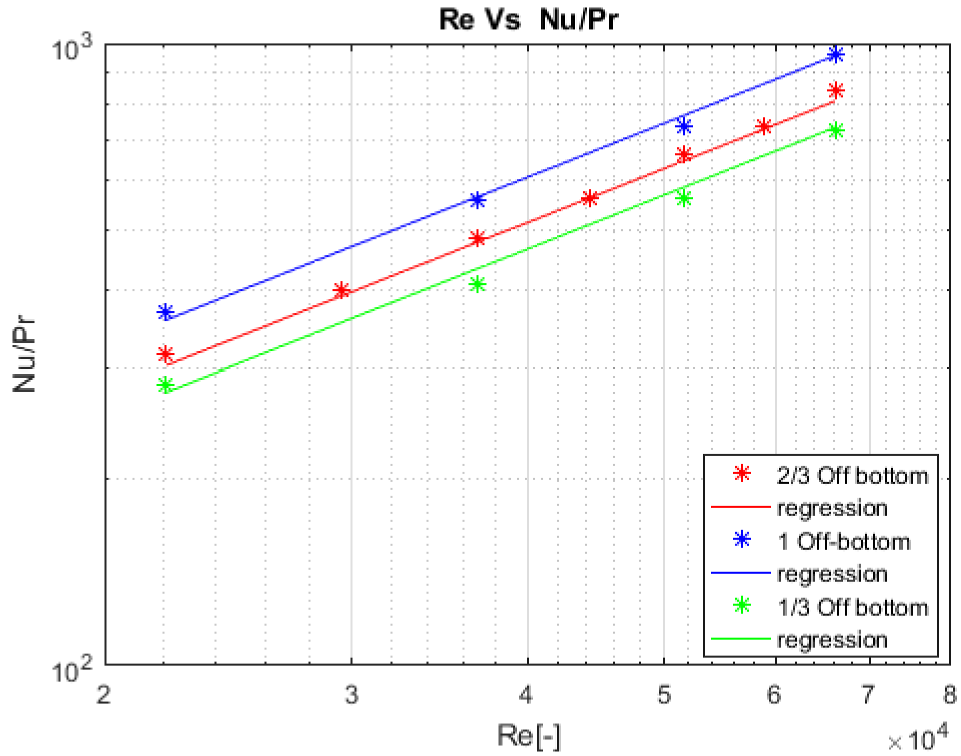


Figure 8.6 Obtained data and fitted correlations compared Nu α (bottom + wall), Off-bottom clearance h/d = 1, 2/3, 1/3.

Nusselt Number	**C**	**Confidence interval of C**	$\boldsymbol{a}$	**Confidence interval of** $\boldsymbol{a}$	$\boldsymbol{\frac{h}{d}}$	**Confidence Interval of** $\boldsymbol{\frac{h}{d}}$
Nu-Mean α (bottom + wall)	0.035	± 0.021 … (60 %)	0.89	± 0.055 … (6.19%)	-0.25	± 0.039 … (16 %)
Nuα bottom	0.139	± 0.115… (82.88)	0.80	± 0.076… (9.56%)	-0.24	± 0.056… (22%)
Nu α wall	0.020	± 0.013…. (63%)	0.93	± 0.058… (6.23%)	-0.23	±0.040 … (16.9%)

Table 8.9 Values of the coefficients for the correlation of Nusselt number, case Off-bottom clearance h/d = 1, 2/3, 1/3.

From the observation of data points and velocity, temperature contours the influence of impeller moving towards the bottom of the vessel the heat transfer rate is slightly increasing towards the bottom of vessel, at wall of the vessel its slightly less heat transfer. It is similarly like impinging jet. [Petera. K el al., 2017].

8.5 Verification of Final temperature

The final temperature can be calculated analytical and compared with results of ANSYS Fluent simulation.

Equation to calculate the heat flux:

$$Q = m\, c_p \frac{dT}{dt} \tag{8.14}$$

Where m is total mass of the heated fluid, this can be calculated as the volume of the tank times the density of the water [998.2 Kg/m^3]. The specific heat capacity (C_p) is 4182 [J/Kg K]. A heat flux of q= 3000 W/m^2 , we need consider the surface area where heat flux is applied bottom and wall of agitated vessel [S]. Therefore, the previous equation [8.14] can be written as:

$$q\, S = V_{tank}\, \rho_{water}\, Cp_{water}\, \frac{dT}{dt} \tag{8.15}$$

This is an ordinary differential equation, which can be solved by separating the variables and integration. The limits for integration for the temperature side are initial temperature, which is known T_w = 300 K and final temperature T_f, mixing time t_m = 0 to 20 seconds.

$$q\, S \int_{0}^{20} dt = V\ \rho\ Cp \int_{300}^{T_f} dT$$

$$q\, S\, (20 - 0) = V\, \rho\, Cp\, (T_f - 300)$$

$$T_f = \frac{q\, S\ (20)}{V\ Cp\ \rho} + 300\ K \tag{8.16}$$

There the surface (S), can be calculated as the sum of the bottom surface [$\pi\, r^2$] and the wall surface [$2\, \pi\, r^2 \times H$]. The diameter of tank 0.2 m and the height is 0.2 m, total surface [s] = 0.157 m^2 and volume of the tank ($\pi r^2 \times H$) is 0.0068 m^3 by calculating the values in equation [8.16]. The final temperature is $T_f = 300\ K$. The final temperature obtained from the simulation with a report of volume integrals is 300.01 K, which tell calculation is correct.

For calculation of the heat transfer coefficient, ANSYS Fluent solver does consider this increase, but takes the temperature of the fluid as constant input parameter (T_{ref}) according to the following equation:

$$\alpha = \frac{q}{T_{ref} - T_w} \qquad [8.17]$$

Where q is heat flux and T_w is temperature at the wall.

CONCLUSION AND FUTURE SCOPE

Conclusion

The following conclusion have been drawn from in this master work:

a) A literature research was done to find scientific work related to heat transfer in an agitated vessel with pitched blade turbine impeller and found out the interesting facts about agitated vessel from past years research made on it with different boundary conditions and with phenomenal development.

b) Geometry of agitated vessel and meshing

i. Created a three-dimensional simulation of heat transfer in given geometry agitated vessel model by using ANSYS Workbench15.0. For three different cases of Off - bottom clearance h/d = 1, 2/3, 1/3 impeller diameter ratio, distance from the bottom of vessel.
ii. The power characteristics of the PBT impeller were determined.
iii. Using sliding mesh technique has been used with tetrahedral mesh and polyhedral mesh.

c) The heat transfer coefficients of transient simulation of agitated vessel

i. The solution strategy of the setting for the ANSYS Fluent solver was determined to perform unsteady heat transfer during heating of batch of liquid.
ii. Three dimensional simulations of heat transfer in a model have been performed using k-ω (SST) turbulence model.
iii. Internal heat source (sink) in ANSYS CFD simulation eliminated change in temperature caused by constant heat flux at bottom and vertical walls of agitated vessel.
iv. Two different simulations for constant heat flux q = 3000 W/m^2 and q = 30000W/m^2 for rotational speed of impeller 500rpm were performed to verify its influence. It was negligible.
v. Evaluated impact of the impeller distance from the bottom h/d= 1, 2/3, 1/3 constant heat flue q = 3000W/m^2 for 300 to 900 rpm.
vi. The mean heat transfer coefficients Nusselt mean α, Nusselt mean α bottom, Nusselt mean α wall was evaluated by performing simulation in ANSYS Fluent 15.0. The

calculated the Power number, Nusselt number, and Reynolds number. Developed were evaluated in each simulation heat transfer correlations using non-linear analysis (nlinfit) in MATLAB.

vii. The developed correlations were compared with the experimental work from the literature of Chapman et al. [1964] for case off-bottom clearance 2/3 and Nagata et al [1972] for case Off -bottom clearance 1, 1/3 and relatively good agreement with the experiment data was observed.

viii. The impact of the off-bottom clearance was described by the correlation for the Nusselt number. In general, the smaller is the distance the larger is the heat transfer rate which is in accordance with the negative power of h/d term in the correlation. It is similar to impinging jet case.

Future Scope

This work was focused on heat transfer simulation and optimising the agitated vessel design with different rotational speed of impeller. In addition to this work can be done in future:

- By increasing the run time simulation Δt_m and decrease the time step size to perform simulation for case h/d =1 and h/d= 1/3 Off bottom clearance we can assess better accurate results.
- Simulation based on other turbulence models like LES (Large eddy simulation) and RSM (Reynolds Stress Model) with fine mesh quality for that high computational servers are need and more number of simulations days.
- In present work baffles employed in agitated vessel are used, so unbaffled and with round bottom tank with same geometry heat transfer simulation can be done which is most used geometry in food processing industries.
- Considering thermos – Physical properties of fluid and Pr Prandtl number, and other type of radial impeller (Rushton disk turbine).

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APPENDIX

A) The ‘nlinfit2’ function written in MATLAB

```
function [ a, resid, Jc, ci, cip, cipp ] = nlinfit2(Xi,Yi,fmodel,Binit)
np = length(Binit);
if  (~ exist('OCTAVE_VERSION'))
  [a,resid,Jc,covb] = nlinfit(Xi,Yi,fmodel,Binit);
  ci = nlparci(a,resid,'jacobian',Jc,'alpha',1-0.95);
  cip = a' - ci(:,1);
else
 % leasqr in Octave expects opposite order of input parameters
  fmodel2 = @(x,a) fmodel(a,x);
  [y2,a,kvg,iter,corp,covp,covr,stdresid,Z,r2] = leasqr(Xi,Yi,Binit,fmodel2);
  %%beta = a;
  resid = Yi - y2; % residua
  N = length(Xi);
  nf = N-np;
  Sv2 = sum(resid.^2)/nf;
  %covp
  Jc = [];
  C = sum(stdresid.^2)/nf*covp;
  t975 = tinv(0.975,nf);
  for i=1:np;
    stde(i) = sqrt(C(i,i));
    cip(i) = stde(i)*t975;
    ci(i,:) = [a(i)-cip(i),a(i)+cip(i)];
  end
end
cipp = cip./abs(a')*100;
for i=1:np;
  fprintf('beta(%d): %12f +- %10f (%.2f%%),   %12f ... %12f\n',i,a(i),cip(i),cipp(i),ci(i,:));
end
```

The MATLAB file for the functional relationship Power number Po vs Reynolds number Re described by null hypothesis.

```
data = load('aa.csv');
%Xi = data(:,1)
%Yi = data(:,2)
fmodel = @(b,x) b(1)*x.^b(2); %power model
[b,resid,J] = nlinfit2(Xi,Yi,fmodel,[1 1]);
b
SSalt = sum( resid.^2 )
N = length(Xi)
DFalt = N - 2
fmodel1 = @(b,x) b(1)*x.^0; %null hypothesis
[b0,resid0,J0] = nlinfit2(Xi,Yi,fmodel1,[1]);
b0
SSnull = sum( resid0.^2 )
DFnull = N - 1
F = ( (SSnull-SSalt)/SSalt )/( (DFnull-DFalt)/DFalt )
Fcrit = finv(0.95,DFnull-DFalt,DFalt)
Pr = fcdf(F,DFnull-DFalt,DFalt)
p = 1-Pr
if ( F < Fcrit )
disp('no significant difference');
else
   disp('significant difference');
end
y1 = fmodel(b,Xi);
y0 = fmodel1(b0,Xi);
log log(Xi,Yi,'r*', Xi,y1);
```

B) Calculation table for off Bottom clearance h/d=23

Heat flux (W/m^2)	N(RPM)	N(rps)	rad/s	Moment (n-m)	Power (P) w	Power number (Po)	Diameter of vessel (d)	diameter of impeller (m)
3000	300	5.00	31.41592654	0.009	0.289	1.76	0.2	0.0667
3000	400	6.67	41.88790205	0.015	0.647	1.66	0.2	0.0667
3000	500	8.33	52.35987756	0.027	1.427	1.88	0.2	0.0667
30000	500	8.33	52.35987756	0.027	1.427	1.88	0.2	0.0667
3000	600	10.00	62.83185307	0.039	2.473	1.88	0.2	0.0667
3000	700	11.67	73.30382858	0.053	3.920	1.88	0.2	0.0667
3000	800	13.33	83.7758041	0.068	5.692	1.83	0.2	0.0667
3000	900	15.00	94.24777961	0.088	8.299	1.87	0.2	0.0667

dynamic viscosity(Pa. s)	Re … Xi	mean alpha (w/m2-k)α	mean alpha bottom	mean alpha wall	Nu (mean α)	Nu (α Bottom)
0.0010	22116	2207.899	3382.499	1912.000	735.966	1127.500
0.0010	29488	2797.980	4226.677	2438.071	932.660	1408.892
0.0010	36860	3404.102	5101.563	2976.487	1134.701	1700.521
0.0010	36860	3404.082	5101.500	2976.477	1134.694	1700.500
0.0010	44232	3927.515	5802.120	3455.275	1309.172	1934.040
0.0010	51604	4644.879	6640.802	4142.077	1548.293	2213.601
0.0010	58976	5149.296	7389.914	4584.852	1716.432	2463.305
0.0010	66348	5860.863	8168.816	5279.456	1953.621	2722.939

Nu (α wall)	Pr^(1/3)	Nu (mean α)/Pr(1/3) … Yi	Nu (mean α bottom)	Nu (mean αwall)
637.333	2.330	315.824	483.842	273.498
812.690	2.330	400.231	604.596	348.749
992.162	2.330	486.933	729.742	425.765
992.159	2.330	486.930	729.733	425.764
1151.758	2.330	561.803	829.952	494.253
1380.692	2.330	664.417	949.920	592.495
1528.284	2.330	736.570	1057.075	655.830
1759.819	2.330	838.355	1168.491	755.189

Calculation table for off -bottom clearance h/d = 1/3

N(RPM)	Angular velocity (rad/s)	Moment (n-m)	Power (P) w	Power number (Po)	Diameter of vessel (d)	diameter of impeller (m)
300	31.4159	0.0110	0.347	2.11	0.20	0.066666667
500	52.3599	0.0296	1.549	2.04	0.20	0.066666667
700	73.3038	0.0569	4.174	2.00	0.20	0.066666667
900	94.2478	0.1077	10.148	2.29	0.20	0.066666667

Re Xi	mean alpha (w/m2-k)α	mean alpha bottom	mean alpha wall	Nu(mean α)	Nu (α Bottom)	Nu (α wall)
22116	2582.866	3839.656	2266.263	860.955	1279.885	755.421
36860	3896.019	5764.561	3425.306	1298.673	1921.520	1141.769
51604	5156.916	7469.290	4574.396	1718.972	2489.763	1524.799
66348	6735.729	9083.646	6144.255	2245.243	3027.882	2048.085

Pr^1/3	Nu (mean α)/Pr(1/3) … Yi	Nu (mean αbottom)/Pr(1/3) … Yi	Nu (mean αwall)…Yi
2.330	369.461	549.236	324.173
2.330	557.298	824.579	489.966
2.330	737.660	1068.429	654.335
2.330	963.498	1299.351	878.892

Calculation table foo off bottom clearance h/d= 1

Nu (mean α)/Pr(1/3) … Yi	Nu (mean αbottom)/Pr(1/3) … Yi	Nu (mean αwall)
283.530	389.676	256.790
408.756	579.043	365.858
562.571	783.071	507.024
724.028	972.843	661.348

C) MATLAB script for h/d = 2/3 nonlinear regression and similar code is used for 1, 1/3

```
Clear
clc
% co-relation code
% Data loading
%

% data1=load('data1.csv')
% Re=data1(:,1)
% Pr=data1(:,2)
% Vi=data1(:,4)
% % chappman co-relation
%Nu_cm= (0.76) .* ((Re).^(0.66)) .* ((Pr).^(0.33)) .* ((Vi).^(0.14))
% % new Xi_1 and Yi_1
% Xi_1=Re;
% Yi_1=Nu_cm ./ (Pr.^(1/3));

%old code
data = load('data_all.csv')
% only h/d = 2/3
disp('--- h/d = 2/3 ---');
Xi = data(1:7,2);
Yi = data(1:7,4);
fmodel = @(b,x) b(1)*x.^b(2);
[b,resid,J] = nlinfit2(Xi,Yi,fmodel,[1 1]);
x = linspace(min(Xi),max(Xi),30);
y = fmodel(b,x);

% Chapman correlation
Xi_1 = Xi;
Yi_1 = 0.53*Xi_1.^0.66;

figure(1);
hold on
loglog(Xi,Yi,'bsq', x,y,'b-')
loglog(Xi_1,Yi_1,x,y,'r-')
xlabel('Re')
ylabel('Nu / (Pr^1/3)')
legend('fluent data','regression','Chapman')
title('Re vs Nu / Pr^1/3')
hold off
axis([20000 70000 100 1000]);

% table
disp('values form fluent')
t1=table(Xi,Yi)
disp('values calculated from chapman')
t2=table(Xi_1,Yi_1)
```