DESIGN OF REACTORS AND COMPARISON OF PERFORMANCE BETWEEN VARIOUS TYPES OF IMPELLERS.

A Graduate Project Report submitted to Manipal Academy of Higher Education in partial fulfillment of the requirements for the award of the degree of

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CERTIFICATE

This is to certify that the project titled **DESIGN OF REACTORS AND COMPARISON OF PERFORMANCE BETWEEN VARIOUS TYPES OF IMPELLERS** is a record of the bonafide work done by **ATHARVA AJAY WANI (170909292**) submitted in partial fulfillment of the requirements for the award of the degree of **BACHELOR OF TECHNOLOGY** in **MECHANICAL ENGINEERING** of Manipal Institute of Technology, Manipal, Karnataka (A constituent unit of Manipal Academy of Higher Education) during the year 2020-2021.

Mr. Krishna Kumar P. | **Dr. Sathyashankara Sharma**

Project Guide | **Head of the department**

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Introduction

ACME process systems pvt. Ltd. designs and manufactures various chemical processing equipment for storage, mixing, heating, or cooling of chemicals. These equipment include reactors, agitators, heat exchangers, pressure vessels, hydrogenators etc. All these equipment are involved in highly critical processes and handle chemicals that can be toxic, inflammable or could be harmful to environment like concentrated HCL, Hydrogen, Petroleum products etc. In many cases, these equipment are pressurized to a very high pressure as it is vital to the process of the chemical. The equipment is also supplied to food and pharmaceutical companies which requires special materials so that all components coming in contact with the process fluids are food grade.

It is necessary that these equipment are manufactured with these factors in mind. Such highly critical equipment needs to be designed and manufactured to a great level of precision so that it performs efficiently in the process and does not undergo a catastrophic failure. Also, it is designed in a way that it reduces batch times and capital investment for the customer.

Although process systems is a chemical engineering subject, the actual design of pressure vessels and other components requires the knowledge of mechanical engineering. At this company, chemical and mechanical engineers work together to design and manufacture these process equipment. The chemical engineers look into the aspects related to the actual process such as which impellers will create the best flow and mixing patterns to improve the efficiency of mixing and heat exchange. The mechanical engineers design the shafts, vessels etc so that the equipment can support the process requirements. Mechanical engineers are also involved in the manufacturing process. The strength of the vessels and other components largely depend on the manufacturing quality. A lot of attention is given to the quality of welds and correctness in the dimensions. Since a lot of the chemicals are very sensitive to the conditions they are being processed in, slight fluctuations in the equipment can result in a bad batch which can cause a negative effect on the whole production cycle. The materials being used to manufacture the equipment must be compatible with the process fluids, so the type and quality of materials used also need to be closely monitored.

The process engineering sector has a very wide range of application. Almost every industry like food, pharmaceuticals, petrochemical industry, automobile industry etc has the requirement of storage or mixing of some ingredients or chemicals. As this is such a diverse field, the customers of this company are also very diverse. Some of the major customers include [1]:

- Pharmaceuticals
    - Biocon Ltd.
    - Sun Pharmaceuticals.
    - Anthem Biosciences.
    - Unique Biotech Ltd.
- Chemicals and Petrochemicals
    - 3M.
    - Avery Dennison.
    - Alfa Chem Group, Ukraine.
    - Castrol India Ltd.
    - Reliance Industries Ltd.
    - Unilever Ltd.
- Paints and Dyes
    - Asian Paints Ltd.
    - Berger Paints Ltd.
    - Kansai Nerolac paints Ltd.
    - Lakhani Dyestuff Ltd.
- Food
    - Mondelez International (Cadbury).
    - Tetrapak India Ltd.

Importance of proposed work

The products manufactured by the company are used in highly critical applications so designing and optimizing the design to the highest degree is important. If the agitator is not designed correctly, the mixture does not mix homogeneously which results in a bad batch or is the vessel its supports are not designed correctly it might fail and cause damage to other equipment around it causing even more financial loss. Understanding the aspects that matter the most and then applying that knowledge in designing the reactors is essential.

The company was started about 12 years ago and designs and manufactures these reactors. To further develop in the market to provide innovative solutions the company is setting up an R&D department. This department is currently in its infancy with very few employees directly working in it. By working in the R&D department I can directly contribute to the progress.

To come up with new ideas first the old ideas and research needs to be studied. By curating relevant information future research becomes easier. Analysis of existing designs using CFD can be used to compare new innovative designs. Hence creating a database of CFD simulations with different types of impellers can be very important to come up with new designs and optimize current designs.

Working of present system

As this company serves to such a wide variety of industries and customers, every new project is unique from others in some or the other way. To make sure all projects run on schedule a standard procedure is followed for every project be it a brand-new customers project or a repeat order from an old customer.

The first step to any project is getting the order from the customer by offering the best price and service compared to the competitors. The sales team looks after this by talking with the customers and understanding their requirements. After getting detailed information about the requirements of the customer the sales team does some preliminary design work to make a quotation. This preliminary design includes the choosing the required impellers, heating and cooling elements, shaft, motor requirement, gearbox, vessel design and other essential components (Fig 1.).

Impeller type	Np	RPM	Diameter mm	Diameter2 in	Sp. Gravit	Viscosity facto	Proximity facto	Shaft power KW	Shaft power HP	No. of Im	Motor powe KW
PBT w/o fin	1.225	85	740	29.13385827	1.7	1	1	1.313852569	1.761876296	1	1.642315712
AA304	0.65	85	770	30.31496063	1.7	1	1	0.850391538	1.140375052	2	2.125978844
PBT	1.27	85	375	14.76377953	1.7	1	1	0.045521022	0.061043691	1	0.056901278
	0	85		0	1.7	1	1	0	0		0
							Total	2.20976513	2.963295039		3.825195834

Over desig
25

Motor Power	RPM	Torque	Reduction require	Selected reductio	Actual RPM
KW		Nm			
7.5	1740	41.16076114	20.47058824	20.32	85.62992126

Flow Calculation

Impeller Type	Nq	RPM	Diameter (mm)	Sp. Gravity	Viscosity	No. of Imp	Flow (m3/min)	Reynolds Numbe
PBT w/o fin	0.743	85	740	1.7	5	1	25.59192172	263760.6667
AA304	0.68	85	770	1.7	5	2	52.7752148	571160.3333
PBT	0.787	85	375	1.7	5	1	3.527666016	67734.375
0	0	85	0	1.7	5	0	0	0
						Total	81.89480254	902655.375

Tip speeds

Impeller type	Diameter (mm)	RPM	Tip speed
PBT w/o fin	740	85	3.293436299
AA304	770	85	3.426953986
PBT	375	85	1.668971097
0	0	85	0

Tank Geometry								
		L/D	3	Liquid level	4097.510189			
Diameter (mm)	1500	D/T	0.493333333	Z/T	2.731673459			
St. height (mm)	4500	Work vol/Act vol	0.851012339					
Beam height (mm)	50							
Top type	Flat	120	<- Cone angle					
Bottom type	ASME	120	<- Cone angle					
Top volume	Bottom volume	Working volume	Gross volume					
0	273.34125	7000	8225.497654	Jamming Factor	1			
Top height	Bottom height	Gap from bottom	Appx shaft height	Deflection	Shaft dia	Rigidity	Chosen dia	Actual Deflection
0	291	50	5791	5.7	96.22161752	70.3	95	2.457146188
					Over design factor			
					25			

Fig 1. Sample agitator design calculation excel sheet.

Based on the power requirements motor, gearbox, bearings etc are selected. After this, costing is done for the project and a budgetary quote is given to the customer (Fig 2.). Within this quote, transportation charges, installation charges etc are also included. The customer then approves the design or asks for some redesigning.

Sr No	Particulars	Dia (mm)	St. Ht (mm)	Thk (mm)	MOC	Density	Rate (Rs/Kg)	Qty	Weight (Kg)	Cost	Limpet Coil		
1	Shell	1500	4500	5	SS304	8027	230	1	856	1,96,956	Limpet OD	60.0	
2	Top - Flat	1650	1650	100	SS304	8027	230	1	1716	3,94,765	Length of limpet/turn on shell	5176	
3	Bottom-10% Torispherical	1750	1750	6	SS304	8027	230	1	147	33,924	Limpet Height	3375	
4	Baffles	80	4500	5	SS304	8027	230	4	58	13,293	Limpet Pitch	80	
5	BODY FLANGES								328	19,205	No. of Turns	42.19	43.00
6	Limpet				SS304	8027			0	0	Total Length Of Limpet on Shell	222580	223
7	Nozzles				SS304	8027				10,350	Total Length Of Limpet on Dish	29	31
8	Nozzle Wt.						50		30	1,500	Total Length of Limpet in meters	252	252
9	Handhole	SS304							7	4,500	width of Limpet	0.094	0.094
10	Agitator Mounting	SS304	400	50			300	1	49	14,789	Thickness	0	0
11	Internal-Polishing/External-Pickling						1000		31	31,189	Limpet MOC	SS304	8027
12	Lug Supports				SS304		1573	4	63	6,293	Limpet Wt.	0	0
13	Radiography	SPOT								5,000	Limpet Raw Material Cost	0	0
14	Misc									5,000	Limpet on Shell Cost	0	0
									Cost	**7,36,765**	Limpet On Dish Cost	0	0
									Factor	**1.28**	**Total Limpet Cost**		**0**
									Price	**9,44,000**			
									Agitator	**1,70,000**			
									Total Price	**11,14,000**			
									F.O.R	**5,80,000**			

BODY FLANGE						
Description	**MOC**	**Dimensions**	**QTY.**	**Wt**	**Rate**	**Cost**
Flat	IS:2062	3500 x 90 x 60	2	297	0	0
Rolling/Welding/Straightening				297	0	0
Liner/T&G	SS316L	3500 x 40 x 14	2	31	0	0
Machining/Drilling/Fitting to Shell				328	25	8205
Gasket			1		5000	5000
Hardware			30		200	6000
					Total	**19205**

Lug Support					
Particulars	MOC	Size	Wt	Rate	Cost
RF Pad	SS304	250X200X6	2	100	241
Base Plate	IS:2062	250x200x14	6	100	562
Vertical Gusset	IS:2062	200x200x12	8	100	771
				Total	**1573**

Fig 2. Sample costing sheet

Once the customer approves the design and accepts the offer the engineering team prepares detailed drawings of the project on AutoCAD and in some cases prepare a 3D model on SolidWorks. The designing of the vessel is done using a software called PV elite. Using all these tools the detailed drawings are submitted to the customer and forwarded to the manufacturing team.

Usually the bought-out items like the motor, gearbox, seals, bearings etc have longer lead times hence they need to be ordered early. Once the sales team gets a primary confirmation from the customer, the procurement team orders the bought outs. After getting the detailed drawings from the engineering team, the manufacturing team uses AutoCAD to optimize material usage while cutting sheets of metal to be formed into various shapes. Other components like flanges, couplings, shafts, impellers etc are also manufactured in-house using latest technologies like CNC plasma cutter and conventional machinery like lathe machines, universal drilling machines, milling machines etc. (Fig 3.)

(a) (b) (c)

Fig 3. Stages in manufacturing: (a)Raw material, (b)Rolled sheet metal, (c)Finished product. [9]

The manufacturing team finishes installing all components and getting it ready for testing. The quality control team performs lot of checks and tests all along the manufacturing process and after manufacturing as well. It performs material checks to see if the material meets the requirements of the customer. It also keeps making periodic checks if all welds and joints fulfil the quality standards. Once the manufacturing is complete the QC team performs internal checks on the quality of manufacturing and in some cases the customer assigns a third-party inspector who oversees the tests and gives his approval or suggests improvements.

After the equipment passes all quality control checks it undergoes a final finishing process where the equipment is cleaned thoroughly, and protective paint or coating is done. The dispatch team prepares the equipment for a safe transport and loads it onto a truck for its delivery to the customer. Overseas shipment is done using ships. Once the equipment arrives at the customers site, a team is arranged at the site for installation and a quality control team member is present during the installation to make final checks and commission the equipment into service. The accounts team receives and tracks the payment. The smooth running of the entire project is taken care by the projects team.

Literature review

Reactor:

A reactor is a process equipment in which two or more chemicals are mixed under specific temperature and pressure conditions. A reactor consists mainly of two components: a vessel and an agitator. Based on the process requirements it may consist of other components for heating or cooling namely limpets or internal coils.

The design of a reactor is crucial to achieve high performance. It is essential that the vessel is made of a compatible material to safely contain the process fluids without reacting with them. It is also important that the vessel can cope with various loads on it like internal pressure, static weight of fluid, forces caused by movement of fluid during mixing, weight of motor, gearbox nozzles etc. The vessel should be able to develop and maintain high pressure or full vacuum based on requirement. The thickness required for the vessel to be structurally sound, a specialized program called PV elite used. All the required process data is fed to the program and based on that it performs various calculations and gives the minimum required thickness of metal sheet to manufacture the vessel.

The design of an agitator is just as important as this is the device that achieves the mixing of the chemicals and other ingredients in the process. The impellers must be designed in a way that they can stand up to the forces on them while moving through the fluid. There are various types of impellers, and they should be chosen so that they achieve the best possible mixing while requiring the least power to move through the fluid. Baffles are provided inside the vessel at regular intervals that break the vortex created during mixing and improves the mixing characteristics.

There are various types of motors, and the required motor is selected based on the power requirement of the impellers. Power requirements depend on various factors like density, viscosity, speed of rotation, type of impellers etc. Other than power requirement the working conditions are also kept in mind. If the reactor is mounted in an open environment it needs to be weatherproof or if it is working in place where the chemicals are flammable or corrosive the motor needs to be flameproof.

In case the process requires high pressure, or a full vacuum proper sealing needs to be done. These seals have different ratings for different pressures and type of process. These seals may need cooling as the faces of the seal can get hot due to the process temperature so to prevent this a cooling device called thermosyphon pot is provided which circulates coolant around the face of the seal and stops it from overheating. Required bearings and couplings are also chosen based on shaft diameter and amount of transmitted torque.

Many processes require have a specific temperature requirement. The contents of the vessel need to be heated or cooled. This is achieved by using hot steam or chilled water or coolant from the utilities at the customer's site. The steam or coolant is fed into devices like limpets or jackets on the outside of the vessel or internal coils. The limpets and jackets heat the vessel walls which heats the contents whereas the internal coils are immersed in the fluid. The heating or cooling fluids are continuously circulated in the thermal device. In some cases, layers of insulation are also provided to maintain the temperature inside the vessel and keep the outside of the vessel at a temperature that is safe to touch.

A reactor needs nozzles and inlets for letting in the fluids into the vessel, provide outlet for the mixed fluid, inlet and outlet for thermal devices, manholes etc. These nozzles are basically sections of pipe welded wherever needed. Flanges are then welded to these pipes so that proper connections can be made between the fluid lines at the customers site and the pipes. To remove the mixed batch from the vessel, in some cases valves are given which let out the mixed contents in either a slow regulated flow or as a flood, whichever is required by the customer.

Impellers:

Impellers are the most important component in the mixing of fluids in the vessel. There are many types of impellers, each having its own advantages and disadvantages. Some impellers are good at mixing but consume a lot of power whereas some consume fraction of the power but may not be as good at mixing. Each impeller also works most effectively in a specific range of viscosities and speed. Then there are some special purpose impellers that are good at some tasks like breaking the settled layer of some powder at the top of the liquid surface or making sure particles do not settle down at the bottom.

The blades of an impeller are fixed to the shaft by bolting or welding the blades to a hub and then bolting or welding the hub to the shaft. The impellers and hubs need to structurally strong as they experience a lot of pressure on them while moving through the fluid. As the fluids in the vessel that needs to be mixed can be highly viscous and have high density, it exerts force on the impeller moving through it. These forces can reach very high values if the required rotation speed for mixing is high. Impellers are therefore made of thick sheet metal and hubs are casted in the desired shape and size.

Some of the major types of impellers are as follows [2]:

- Hydrofoils – This impeller gives huge power savings. As seen in Fig. 4a the blades are curved in a way that low drag is experienced and most of power is converted into an axial flow which helps in creating a current in the fluid which mixes the fluids thoroughly. It also helps in reducing batch times. This type of impeller is used in fluids up to a viscosity of about 4000 cps.

Fig 4a. Hydrofoil impeller.[2]

- Wide blade hydrofoils – These are used in high viscosity application. It gives a shear as well as flow type movement of the fluid. It has much better flow properties in high viscosity liquids. It is also good at gas dispersion in liquid.

Fig 4b. Wide blade hydrofoil impeller.[2]

- Gas dispersion turbine – These are used in applications where there is a requirement for good dispersion of gas as in the case of a hydrogenator. This type of impeller is good at gas holdup due to the width and curvature of the blade as seen in Fig4c. and dispersing the gas in the fluid so that the gas can react with the fluid more efficiently and in less time.

Fig 4c. Gas dispersion turbine. [2]

- Pitched blade turbine – The blades of this type of impeller are easier to manufacture as they are just rectangular pieces of metal. They are mounted on the hub usually at 45°

from the axis of the shaft as shown in fig 4d. These can be used for low as well as high viscosity applications where flow and shear are required. These are not as power efficient as hydrofoils.

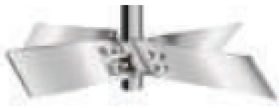

Fig 4d. Pitched bade turbine. [2]

- Curved blade and Flat blade turbines – This type of impeller is used in conditions where high shear is required in the fluid. It is most used in gas-liquid applications. Curved blade turbine (fig 4e (left)) is an improved version of flat blade turbine (fig 4e (right)). It uses lower power for same level of performance as a flat blade turbine.

Fig 4e. Curved blade turbine (left), Flat blade turbine (right). [2]

- Anchor – It is generally used in high viscosity applications. It is also used in case the material in the vessel tends to sick to the wall. It has three common types: Full anchor, Half anchor, and Baby Anchor. A baby anchor is used to mainly prevent heavy suspension particles to settle down in the bottom. The type of anchor shown in fig 4f is a full anchor.

Fig 4f. Anchor. [2]

- Spiral helix – Its finds application in processes where crystallisation takes place, or the material is highly viscous like in case of mixing clay with a dye. It is also used in processes where the material tends to stick to the wall.

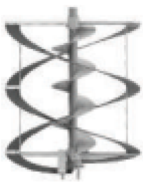

Fig 4g. Spiral helix impeller. [2]

Agitators:

As a reactor is a complete product made of the vessel, heating or elements and the agitator, the agitator is also a complete product. Many customers already have tanks and vessels installed at their site and they tend to repurpose these vessels for a new process once the old one gets obsolete. In such case there may be a need to redesign the agitator alone so that it is compatible with the new process.

Agitators are generally of three types: Top entry agitator, Bottom entry agitator and side entry agitator. The choice of which type of agitator is based on the customer and the process.

An agitator is a device made up of a motor, a gearbox, a shaft, and the impellers along with some other parts like bearings, seals, etc. In designing the agitator lot of factors need to be considered. First, type of impeller is selected based on the process. Each impeller has a different power consumption factor which affects the required motor power. Next, based on the dimensions of the vessel number of impellers is decided. It depends on the ratio of the diameter of the vessel to the Liquid level in the vessel. Then depending on the process, if there is a chance of suspended particles to settle down at the bottom, a Baby anchor or a kicker is provided which further increases the power requirement.

After deciding the type and number of impellers required its sweep diameter are decided for maximum performance which is usually kept at 50% the diameter of the vessel but is optimized by increasing or decreasing its diameter and checking for mixing characteristics and power consumption. The rotation speed also plays a big role in mixing and power consumption. The speed is also optimized along with the diameter based on the level of mixing required by the process.

Once the required speed and diameter are determined, the power requirement is calculated and accordingly a suitable motor is selected. As the motor speed are generally much higher than the required speed, a gearbox is also selected with a reduction ratio that gives the output speed as close to required speed as possible.

There are various types of gearbox types that are used namely, Inline helical, bevel helical and parallel helical. Out of these, inline helical is the most commonly used type. In case where there is space constraint on the top the vessel or to the side of the vessel in side entry agitator, a bevel helical or a parallel helical gearbox is used.

Next, the dimensions of the shaft are decided based on the power and torque from the motor and gearbox and the loads on it due to the impellers. The diameter of the shaft is calculated by using a program called lightning design suit which considers all the forces and bending moments on the shaft due to the movement of the impeller through the fluid and returns the required shaft diameter.

Based on the diameter of the shaft, the bearings and couplings are selected. Usually, the shaft is split into two sections, the driving side, and the driven side. The output shaft of the gearbox is connected to the driving shaft using a flexible coupling to reduce shocks, jerks, and slight misalignment. The driven shaft is connected to the drive shaft by a rigid coupling.

In some cases, where the shaft is too long or is running at high speed, the required diameter of the shaft is very large. This is because the shaft is generally supported at only one end as it is sufficient in most cases. If the shaft diameter is coming out to be too large with the conventional design, a support called steady bearing is provided at the bottom of the shaft. This helps support the shaft on both ends which reduces stresses on the shaft and we can use a lower diameter shaft.

Along with these a few other parts need to be selected like the seals and bearings. The bearings are selected based on the diameter of the shaft and a bearing housing is selected based on the bearing selected. Depending on the load either single or double bearing is selected. The seals are chosen based on the pressure required in the vessel for the process. For lower pressures single mechanical seal is chosen and for higher pressures a double mechanical seal may be used. In case the temperature inside the vessel is too high a coolant needs to be provided to seal face so that it does not break due to intense heat. This is done using a thermosyphon pot which circulates a coolant through a heat trap and keeps the seal face cool. When the process works at atmospheric pressure, a mechanical seal is not required, and a device called a stuffing box can be used so that there are no gaps around the shaft.

Power and flow calculations [3]:

In the design of an agitator for a vessel, power and flow calculations are extremely important as the design is optimized based on the power required. The power required by the impeller proportional to the density of fluid, cube of speed of rotation, fifth power of diameter of the impeller and number of impellers.

$$P \propto n^3 \times D^5 \times \rho \times i$$

We multiply a constant called power factor which is constant for each type of impeller.

$$P = N_p \times n^3 \times D^5 \times \rho \times i$$

N_p – power factor

n – speed of rotation (RPS)

D – diameter of impeller (m)

ρ – density of fluid (kg/m^3)

i – number of impellers

Flow rate is proportional to the speed of rotation, cube of the diameter of the impeller and number of impellers.

$$\text{Flow } (m^3/min) \propto N \times D^3 \times i$$

To get equation of flow we use the flow constant which is specific to each impeller type.

$$\text{Flow } (m^3/min) = N_q \times N \times D^3 \times i$$

N_q – flow factor

N – speed of rotation (RPM)

D – diameter of impeller (m)

i = number of impellers

Tip speed of the impeller also gives an indication of how well the fluid can get mixed. The tip speed is given by the following equation.

$$S_t = \pi \times D \times n$$

Higher tip speed usually means a higher level of mixing.

To achieve mixing, agitation, or suspension of particles in fluid, the fluid needs to be in a turbulent regime. To determine this, we use Reynolds number to determine how turbulent the flow in vessel is. It is given by the following formula.

$$N_{Re} = \frac{n \text{ x } D^2 \text{ x } \rho \text{ x i x } 1000}{\upsilon}$$

n – speed of rotation (RPS)

υ - viscosity (cp)

ρ – density (kg/m^3)

In order to achieve proper mixing highly turbulent conditions are required. A Reynolds number greater than 50000 is desirable. To further increase the turbulence, baffles are provided in the tank to break the flow and create turbulence.

All these metrics give us means to make the agitator more power efficient and achieve good mixing. The calculations for power and flow calculations are done using excel sheets as these calculations are simple and do not need specialized software's.

Shaft calculation [4]:

Shaft is designed by using ASME standard. Maximum of 1mm/m deflection is allowed in the shaft. The diameter of the required shaft can be found by using the following formula.

$$\theta = \frac{584 \text{ x T x L}}{\text{G x } d^4}$$

ɵ - shaft deflection (rad)

T – torque (Nm)

L – length of shaft (m)

G – modulus of rigidity

d – diameter of shaft

A software called Lightning design suite is used to determine shaft diameter precisely, but the above formula can also be used since it also gives highly accurate results.

Shell and end thickness calculation [5][6]:

Vessel shell and end thicknesses are calculated by the ASME standards. The following formulas are used.

$$\text{Shell thickness} = \frac{\text{Internal pressure x 0.0981 x Radius of tank}}{\text{Allowable Stress x Weld efficiency} - \text{0.6 x Internal pressure x 0.0981}}$$

Or

$$\frac{\text{External pressure x 0.0981 x Radius of tank}}{\text{Allowable Stress x Weld efficiency} - \text{0.6 x External pressure x 0.0981}}$$

Maximum of the two is chosen.

For ends the formula for varies for each type of end.

$$\text{Flat end} = \frac{\text{Pressure x 0.0981 x Radius of tank}}{\text{Allowable Stress x Weld efficiency} - \text{0.6 x Pressure x 0.0981}}$$

$$\text{Tori-spherical End} = \frac{\text{Pressure x 0.0981 x Radius of tank}}{\text{Allowable Stress x Weld efficiency} - \text{0.2 x Pressure x 0.0981}}$$

$$\text{Elliptical End} = \frac{\text{Pressure x 0.0981 x 0.9 x Radius of tank}}{\text{Allowable Stress x Weld efficiency} - \text{0.2 x Pressure x 0.0981}}$$

$$\text{Hemi-spherical head} = \frac{\text{Pressure x 0.0981 x Radius of tank}}{\text{2 x (Allowable Stress x Weld efficiency} - \text{0.2 x Pressure x 0.0981)}}$$

$$\text{Conical head} = \frac{\text{Pressure x 0.0981 x Radius of tank}}{\cos\left(\frac{\text{Cone angle}}{2}\right) \text{ x (Allowable Stress x Weld efficiency} - \text{0.2 x Pressure x 0.0981)}}$$

Just like in the case of shell thickness, we do the calculation for internal and external pressure and choose the higher value. The calculation of shell and ends is done using a software called PV elite which is an industry accepted software which also generates a report specifying all the intricate calculations and limitations of the design. It performs it calculations according to ASME standards and gives a report as advised by ASME. This report is submitted to the customer as a design validation.

Flange thickness calculation [7]:

Flange thickness is calculated according to ASME guidelines. Flanges are divided into various classes based on their pressure ratings. A class of flange is chosen and then the following formula is used for the calculation of flange thickness.

$$\text{Flange thickness} = \frac{1.5 \text{ x Flange class x Diameter of flange}}{2 \text{ x } 7000 - 1.2 \text{ x Flange class}}$$

For a particular class of flanges with a certain diameter other dimensions other than the thickness are mentioned in the ASME code and that is used to determine other dimensions like bolt size, bolt circle diameter, outer diameter etc.

Computational fluid dynamics:

CFD is tool that finds its application in a wide variety of industries from designing wings of an aircraft to checking the flow of fluids through pipes. In case of designing a reactor and an agitator it can be used for multiple reasons. In a reactor, various types of vessel ends can be used, and each type of end affects the flow pattern differently. For example, a flat end is opted because it is easy to install, can be moved easily and costs less whereas a cone end is used as it allows complete drainage of fluids in the and does not allow solid particles to settle easily [8].

Every type of impeller has different power requirements and different applications. Since the blades of the impellers are of different shapes, they create different flow patterns. For example, a cowl disc impeller is used to mix solid powders into viscous liquids and a pitched blade turbine is used to maintain a suspension of solids in liquids. In some cases, multiple types of impellers may be used for the same application. To find the required power we need the power number for the impellers. This power number needs to be found experimentally but, making prototypes and testing each case is expensive and can take a lot of time. Hence, by using CFD not only time and money are saved but also different designs can be tested easily.

Types of flows in a reactor:

Flows in a reactor are mainly of two types: Laminar and Turbulent. Although there are many types of flows found in nature, these two are the most commonly seen and used in a reactor.

In very high viscosity (>8000 cps) fluids like in resins, adhesives, paints etc. laminar flow is seen. For effective mixing in this condition impellers like anchor, spiral helix, and screw, intermig impellers etc. are used with a high impeller diameter to tank diameter ratio. The high ratio makes sure of proper mixing even when the speed of impeller is low (<80rpm).

In lower viscosity fluids we achieve good mixing by taking advantage of the turbulent flow. Impellers at medium (80-100 rpm) to high speeds (>100 rpm) create a turbulent flow in the fluid. This turbulence helps in thorough mixing of fluids.

Multiphase flow regimes [10]:

Multiphase flow regimes are divided mainly into four types:

1. Gas – liquid
   - Hydrogenation
2. Liquid – liquid
   - Water + methanol
3. Gas – solid
   - Fluidized bed
4. Liquid – solid
   - Slurry of calcium carbonate and water

Multiphase models:

1. VOF model [11] – The VOF model is used in case of mixture of immiscible fluids. It solves a single set of momentum equations and tracks volume fraction for each of the fluid in the domain. Eg. Motion of large bubbles in water.
2. Mixture model [12] – The mixture model is a simplified version of the multiphase model. It can be used to model flows where each phase has a different velocity but attains equilibrium in small areas in the mixture. It is used when a full multiphase model is not required. Eg. Mixture of oil and water.
3. Eulerian multiphase model [13] – It allows modelling of multiple phases that interact with each other. The phases can be gas, liquids, or solids in any combination. It solves

momentum and continuity equations for each phase. Eg. Suspension of solid particles in a solvent.

Geometry modelling and meshing:

Geometry can be modelled using any of the 3D/2D designing software and stored as a STEP file which can be opened in ansys. The inbuilt modeler in ansys called “Design Modeler” may also be used. The geometry used for CFD is somewhat different from the actual geometry. To make it easier and more accurate to mesh and solve the problem, the geometry is simplified by removing small curves, complicated intersections of parts, etc. This makes it easier for the meshing tool and the fluent solver to complete the calculation.

Meshing is done in the meshing tool within ansys itself. First a base mesh is created by the algorithm and then we can add enhancements to make the mesh uniform. The meshing tool uses one of two algorithms to create the mesh- 1) Patch confirming 2) Patch independent.

1) Patch confirming meshing: In this technique the algorithm all faces, and boundaries are respected. Small features are approximated based on the geometry around it. [14]
2) Patch independent: In this technique the algorithm ignores faces and boundaries unless there is some load or boundary condition acting. It is dependent on named selections, loads and boundary conditions. [14]

Once the base mesh is created various mesh control options can be used to refine the mesh further. Some of these options include changing method of meshing (Tetrahedral, hex dominant, cartesian etc), changing the size of elements in a particular region, changing the numbering of the nodes etc. once these changes are made the mesh is updated to fluent and then the CFD conditions can be set, and calculations are done.

Problem statement and objectives

Problem statement – Understand the user requirements and design a reactor based on the inputs from the customer and perform CFD analysis of critical designs.

1. Design a reactor based on customer's requirements using conventional methods.
2. Perform CFD analysis of critical application designs.

Methodology

Reactor design:

The design of reactor is to be done using conventional methods used by the company. This is done using the same tools as used by the employees. First, a customer sends a user requirement sheet which is studied, and critical aspects needed for the design are noted down.

Next the information is fed into an excel sheet for the design of the agitator as shown in fig 5. It takes data about type of impeller, speed of rotation, vessel dimensions, fluid properties etc. and gives the power requirement for the agitator.

Impeller type	Np	RPM	Diameter mm	Diameter2 in	Sp. Gravit	Viscosity facto	Proximity facto	Shaft power KW	Shaft power HP	No. of Im	Motor powe KW
PBT w/o fin	1.225	94	800	31.49606299	1	1	1	1.543532696	2.069877345	2	3.858831739
Kicker	1.15	94	800	31.49606299	1	1	1	1.449030694	1.943150161	1	1.811288367
	0	94		0	1	1	1	0	0		0
	0	94		0	1	1	1	0	0		0
							Total	2.99256339	4.013027505		5.670120107

Over desig
25

Motor Power KW	RPM	Torque Nm	Reduction require	Selected reductio	Actual RPN
15	1460	98.1092115	15.53191489	15.65	93.29073482

Flow Calculation

Impeller Type	Nq	RPM	Diameter (mm)	Sp. Gravity	Viscosity	No. of Imp	Flow (m3/min	Reynolds Numbe
PBT w/o fin	0.743	94	800	1	1	2	71.518208	2005333.333
Kicker	0.4	94	800	1	1	1	19.2512	1002666.667
0	0	94	0	1	1	0	0	0
0	0	94	0	1	1	0	0	0
						Total	90.769408	3008000

Tip speeds

Impeller type	Diameter (mm)	RPM	Tip speed
PBT w/o fin	800	94	3.937462792
Kicker	800	94	3.937462792
0	0	94	0
0	0	94	0

Tank Geometry

		L/D	1.181818182	Liquid level	305.1631331			
Diameter (mm)	2200	D/T	0.363636364	Z/T	0.138710515			
St. height (mm)	2600	Work vol/Act vol	0.03445836					
Beam height (mm)	1							
Top type	ASME	120	<- Cone angle					
Bottom type	ASME	120	<- Cone angle					
Top volume	Bottom volume	Working volume	Gross volume					
862.38152	862.38152	400	11608.21353	Jamming Factor	1			
Top height	Bottom height	Gap from bottom	Appx shaft height	Deflection	Shaft dia	Rigidity	Chosen dia	Actual Deflection
426.8	426.8	50	4404.6	4.4	88.99205526	70.3	90	4.206177405

Over design factor
0

Fig 5. Agitator design calculation sheet.

After this, using the software PV elite the shell thickness of the vessel is decided, shaft diameter is decided, and the costing is done accordingly. As shown in fig 6 many factors are taken into consideration like raw material cost, machining cost, transport cost etc.

Sr No	Particulars	Dia (mm)	St. Ht (mm)	Thk (mm)	MOC	Density	Rate (Rs/Kg)	Qty	Weight (Kg)	Cost
1	Shell	2200	2600	10	SS316L	8027	300	1	1455	4,36,446
2	Top-10% Torispherical	2520	2520	12	SS316L	8027	300	1	612	1,83,509
3	Bottom-10% Torispherical	2520	2520	12	SS316L	8027	300	1	612	1,83,509
4	Baffles	80	2600	10	SS316L	8027	300	4	67	20,035
5	BODY FLANGES								328	59,801
6	Limpet				SS304	8027			800	2,37,705
7	Nozzles				SS316L	8027				13,450
8	Nozzle Wt.						50		70	3,500
9	Handhole	MS + SS316L Lined							30	15,000
10	Agitator Mounting	MS + SS316L Lined	400	50			300	1	49	14,789
11	Internal-Polishing/External-Pickling						1000		35	35,449
12	Lug Supports				SS304		1573	4	63	6,293
13	Radiography	SPOT								5,000
14	Misc									5,000
									Cost	**12,19,487**
									Factor	**1.28**
									Price	**15,61,000**
									Agitator	**1,70,000**
									Total Price	**17,31,000**
									F.O.R	**20,77,200**

Limpet Coil		
Limpet OD	90.0	
Length of limpet/turn on shell	7616	
Limpet Height	1950	
Limpet Pitch	120	
No. of Turns	16.25	17.00
Total Length Of Limpet on Shell	129473	130
Total Length Of Limpet on Dish	44	46
Total Length of Limpet in meters	174	174
width of Limpet	0.141	0.141
Thickness	4	0.004
Limpet MOC	SS304	8027
Limpet Wt.	790	800
Limpet Raw Material Cost	175	140000
Limpet on Shell Cost	300	39000
Limpet On Dish Cost	600	27700
Total Limpet Cost		**237705**

BODY FLANGE						
Description	**MOC**	**Dimensions**	**QTY.**	**Wt**	**Rate**	**Cost**
Flat	IS:2062	3500 x 90 x 60	2	297	85	25222
Rolling/Welding/Straightening				297	20	5935
Liner/T&G	SS316L	3500 x 40 x 14	2	31	300	9440
Machining/Drilling/Fitting to Shell				328	25	8205
Gasket			1		5000	5000
Hardware			30		200	6000
					Total	**59801**

Lug Support					
Particulars	MOC	Size	Wt	Rate	Cost
RF Pad	SS304	250X200X6	2	100	241
Base Plate	IS:2062	250x200x14	6	100	562
Vertical Gusset	IS:2062	200x200x12	8	100	771
				Total	**1573**

Fig 6. Costing sheet.

Once the customer approves the design and agrees on the quoted price, detailed design of the vessel is done using AutoCAD as shown in fig 7 and bought out parts are ordered.

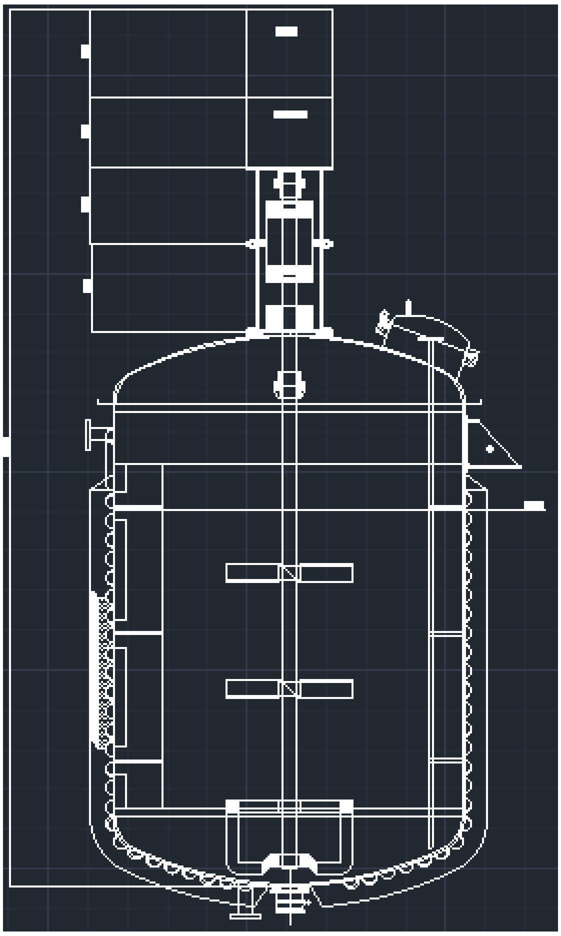

Fig 7. CAD General Arrangement drawing.

After this the manufacturing and quality control teams manufacture the reactor and dispatch it to the customer. The reactor is then installed at the customers site under the supervision of a quality control team member and the reactor is commissioned into service.

CFD analysis:

For the second part of the problem, the existing design is modeled in 3D using SolidWorks. The geometry is a simplified version of the actual geometry. The geometry is simplified to make it easier for the program to solve the problem. Very minute parts, complicated intersections between components etc. are neglected or merged with the larger geometry. This approximation does not change the results in any way as these have insignificant effect to the flow. In fact, by removing these features it helps the program to give more accurate results.

In the geometry of a reactor, first the vessel geometry is drawn and then rotated to form a solid body. Next with reference to the main vessel body, impellers are modelled by creating reference planes at specified distances from the origin. The “Merge” option is deselected so that the impellers are formed as a separate body from the vessel. To use the impeller body to interact with the fluids in CFD we need them to rotate and cause a disturbance in the fluid. To do this we need to create a rotating zone around the impeller. This is also formed as a separate body from vessel and impellers.

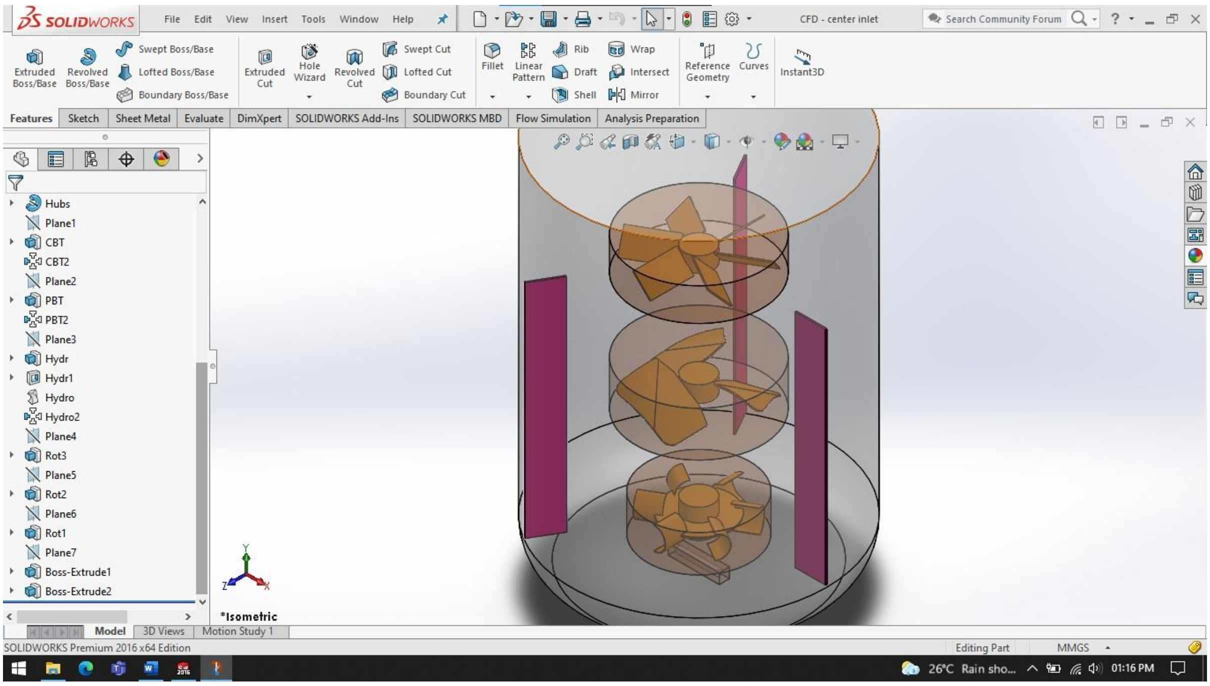

Fig 8. 3D Cad model of a hydrogenator in SolidWorks.

Once the model is created in SolidWorks, it is exported as a STEP file so that it can be read by ansys. In ansys, the geometry is opened in Design Modeler to make it relevant for CFD analysis. In Design Modeler, using the option of creating “Booleans”, the rotating zones are subtracted from the vessel body, but the geometry is retained. Next, the impeller bodies are subtracted from the rotating zones, but their geometry is not retained and hence a void is left in the geometry. This void is important because this is how the software knows where the fluid cannot flow through and the rotation of this void through the fluid causes disturbance in the fluid simulating the movement of the impeller.

The geometry is brought into the meshing tool and a base mesh is created. The automatic method of meshing is set to CFD so that the software itself creates a geometry that is suitable for CFD analysis. Since the latest version of ansys is being used (ansys 2020R student version) the base mesh generated is already of good quality, but a few changes are made to improve the mesh like changing the element size in the rotating zone as this area has more effect to the fluid. Overall element sizes are adjusted to reduce the number of elements but keep the mesh relevant so that computation time is reduced, and the correct solution is achieved more efficiently.

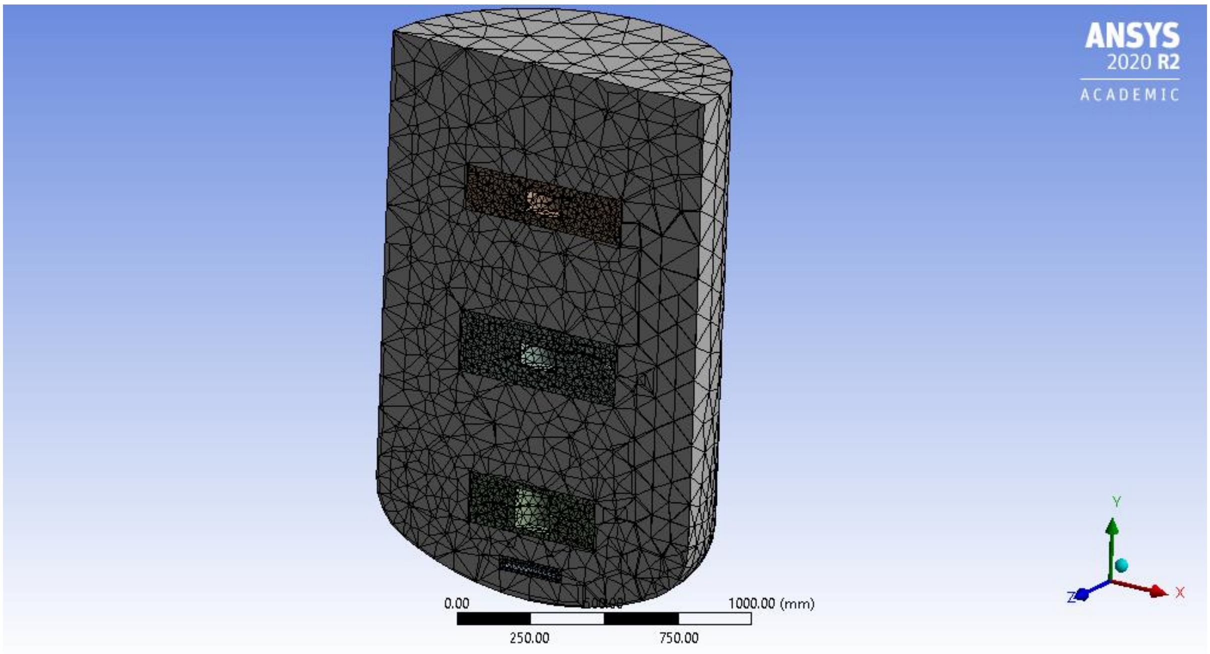

Fig 9. Mesh for hydrogenator model.

The mesh is transferred to fluent to perform CFD analysis. In fluent, the mesh is further refined by the fluent algorithm to make it even more efficient to solve. The option used to do this is called “Make polyhedral”. This converts the mesh elements to polyhedral elements by merging some elements. This significantly reduces the number of elements and consequently the computation time. After this, the physics for CFD are setup.

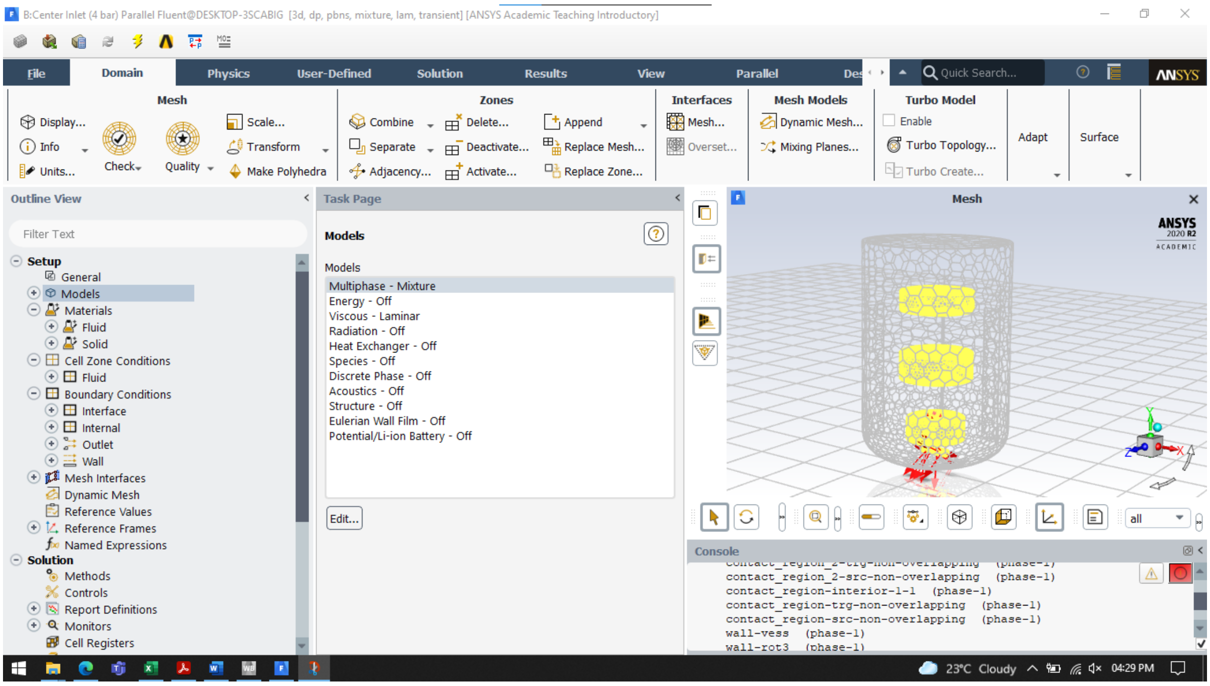

Fig 10. Fluent setup for hydrogenator.

First, transient state solution is selected as we do not know when the system will reach steady state. An approximate time is chosen in which the system is expected to reach steady state and used to model the transient solution. The value of gravity is set to 9.81 m/s^2 and operating pressure is set based on the conditions in the reactor vessel. After this, the material properties are defined for each entity in the mixture. Multiphase model is selected based on the criteria mentioned in the literature review [11,12,13] and viscosity model is also selected. To select the viscosity model as laminar or turbulent, we find the value of Reynold's number (N_{re} < 4000 – Laminar, N_{re} > 4000 – Turbulent). Based on the value of the Reynold's number the appropriate viscosity model is chosen.

The rotation of the impellers is set under the "cell zone conditions" by specifying the rpm of rotation. This speed is decided during the initial design phase of the reactor and can be tweaked based on the results obtained. In some cases, there is an inlet of some gas like in the case of a hydrogenator. In such a situation under "boundary conditions" section, a gas inlet is modeled and either constant pressure or constant velocity inlet is selected. The location of the inlet is defined during the geometry modelling stage.

Once the setup is complete, the solution conditions need to be specified. This includes initializing the problem with the conditions like the volume fraction of each phase in the vessel, initial pressure and a region is defined to specify the height up to which the fluid is filled. Next, the number of timesteps is chosen based on how large each timestep is and what is the expected time to achieve steady state. The "Calculate" button is clicked to start the calculation.

$$\text{Number of timesteps} = \frac{\text{Expected steady state time}}{\text{Timestep size}}$$

After the calculation is completed, it is updated in CFD-Post, which is a software that interprets the solution and gives required information. Many types of 2D and 3D graphs can be plotted to visualize the flow parameters like fluid velocity, volume fraction distribution, particle streamlines etc. Power, Torque, particle velocities etc. can also be calculated in tabular format. A video is also be generated showing the timely progress of any parameter so that it can be used to visualize the how the fluid will flow.

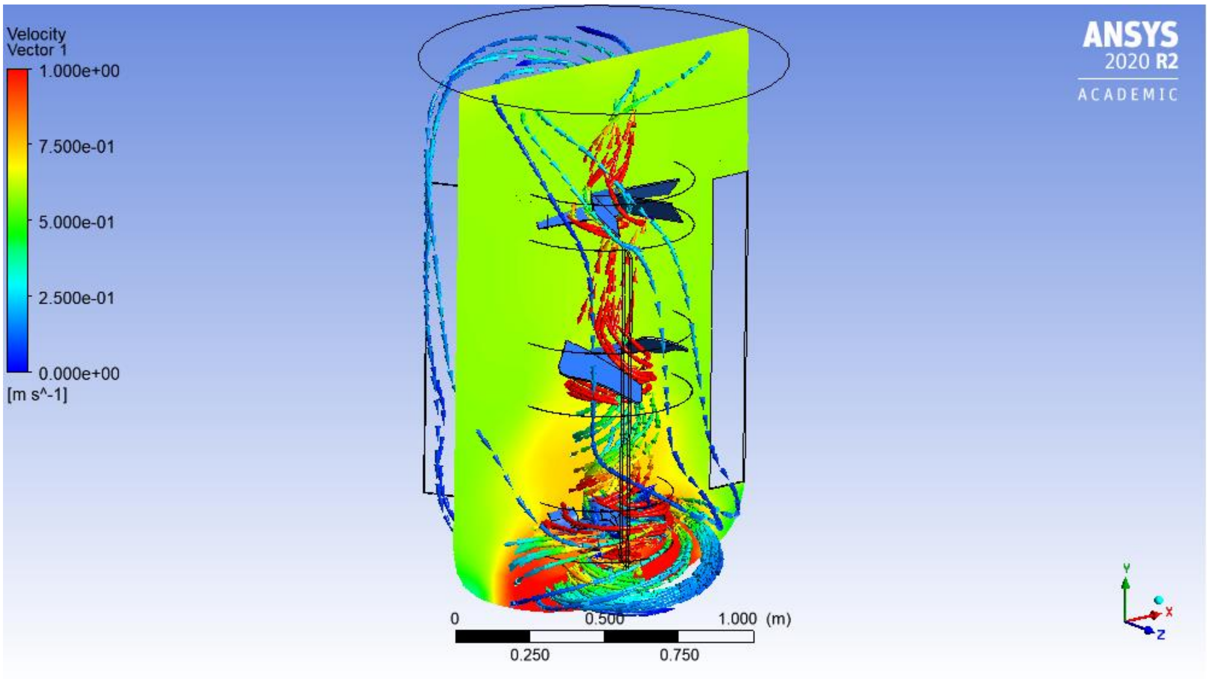

Fig 11. Volume fraction distribution and streamlines of H2 gas in the vessel.

Verification study:

As a study to verify if the methodology is correct, a simple study to compare power number vs Reynolds number graph with actual results is conducted. A 3D model of a single 4-bladed pitched blade turbine impeller and a simple vessel with baffles is created in SolidWorks and imported into ansys-fluent. The physics of the experiment are setup to rotate the impeller in water at certain velocity so that it achieves laminar, transient, and turbulent flow characteristics. Power and flow number for each condition is calculated using the CFD-post software and a graph is plot using Microsoft excel.

The simulation is run at the RPMs in Fig 13. to achieve the desired flow regime. Torque and mass flow at the impeller is calculated using the CFD-post software and power number and flow number is calculated using excel sheet. Next, the Np vs Reynolds number and Nq vs Reynolds number graph is generated and compared with the experimental graphs.

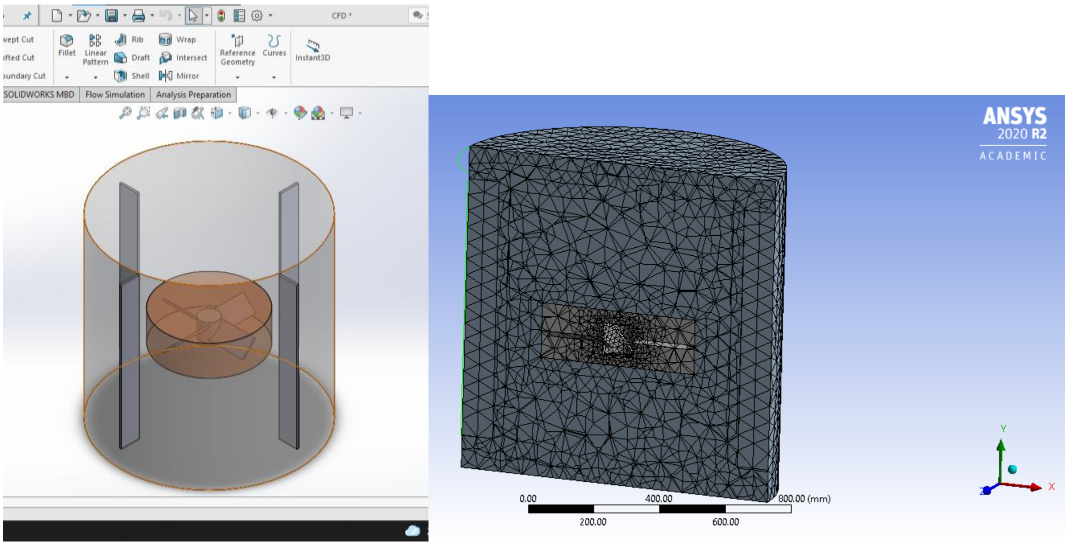

Fig 12. 3D Cad model and mesh for verification study.

Reynolds no.	RPM	Torque(Nm)	Power(kW)	Np	Mass flow(kg/s)	Nq
1	0	0	0	5000	0	0.00001
10	0.0024	8.75E-08	2.19911E-14	18.62110161	8.77E-06	6.69E-01
15	0.0036	7.098E-08	2.67588E-14	6.713527832	1.01E-05	0.512868973
20	0.0048	7.438E-08	3.73875E-14	3.957250107	5.33E-06	0.203174821
40	0.0096	2.131E-07	2.14231E-13	2.83439768	9.52E-06	0.181287342
100	0.024	0.000001179	2.96315E-12	2.509060434	7.04E-05	0.53654321
1000	0.24	0.00009518	2.39213E-09	2.02555023	0.00212713	1.621041
10000	2.4	0.009015	2.26572E-06	1.918505497	0.0163364	1.244962658
100000	24	0.9072	0.002280042	1.930635815	0.136196	1.037921049
1000000	240	91.01	2.287330779	1.93680738	1.273	0.970126505
	Tank dim					
	height	1000	mm			
	dia	1000	mm	sweep dia	0.45	m
				no of imp	1	
	Density	1000	kg/m3			
	viscosity	1	cps			

Fig 13. Verification study condition and results.

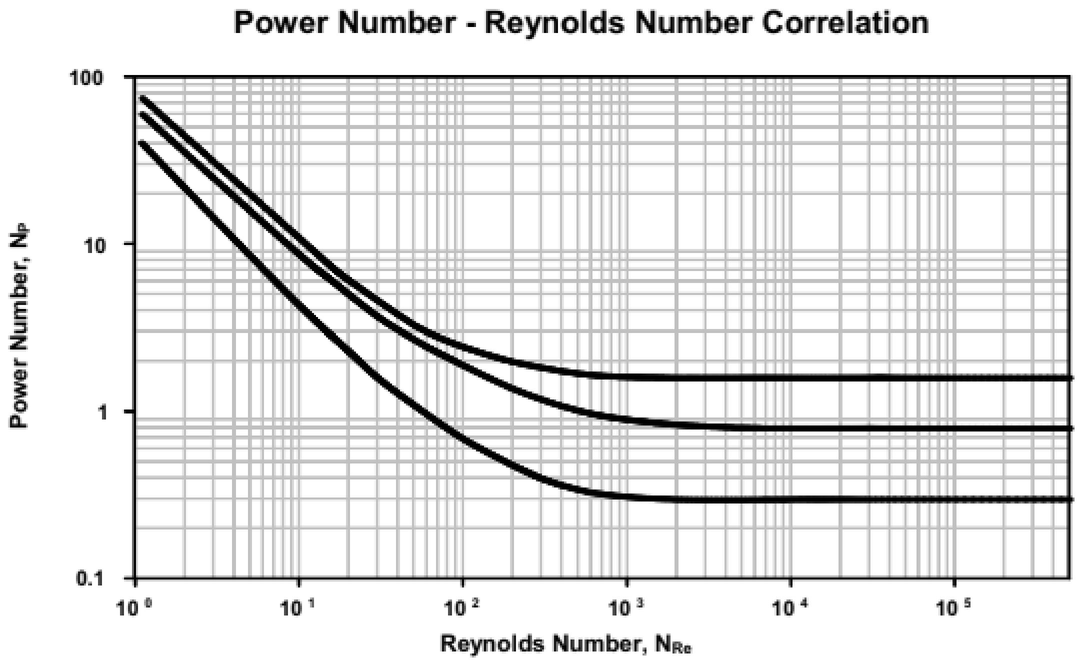

Fig 14. Power number vs Reynold's number experimental graph. [15]

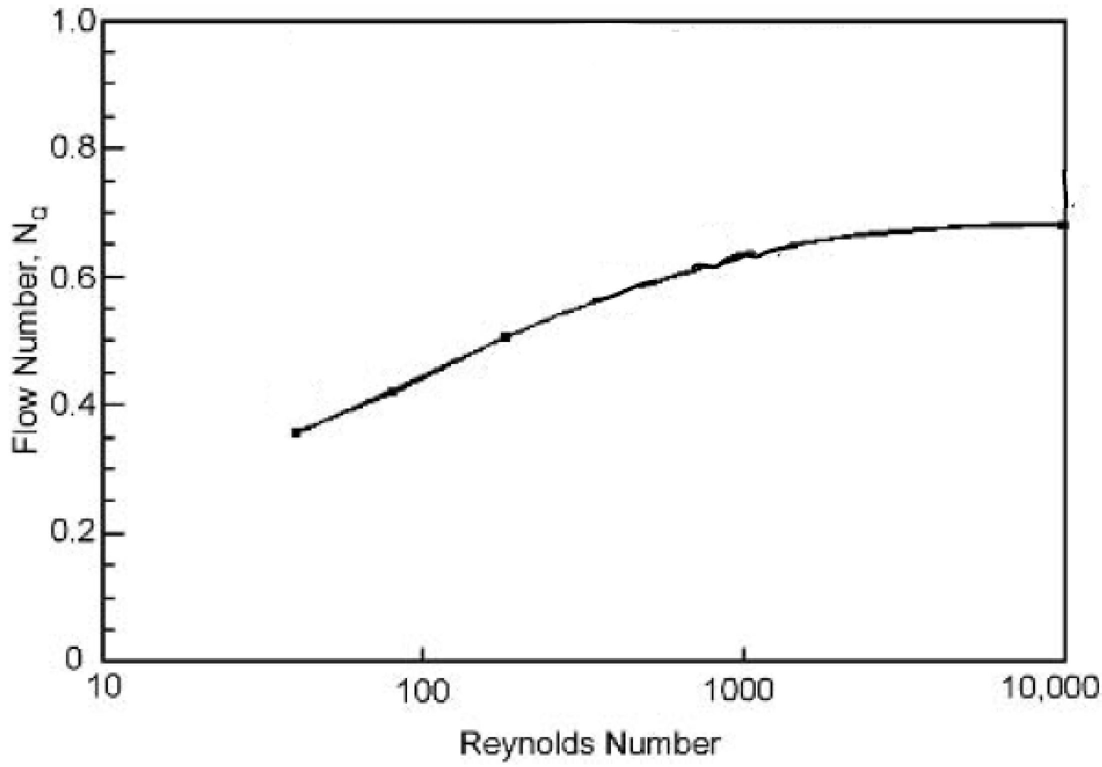

Fig 15. Flow number vs Reynold's number experimental graph. [16]

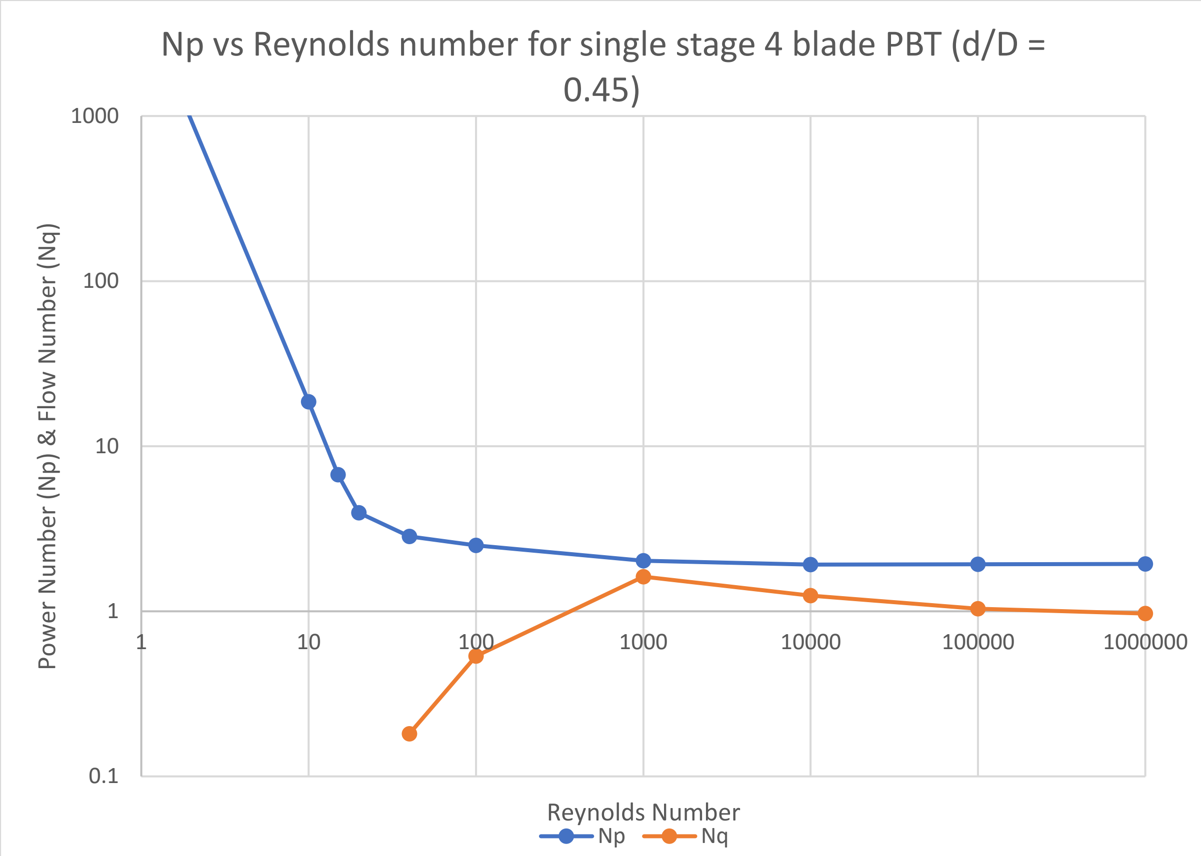

Fig 16. Power number and Flow number vs Reynold's number simulation graph.

After the verification study, the focus of the CFD analysis was on the design of hydrogenators. Various combinations and configurations of type and placement of impellers are analyzed. Mixing patterns and distribution of hydrogen in the fluid are studied to compare different configurations of the impellers.

	2KL side inlet				2KL bottom inlet				50KL bottom + middle inlet		
	CBT 6bld	PBT 6bld	AA405		CBT 6bld	PBT 6bld	AA405		CBT 6bld	CBT 6bld	CBT 6bld
no of imp	1	1	1		1	1	1		1	1	1
density (Kg/m^3)	1000	1000	1000		1000	1000	1000		1000	1000	1000
speed (RPM)	178	178	178		178	178	178		145	145	145
torque (Nm)	92.72	144.3	129.9		85.18	154.6	161.6		755.7	785.9	860.6
power (kW)	1.728312	2.689769	2.421351		1.587765	2.881762	3.012243		11.47482	11.93339	13.06766
dia (m)	0.44	0.565	0.565		0.44	0.565	0.565		0.924	0.924	0.924
np	4.013769	1.789231	1.61068		3.687369	1.916945	2.003741		1.20708	1.255318	1.374636

Fig 17. Power calculations for various hydrogenators.

Reactor capacity	Gas inlet type	Impellers used	RPM	Total power required (kW)
2 KL	Bottom-side	CBT (6 blade), AA405, PBT (6 blade)	178	6.839431514
2 KL	Bottom-center	CBT (6 blade), AA405, PBT (6 blade)	178	7.481769925
50KL	Bottom center and middle rotating	3 PBT (6 blade)	145	36.47588038

Fig 18. Power comparison for various hydrogenators.

Results obtained / expected.

1. In the first part of the project, a reactor is successfully designed and manufactured based on the customer requirements. The manufacturing quality is monitored throughout the process.
2. In the second part of the project, the methodology is verified by comparing the Np vs Reynolds number and Nq vs Reynolds number graphs from the simulation to the experimental graphs. This proved that the steps taken in setting up the simulation are correct and can be applied in simulating other designs.

   The same methodology is applied in simulating hydrogenator designs to visualize the flow and gas distribution patterns in the vessel by using different types of Impellers. The effects of these changes are documented for future reference.

Conclusion

Designing and manufacturing a reactor that meets the customers' requirements as closely as possible is a complex task involving many people. From the start of an order till the end there are many small details that need to be taken care of to produce an acceptable product.

Learning to do one task like designing an agitator requires the knowledge of all other tasks that go in the designing and manufacturing of the product. Each element of a reactor needs to comply with other elements and parts of the reactor so that the entire system performs to its maximum potential.

Furthermore, performing a CFD analysis on the existing and new designs is a very complex task. The first part of the project was a crucial step in performing the second part of the project successfully. The type of impeller used makes a huge difference in performance and cost of running the equipment hence it is important to know the pros and cons of each type of impeller so that correct impeller for a given task is chosen and new designs are explored to improve the performance.

Future work

Future scope of performing successful CFD simulations is developing new innovative solutions for mixing requirements. These new designs will be more efficient in terms of performance and cost. Performing the analysis by changing the type of impellers, position of gas inlets, changing the inlet pressure etc. help in improving the designs by allowing quick testing of multiple configurations. Developing new impeller shapes to achieve better mixing at lower power and less mixing times which improve batch times and batch quality to maximize customer's production efficiency.

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