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FEA and Optimization of Catalyst Bed Reactor Vessel

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ABSTRACT: ACatalyst Bed Reactor (CBR) is a reactor compartment incorporated in a pressure vessel that can be used to carry out a variety of multiphase chemical reactions. In this type of reactor, a fluid (gas or liquid) is passed through a granular solid material (usually a catalyst possibly shaped as tiny spheres) at high enough velocities to suspend the solid and cause it to behave as though it were a fluid. Catalyst bed is a popular technique to speed up chemical processes. However current designs of a bed are stagnant designs where the chemical reaction occurs while the fluid is stationary, as if in a storage vessel. This process is time expensive and hence there is need of speeding up the process in which the fluid flow is present. This can be achieved in a reactor vessel where the Catalyst bed is embedded in the design. This design has its own challenges. When the reaction takes place, some quantity of the catalyst stagnates, and this stagnation has to be removed, which is done using inclined nozzles. These inclined nozzles are a design headache as they create a lot of stress zones. Thus, our objective is to find out the best solution out for this problem so as to enhance the process and to get the best results while performing actual analysis for the vessel under consideration.

KEYWORDS: Pressure vessels, Nozzles, Reactor vessel, FEA, Optimization, Stress distribution, Stress concentration, Stress concentration, Equivalent Von Mises stresses.

I. INTRODUCTION

A. Pressure vessel

A pressure vessel is a closed container designed to hold gases or liquids at a pressure substantially different from the ambient pressure. Pressure vessels are used in a variety of applications. These include the industry and the private sector. They appear in these sectors respectively as industrial compressed air receivers and domestic hot water storage tanks, other examples of pressure vessels are diving cylinder, recompression chamber, distillation towers, autoclaves and many other vessels in mining or oil refineries and petrochemical plants, nuclear reactor vessel, habitat of a space ship, habitat of a submarine, pneumatic reservoir, hydraulic reservoir under pressure, road vehicle airbrake reservoir and storage vessels for liquefied gases such as ammonia, chlorine, propane, butane and LPG [1].



B. Nozzle

Figure 1: Pressure vessels [2]

In pressure vessels, nozzles are required for inlet and outlet of fluid. Pressure vessels find wide applications in thermal and nuclear power plants, process and chemical industries, in space and ocean depths, and fluid supply systems in industries. Due to practical requirements, pressure vessels are often equipped with nozzles of various shapes, sizes and positions, at various angles.



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Figure 2: Nozzles welded cylindrical pressure vessel (Cross section) [3]

A nozzle is a cylindrical component that penetrates the shell or heads of a pressure vessel. The nozzle ends are usually flanged to allow for the necessary connections and to permit easy disassembly for maintenance or access. However sometimes process requirements dictate that some nozzles be placed on the periphery of the pressure vessel [4].



Figure 3: Pressure vessel model with nozzles on the periphery [5]



Figure 4: Section of Reactor pressure vessel with a protruding nozzle [6]

Nozzle is a part designed to control the direction or characteristics of fluid (especially to increase velocity) as it exits (or enters) an enclosed chamber or pipe. Under different loading conditions, the stress will occur at the nozzle to head or shell junction area. Thus reliable and accurate design calculation for head or shell to nozzle junction is necessary. The calculation for nozzle design gives the information whether the design is adequate for givenparameters. The figures below shows various types of nozzle geometries incorporated on the vessel. Two types of intersecting structures, distinguished by flush and protruding nozzles. It is shown that the design with a protruding nozzle would produce a better stress distribution than the design with a flush nozzle [7]



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Figure 5: Section of pressure vessels with a flush and a protruding nozzle [7]

When the head is provided with a nozzle, the stress in the head/nozzle connection remains high and may be reduced with the help of other means. The zone of the head/nozzle connection is subject to disturbance of the membrane stress state existing in the vessel. In the case of symmetrical location of the nozzle, i.e. when the vessel axis and nozzle axis are identical, the stress distribution may be determined analytically (Magnucki, 1998). Otherwise, when both symmetry axes are shifted one with respect to another, the analytical approach would be extremely difficult [8].



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Figure 6: Pressure vessel with head and protruding nozzle [8]

C. Catalyst Bed Reactor

The reactor pressure vessel (RPV) is the central and the most important component of the pressurized reactor vessels since it contains mechanisms at high temperature and under high pressure. Almost all industrial pressure vessels including the RPV have openings, nozzles and other attachments which produce geometric discontinuities in them. The effect of stress concentration because of geometric discontinuities is one of the basic considerations in the design of pressure vessels. These geometric discontinuities alter the stress distributions in the localized area [9].

A Catalyst Bed Reactor (CBR) is a type of reactor device that can be used to carry out a variety of multiphase chemical reactions. Catalyst bed is a popular technique to speed up chemical processes. However current designs of a bed are stagnant designs where the chemical reaction occurs while the fluid is stationary, as if in a storage vessel. This process is time expensive and hence there is need of speeding up the process in which the fluid flow is present. This can be achieved in a reactor vessel where the catalyst bed is embedded in the design. As the reaction takes place, some quantity of the catalyst stagnates, and this stagnation has to be removed, which is done using inclined nozzles. In this subject, these inclined nozzles are of primary interest for their locations in the vessel as we have to look after the symmetry and stresses generated in the vessel because of them.

II. PROBLEM STATEMENT

Catalyst bed reactors are mostly used to speed up the chemical processes. But if the designs of bed are stagnant designs then fluid becomes stationery and it results in slowing down the chemical reaction, which usually occurs in storage vessel. While going through all the paper listed above, it was found that there was no such design till date which will avoid the slowing down of the chemical reaction of the reactor vessel and enhance or speed up the chemical reaction happening inside of the vessel. Thus there is need of speeding up this process which can be achieved in a in a reactor



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vessel where our catalyst bed is embedded in the design. This bed has inclined nozzles which are our primary interest and these are design difficulties as they create a lot of stress zones and may disturb the symmetry of the vessels too.



Figure 7: Ellipsoidal head & nozzle shell intersection (Unsymmetrical geometry) [10]

III.METHODOLOGY

The route below shown defines the methodology with help of flow chart as shown



IV.FINITE ELEMENT ANALYSIS

Finite element analysis (FEA) is a fairly recent discipline crossing the boundaries of Mathematics, physics, engineering, and computer science. The method has wide application and enjoys extensive utilization in the structural, thermal and fluid analysis areas. Finite element analysis (FEA) is a computer based numerical technique for calculating the strength and behaviour of engineering structure. It can be used to calculate deflection, stress, vibration, buckling behaviour and many other phenomena [13]. It also can be uses to analyse either a small or large scale deflection under or applies displacement. It uses a numerical technique called the finite element analysis method (FEA). In finite element method, the actual continuum is represented by the finite element. These elements are considered to be joined at specified joints called nodes or nodal solution. As the actual variation of the field variables (like displacement, temperature and



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pressure or velocity) inside the continuum is not known, the variation of the field inside a finite element is approximately by a simple function. The approximating functions are also called as interpolation models and are defined in terms of field variables at nodes.

When the equilibrium equations for the whole continuum are known, the unknowns will be the nodal values of the field variable. In this dissertation work finite element analysis was carried out using FEA software ANSYS.

The finite element method is comprised of three major phases

- 1. Preprocessing
- 2. Solution
- 3. Post processing

V. MODEL SELECTION AND FEA OF CATALYST BED REACTOR VESSEL

A. Modelling

The first step of pre-processing is to generate the 3-D model of the given component which is compatible to import in the solver. The 3-D model of the Pressure vessel is created in Ansys 15 work bench using the calculated dimensions and using some input given by the company. The model of vertical pressure vessel was created in first step. The vessels is not able to sustain the horizontal wind load of 41 km/hr and hence it was suggested to lay the vessel in horizontal position. Therefore, as per the recommendation we need to incorporate the saddles for the horizontal support. Saddles are provided to lay the pressure vessel in horizontal position, since pressure vessel was unable to withstand the horizontal wind loads and the generated equivalent stress and the deformation were more than the allowable values.

The next step involved with the horizontal pressure vessel was to design the saddle supports for the vessel. Looking at the large height (now length) of the vessel 3 saddles were recommended to support the vessel [24]. The saddles were designed are now working as supports.

Now we can further proceed with the analysis of the vessel.



Figure 8: Pressure vessel with nonzero frequency (Valid model)

Figure 8 shows the deformation of the model at the true scale. Nonzero frequency makes it sure that the model is valid and hence, we can proceed with the further analysis for the project. The red zone in middle is showing higher values of deformation due to temperature 200°C at which the catalyst bed reactor will be under operation. So, reducing this deformation to normal and uniform values comparable to other sections of the vessel will be point of interest.

Thus, we need to locate the area of the catalyst bed reactor vessel. The greenish area shown in the middle of the vessel below reflect our catalyst bed area. It is imparted a temperature of 200°c to match the exact environmental conditions of the actual catalyst bed reactor area.



Figure 9: Pressure vessel model with Catalyst bed reactor section



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Figure 9 is the final model showing the position of the nozzles and a general structure of the vessel. Out of three sections, the middle section will be taking care of the Catalytic bed reactor. The inclined nozzles will inject the fluid at a velocity which will be different from the velocity of the fluid coming from the nozzle located on the ellipsoidal head. Nodes generated are 33987, the sizing kept for meshing the whole model was 100 mm.



Figure 10: Meshing at nozzles

Snaps above depicts the mesh generated near the nozzle geometry.

The boundary conditions applied are listed below

1. Pressure= -396320 Pa on all the surfaces of the vessel. (Represented with red arrows in first snap) the negative sign shows that the pressure is applied from inside in outward direction. The red vessel indicates the pressure applied onto the vessel. The arrows are seen inward from the vessel surface implies the pressure acting inward.



Figure 11: Vessel with pressure acting outward

2. Standard Earth gravity is applied and represented with the yellow arrow in snaps below and this will count the force due to weight of the vessel.



Figure 12: Vessel showing Earth gravity in downward direction

3. The saddle support bases are kept as fixed supports.

4. The edges of all the nozzles are also kept as fixed supports.

B. Meshing

A generalized meshing is shown in the below snap. The image shows the section of the pressure vessel including the cut section of the nozzle.

The meshing is done with mesh size of 100 mm for cylinder and the saddle supports. The mesh is not over fined.



Figure 13: Meshing of the vessel (body sizing 100 mm)

Also, the Map faced meshing is done at the reinforcement pads for removing non regularity in meshing which affects the end results. The mesh type is Quadrilateral-mesh. Fine mesh is done to get the accurate values of stresses in those regions. This can be viewed in Figure 13, (Nodes- 33987 & Elements- 32947). The material used for pressure vessel is SA 516 Grade 70 (Carbon steel plate) is shown in Table 1.



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rable 1. Final material description	
Description	Values
Material	SA 516 Grade 70
Poisson's ratio	0.29
Allowable stress	137.8951 MPa

Table 1: Final material description

C. Dead weight loading conditions

After the validation of the vessel, the next step was to analyze the vessel with dead weight loading conditions. The load by acceleration due to gravity is applied to find the total deformation and equivalent Von Mises stresses. As shown in above figure, the standard earth gravity 9806.6 mm/s2 is applied downward. The fixed support is given to the middle saddle and the end saddle supports were imparted displacements. Nozzles were kept free. No other force or pressure was applied from inside or outside and no thermal conditions were considered for the dead weight loading. The thickness of the vessel was kept 12 mm and the analysis was carried out.



Figure 14: Dead weight loading (DWL) conditions

It is clearly seen in the above image, standard Earth gravity (A) is acting downward on the vessel i.e. weight of the vessel. After applying the above inputs, the results for Equivalent Von Mises stresses and deformation were noted. The following images were taken to capture the results generated. As per the static structural dead weight analysis shown in figure 15 and figure 16, the deformation and equivalent stress of 9.0653 mm and 126.46 MPa were found respectively. The equivalent stress obtained is less than the allowable stress which is 137.8 MPa and thus the design is safe. But, sometimes the stress Concentration is one of the important factors to be studied in the pressure vessels openings, and nozzles are the openings in our case and needs to be taken care of [15].



Figure 16: Total deformation for DWL conditions

Till now we have finalized the model and we are ready to proceed with the further analysis of the vessel with 12 mm thickness. In the next chapter, total 8 cases will be analyzed, 4 cases will be studied with the nozzles fixed as we have done in dead weight loading. In next 4 cases, nozzles will be kept free and results will be studied. We are actually looking for the stable model in terms of stresses and deformation having minimum localized stresses while the model is under the boundary conditions and this is our basic goal from this project. The critical zones are nozzle to vessel intersections because the stresses generated in those areas are much higher than the other areas of the vessel.

Till now we have finalized our model and its requirements to meet our requirements. We made it horizontal, added the saddle supports and came to the conclusion that we can proceed further for the analysis and it is now ready to study under our boundary conditions. Hence, in this chapter, we will be dealing with final analysis of the completely defined



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model while applying the boundary conditions. We will check the results we are getting from all the cases of the analysis process. If the results are satisfactory then we can proceed further for the conclusions. But if the results are poor as far as the stresses generated and the deformation is concerned, then we have to think of modification and optimization to the model.

D. Boundary Conditions

The boundary conditions applied to the model are

- 1. A pressure of 0.39632 MPa is applied to all internal surfaces of the pressurized section.
- 2. Acceleration due to gravity 9810 mm/s² is applied.
- 3. The temperature applied on the catalyst bed reactor section of the pressure vessel is 200°C.
- 4. The middle saddle is fixed and displacement is given to end saddles.
- 5. The thickness of the vessel kept is 12 mm per the ASME section calculations.
- 6. All the nozzles are considered fixed for first four cases and then followed by free nozzles cases.

Our main focus for this analysis was to check the reports for the vessel and check the stability of the vessel in terms of stresses and deformation. Thus, the Equivalent Von Mises stresses and the deformation will be of the prime importance. If those are within the allowable values we can proceed with the nonlinear analysis and final conclusion for this model. But if it is not the case then we have to change the parameters of this model to get the required results and stabilize the model in terms of stresses and deformation.

E. Analysis Phase

The analysis will deliver eight results for 12 mm thickness with linear method. First four will be for fixed nozzles and the next four will cover the free nozzles analysis reports. If the results are within the allowable stress values, then we can proceed for the nonlinear analysis otherwise we will go for thickness optimization in the next chapter and again will repeat the procedure until we find the stabilized vessel in terms of stresses and deformation.

Listed below are the inputs for the first four cases and their results with required snaps showing the deformation (DMX) and Equivalent Von Mises stresses values. These four results are found for fixed nozzle and the vessel is supported on the middle saddle.

Analysis done for 12 mm thickness with nozzles fixed and results reported as below

a] Temperature 200 degrees Celsius, Force 2000N

Body sizing 40 mm, Thickness 12 mm for all components, Number of nodes 206871, elements 204896



Equivalent Von Mises stresses = 4306.5 MPa



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The above case shows the results are much above the allowable values of stress and deformation. The red zone is the indication for unstable zone of the vessel in terms of stresses and deformation. In the stress analysis image we can see that surface around the nozzles are more prone to higher values of stresses and thus the references we studied are going parallel with our analysis. The stresses are more concentrated near the nozzle and vessel junctions. As far as the values of stresses and deformation are concerned, it can be declared to be a failure and we need to study next results of fixed nozzles and free nozzles.

b] Body sizing 55 mm

Number of nodes 109921, elements 108233



Figure 20: EVMS 2

Equivalent Von Mises stresses = 3926.9 MPa

By changing the body sizing we are reducing the number of nodes from 2 lacs to 1, 10,000 thousand and keeping the other boundary conditions as it is we will note the results. The maximum equivalent Von Mises stress found to be somewhat lesser than the previous case, but still the results are unacceptable as the allowable stress is much lower value than what we are getting.

c] Body sizing 60 mm

Number of nodes 92384, elements 90865



Figure 22: EVMS 3 Equivalent Von Mises stresses = 3956.9 MPa



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The next optimization is done with further reducing the body sizing i.e. node numbers to around 90,000. No appreciable change in stress value is noticed and stress value is same as the previous case. d] Body sizing 85 mm

Number of nodes 46914, Elements 45773



Figure 24: EVMS 4 Equivalent Von Mises stress = 4442.4 MPa

Looking at the final optimization of the fixed nozzle case, the values are much beyond the allowable values and we will run the optimization cases for free nozzle cases. In the 4th case, we can see that the stresses are getting uniform but the value cannot be entertained and hence we will move forward to our next cases of analysis.

Analysis done for 12 mm thickness with nozzles free and results reported as below

Listed below are the inputs for the next four cases of free nozzles. All the inputs will be the same as above with the only difference being the nozzles released free which means that the nozzles are free to have infinitesimal small movement in any direction. Their results with required snaps showing the deformation (DMX) and Equivalent Von Mises stresses values. Analysis results are found for free nozzles. All nozzles are free and the vessel is supported only on the middle saddle.

a] Temperature 200 degrees Celsius, Force 2000N, Thickness 12 mm for all components, Body sizing 40 mm, Number of nodes 206871, Elements 204896



Figure 26: EVMS 5



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Equivalent Von Mises stresses = 531.68 MPa

In the first case of free nozzles having 2 lacs of nodes, we can see the stress generated came down to 531.68 MPa which is very good improvement as far as the stresses are concerned. Again, uniform stress distribution is a noticeable change noted and a positive response. The deformation is still having a large value which is not acceptable. The maximum stress concentration found is near the nozzle-vessel junction and also near the saddle-vessel junction. Thus, the path of the results are going the right way but need to be taken care of.



Equivalent Von Mises stresses = 530.47 MPa

The results obtained are for body sizing 55 mm i.e. around 1 10,000 nodes. Not much variation is seen when we compare this case with the previous case of 2, 00,000 nodes. Deformation is slightly increased by 1 mm but the stress is reduced by 1 MPa. Next cases should analyzed for stresses and deformation.

c] Body sizing 60 mm, Number of nodes 92384, elements 90865



Figure 30: EVMS 7 Equivalent Von Mises stresses = 522.56 MPa

The stress is reduced again by around 8 MPa for 92000 nodes and deformation is also reduced by 8 mm. The area of concern are the junctions of nozzle and vessel. The remaining area shows the uniform stress distribution which can be seen by observing at the image. The middle saddle is fixed and hence it is taking all the load and it looks unstable in terms of stresses generated. If we increase the thickness of saddle it will reduce the stresses generated. d] Body sizing 85 mm, Number of nodes 46914, elements 45773



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Figure 32: EVMS 8

Equivalent Von Mises stress = 874.69 MPa

The stress is increased significantly for 45,500 nodes and the deformation as well. And hence considering this case we have to move forward to next level of optimization. Thus, we will have to keep the track of next series of results generated through the change of parameters and if it releases the instability of the stresses and deformation generated then it will help us to conclude this project.

The above cases were analyzed for 12 mm thickness and the results generated were not satisfactory in terms of stresses generated and the deformation. The Equivalent Von Mises stresses generated were much higher than the allowable stress values (138 MPa) when the model was analyzed for fixed nozzles cases and then sudden decrease was noted for free nozzles cases. The decrease is still much above the allowable stress values and it has to be lowered as we are getting higher stresses in some regions viz. regions of nozzles and vessel intersections. It is our prime focus to control these stresses. This means that we have to look beyond the calculated thickness as the results are poor. We have to reconsider the thickness parameter for this analysis as we cannot control the other parameters and hence it was then recommended to increase the thickness. Thus, the role optimization will be on the screen for the new thickness. The thickness recommended by the company was 30 mm. Thus, we now will be dealing with optimization concept.

VI.OPTIMIZATION

Optimization is done by trial and error method by changing thickness of pressure vessel. Design optimization is a technique that seeks to determine an optimum design. An optimum design means, one that meets all specified requirements but with a minimum expense of certain factors such as weight, surface area, volume, stress, cost, etc. in other words, the optimum design is usually one that is as effective as possible and meeting the requirements. Virtually any aspect of design can be optimized viz. dimensions, shape (fillet radii), and placement of supports and cost of fabrication, natural frequency, material property, and so on. The ANSYS program offers two optimization methods to accommodate a wide range of optimization problems.

The 'sub problem approximation method' is an advanced zero-order method that can be efficiently applied to most engineering problems.

The first order method is based on design sensitivities and is more suitable for problems that require high accuracy.

For both the sub problem approximation and first order methods, the program performs a series of analysis-evaluationmodification cycles. That is, an analysis of the initial design is performed, the results are evaluated against specified design criteria, and the design is modified as necessary. The process is repeated until all specified criteria are met.

In our case, we will be performing the single variable optimization method which comes under Classical optimization techniques. The thickness will be our variable which will be under consideration and we will optimize it for stabilizing the vessel.



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A. Results Statistics-Bar chart

The results statistics studied for optimization are shown with the help of bar charts below. Trial considering thickness 30 mm while linear approach with nozzles fixed



Trial considering thickness 30 mm while linear approach with nozzles free



Analysis for 30 mm thickness with nozzles free (Nonlinear analysis)



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With previous experience of the increasing trend of the value of stresses generated and the deformation formed, we are getting the same result for nonlinear analysis of the 46,000 nodes and the result is satisfactory with stress being equal to 226.21 MPa and deformation magnitude is equal to 8.3093 mm. Both these values are within the respective allowable zone. The vessel looks stable as far as the stresses are concerned, the only concern being the middle saddle which needs special care to be taken while manufacturing. From the above iterations, it was learnt that the vessel with thickness 30 mm is more stable in terms of stresses generated, deformation at various sections of the vessel. Again, it was found that the vessel with free nozzles are having more stabilized, uniformly distributed and safe results than that for vessel with fixed nozzles. Now, it can be considered to be an optimum design.

Thus, from the above analysis it is reflected that, 30 mm thickness will work far better than the theoretical 12 mm thickness and hence we can proceed with the same. The nozzles added for the purpose of speeding up the flow of the reaction can now considered to be safe for the operation of catalyst bed reactor vessel.

The above images also tells us that the cases with free nozzles are having Von Mises stresses generated less than 400 MPa and are much uniform than for the fixed nozzles. The stresses in the range of allowable stress value (414 MPa) for some zones of vessel like middle saddle base.

VII. VALIDATION OF RESULTS

Validation of FEA Results with Experimental Results

A. Deformation validation

Deformation results obtained from FE model is verified by experimental deformation testor displacement sensor. The actual deformation developed over the nozzle vessel junction the surface of CBR is 9.5 mm. Looking at the deformation value (DMX 8.3093 mm) near the nozzle vesseljunction, we can say that a difference of 1.19 mm is observed when we compared it against experimental reading of 9.5 mm i.e. 12.5% difference is noted between FEA readingand actual reading. This difference is acceptable since the 15% of deformation difference allowed as per the company's recommendation.

B. Stress validation

The stress values (EVMS) obtained from FEA results are 200.04 MPa, 187.6 MPa and 226.21 MPa. Experimental



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measurement of the stress values on site is not possible sincethere is no such equipment or sensing device which will give us directly the stress valuefrom the part or section of pressure vessel under consideration. To validate the above values of the stresses, the analytical value of stress is taken from ASME SECTION-VIII.

Thus, from ASME section we have, 414 MPa (138 X 3) [20].

As per ASME SECTION-VIII, Div-I, UG-23(e),

Where,

S = Allowable stress of pressure vessel material at design temperature

Sps = Allowable primary plus secondary stress at design temperature (Maximum allowable

Design stress).

For SA-516 Grade 70,

S=138 MPa

Sps= 3 X 138= 414 MPa

Now, taking the maximum value of stress from FEA results i.e. 226.21 MPa. This value is then increased by 12.5%. This increment is taken from the deformation deviation of 12.5% (as per the company's recommendation). So, the effective stress value obtained is 282.76MPa. Thus, the values of Equivalent Von Mises stresses observed are lower than the allowable analytical stress value (414 MPa). Hence, the nozzle and vessel junction can said to be safein terms of deformation and stresses generated.

VIII.CONCLUSION

The FEA has been carried with 12 mm thickness and then followed by 30 mm thickness. The results obtained with 12 mm thickness were not satisfactory since the deformationfound was high and the Equivalent Von Mises stresses were much more than the allowablestress value (i.e. 414 MPa). The critical zones occurred near the nozzle vessel intersections and the stresses were huge the near such areas.

Hence, looking at the stresses and the deformation with 12 mm thickness, FEA has beencarried out with 30 mm thickness as per the company's recommendation. Again all thecases were carried out for 30 mm thickness. A mark able decrease in the stresses was noted.Deformation is also having much lower value which is allowable. FEA and Experimentalresults are in close resemblance. No damage and leakage detected during the tests. Pressurevessel with Catalyst Bed reactor is working properly in the field within the permissible limits of deformation and stresses. Improved results are obtained for reactions occurring in the reactionary pressure vessel with the help of these added nozzles. The vessel is morestable in terms of stresses generated and the deformation occurred.

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