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Analysis and Optimization of Reactant Column with Thermo – Structural Coupled FEA

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***Abstract*-A reactant column is typically a vertical duct, from which reactant at high pressure is pushed from top to bottom. At the bottom of the column there are holes allowing the reactant to flow out, and mix with the other reactant and chemical process is underway. The advantage of such a design is that the rate of reaction is directly controlled by the pressure in the column, as this indirectly controls the mass flow rate. So more the number of holes more will be efficiency of the process. The design problem is that, typically the holes are the weak regions structurally and in addition they also experience high thermal zones, making them more vulnerable. The thesis focuses on optimizing the location of these holes for maximum structural safety. Also the objective of this paper is to analyze reactant column and determine their strength, and also will be to optimize the design in a manner that all failures can be avoided.**

Keywords: Non – Linear, Reactant Column, Thermo – Structural FEA, Static structure analysis.

1. INTRODUCTION

1.1 Fischer–Tropsch process

Fischer–Tropsch synthesis is a collection of chemical reactions that converts a mixture of carbon monoxide and hydrogen into liquid hydrocarbons. The process, a key component of gas to liquids technology, produces a synthetic lubrication oil and synthetic fuel, typically from coal, natural gas, or biomass ·The F–T process has received intermittent attention as a source of low-sulfur diesel fuel and to address the supply or cost of petroleum-derived hydrocarbons.

A. Process conditions

High-temperature Fischer–Tropsch (or HTFT) is operated at temperatures of 300°C-350°C and uses an iron-based catalyst. This process was used extensively by Sasol in their Coal-to-Liquid plants (CTL). Low-Temperature

A variety of catalysts can be used for the Fischer–Tropsch process, but the most common are the transition metals cobalt, iron, and ruthenium. Nickel can also be used, but tends to favor methane formation.

1.2. Bergius Process

The Bergius Process is a method of production of liquid hydrocarbons for use as synthetic fuel by hydrogenation of high-volatile bituminous coal at high temperature and pressure.

A. Process conditions

The coal is finely ground and dried in a stream of hot gas. The dry product is mixed with heavy oil recycled from the process. Catalyst is typically added to the mixture. A number of catalysts have been developed, including tungsten or molybdenum sulfides, tin or nickel oleate, and others. Alternatively, iron sulphides present in the coal may have sufficient catalytic activity for the process, which was the original Bergius process. Then the mixture is pumped into a reactor. The reaction occurs at between 400 to 500 °C and 20 to 70 MPa hydrogen pressure. The reaction produces heavy oils, middle oils, gasoline, and gases

2. MAIN PRESSURE VESSEL COMPONENTS

Pressure vessels are containers for fluids that are under pressure. They are used in a wide variety of industries (e.g., petroleum refining, chemical, power, pulp and paper, food, etc.) Pressure vessels are design with ASME Boiler and Pressure Vessel Code, Section VIII.

2.1 Shell

The shell is the primary component that contains the pressure. Pressure vessel shells are welded together to form a structure that has a common rotational axis. Most pressure vessel shells are cylindrical, spherical, or conical in shape.

2.2. Skirt Supports

Tall, vertical, cylindrical pressure vessels (e.g., the tower and reactor are typically supported by skirts. A support skirt is a cylindrical shell section that is welded either to the lower portion of the vessel shell or to the bottom head (for cylindrical vessels). The skirt is normally long enough to provide enough flexibility so that radial thermal expansion of the shell does not cause high thermal stresses at its junction with the skirt.

2.3. Head

All pressure vessel shells must be closed at the ends by heads. Hear heads are typically used flat head.

2.4 Nozzle

A nozzle is a cylindrical component that penetrates the shell or heads of a pressure vessel.. Nozzles are used for the following applications:

Attach piping for flow into or out of the vessel. Also provide for direct attachment of other equipment items, (e.g., a heat exchanger or mixer).

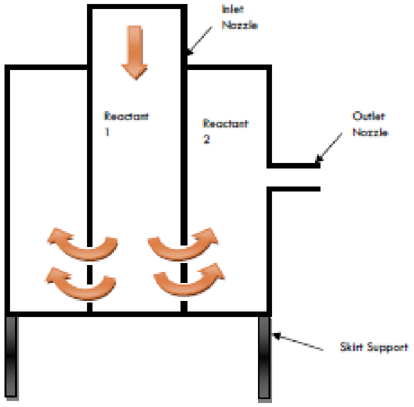

Figure1.Block Diagram of Reactant Column

3. BRIEF OVERVIEW OF SOME RESEARCH

As there are lot of work is done on the pressure vessels. A brief review of some selected references.

3.1 By E. 0. Bergman, Alhambra, Calif have suggested that External loads applied to vertical pressure vessels produce axial loading and bending moments on the vessel. These result in axial tensions and compressions in the shell, which must be combined with the effects of the pressure loading to give the total longitudinal stress acting in the shell.

The design method to be used depends on whether the longitudinal Stress in the shell is tension or compression, and on whether the vessel is subjected to internal or external pressure.

3.2 Pedro Marcal,Dennis H. Martens,Michael A.P

On this paper represents a practical review of the use of PC-based Finite Element software in the analysis of typical pressure vessel components. The authors discuss element type selection criteria and features. Some of the different element formulations are discussed. Modeling parameters and convergence procedures are examined. Practical evaluation tolerances are discussed

4. FINITE ELEMENT ANALYSIS

When the FEM is applied to a specific field of analysis like stress analysis, thermal analysis, or vibration Analysis, it is often referred to as finite element analysis (FEA). FEA is the most common tool for stress and structural analysis. Various fields of study are often related. For example, distributions of non-uniform temperatures induce non-obvious loading conditions on solid structural members. Thus, it is common to conduct a thermal FEA to obtain temperature results that in turn become input data for a stress FEA. FEA can also receive input data from other tools like motion (kinetics) analysis systems and computation fluid dynamic (CFD) systems.

5. NEED OF ANALYSIS

In industry the component produced may be of different sizes, from flat plates of very simple shape to complex 3 dimensional solid bodies. During operation they may be subjected to various types of applied loading conditions which include centrifugal

force, pressure and temperature loading and prescribed boundary conditions. With rising cost of material over design, the resultant wastage may be extremely costly. Failure of component during service may produce a high service return rate, which is extremely undesirable both from high replacement cost and damage to the prestige of product. So stress analysis at the design stage is essential, if service failures are to be avoided and near optimum designs are to be achieved for specified

6. SOLUTION PROCEDURE FOR NON -LINEAR ANALYSES

ANSYS employs the "Newton- Raphson" approach to solve nonlinear problems. In this approach, the load is subdivided into a series of load increments.

The load increments can be applied over several load steps. Figure "Newton- Raphson Approach" illustrates the use of Newton-Raphson equilibrium iterations in a single DOF nonlinear analysis.

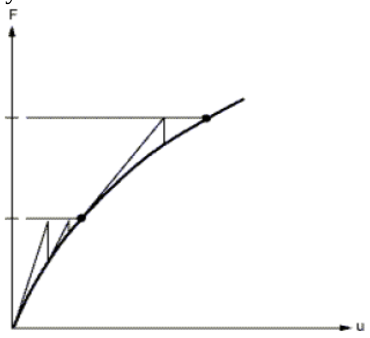

Figure 2**:** Newton-Raphson Approach

Before each solution, the Newton-Raphson method evaluates the out of- balance load vector, which is the difference between the restoring forces (the loads corresponding to the element stresses) and the applied loads. The program then performs a linear solution, using the out-of-balance loads, and checks for convergence. If convergence criteria are not satisfied, the out-of-balance load vector is reevaluated, the stiffness matrix is updated, and a new solution is obtained. This iterative procedure continues until the problem converges.

7. DETAILS OF REACTANT COLUMN ASSEMBLY

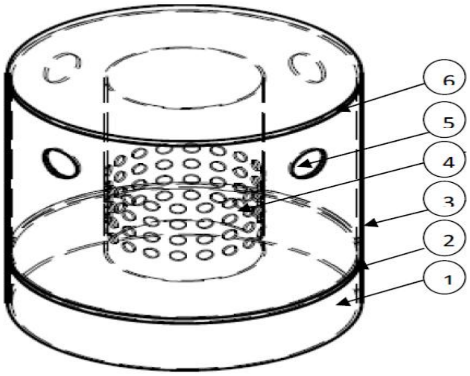

Figure 3-D Drawings of reactant column

1. Skirt Support, 2.Base Plate, 3.Shell,4.Inner Reactant Column , 5.Nozzle,6.Top Plate

8. MODELLING AND ANALYSIS

3-D model of reactant column assembly is created in ANSYS Workbench & CATIA, which is required for the purpose of further analysis. ANSYS Workbench provides a highly integrated engineering simulation platform, supports multi-physics engineering solutions and provides bi-directional parametric associability with most available CAD systems.

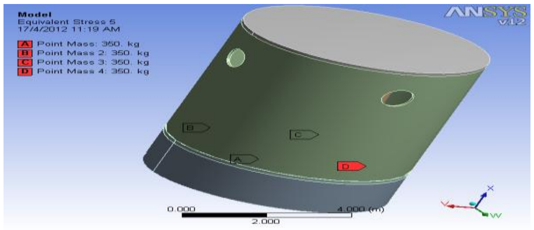

Figure 4. Reactant Column Assembly

Material properties SA516 Grade 70 applied to the body contains:

8.1 Mechanical properties

TABLE I. Mechanical property of material SA516 Grade 70

Yield Strength	240 MPa
Ultimate Strength	460 MPa
Thermal Conductivity	60.5 W/mk
Poisson's Ratio	0.3

8.2. Chemical Composition

TABLE II. Chemical Composition of material SA516 Grade 70

Carbon(c)	0.30%
Manganese(Mn)	0.80-1.3%
Phosphorous(p)	0.035%
Sulphur (s)	0.035%
Silicon(si)	0.13-0.45%

8.3 Meshing

The Reactant column assembly model is meshed with 20 node hexahedron SOLID186 element. It is a higher order 3-D 20-node solid element that exhibits quadratic displacement behavior. The element is defined by 20 nodes having three degrees of freedom per node: translations in the nodal x, y, and z directions.

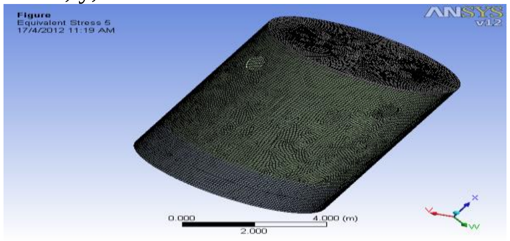

Figure5. Fine Hexahedron Meshed Model of Reactant Column Assembly

8.4 Defining The Contacts

Highly nonlinear problems Contacts are necessary. So it requires proper attention to define the correct contact pairs and target and contact surfaces. When two surfaces are in contact one is target surface and another is contact. Contact surface is one from which forces get transfer to target surface. Target surface is that to which forces get transfer. Reactant column assembly consists of different components like top plate, inner reactant column, shell, bottom plate, skirt support.
These components are connected to each other have number of contacts pairs. All contacts defined are of bonded type.

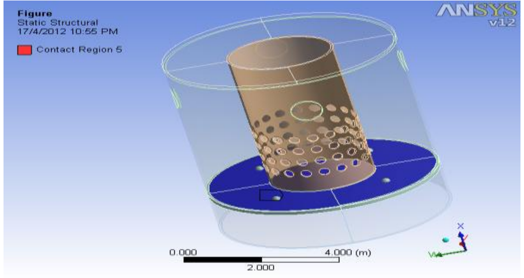

Figure 6. Bonded contact between inner reactant Column & base plate.

8.5 Boundary Conditions

Boundary Conditions are as follows:
1. Bottom there is skirt support which is considered as Fixed.
2. Weight of cobalt meshing 1400 kg applies on the base plate. Which is equally divided into 4 parts that is 350 kg on equally each divided faces.

3. Internal pressure 0.2 MPA apply on top & bottom plate also on shell faces.
4. There is pressure differences 0.09 MPA during flow of pressure raised fluid that is apply on internal faces on inner reactant column.
5. Standard earth gravity 9.81 m/s^2 apply at centre of pressure vessel.
6. Process Temperature 500k

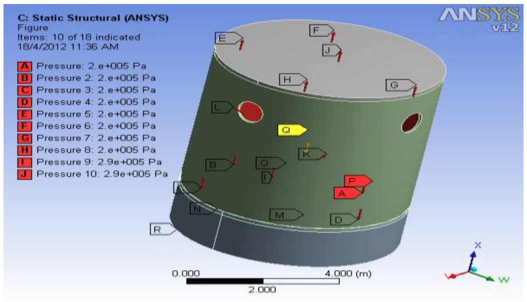

Figure 7. Reactant Column with Boundry Condition

9. RESULT AND DISCUSSION

After giving the solution, the problem is being solved in ANSYS by giving the number of sub steps for nonlinearity. The resulting stress and deformation plots after solving the problem for all boundary conditions.

The stress and the deformation color counters plots for considering above all boundary conditions. by changing meshing size & substeps. Maximum von-mises Stress & deformation color counters plotted as shown below. in fig.

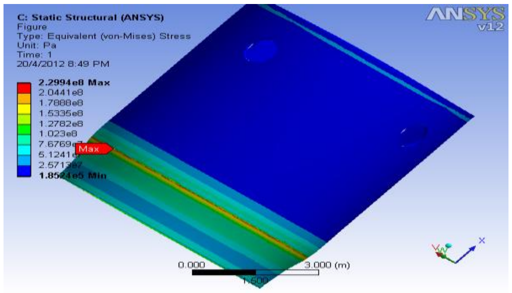

Figure 8.Von-Mises Stress Plot on skirt support

Maximum Equivalent Stress = 2.299e8 Pa

Maximum Deformation = 0.018m

The maximum stress value shown by the red color plot is acting at very small portion of skirt support. In actual practice this type of stresses due to the stress concentration and can be neglected. That also less than allowable stress of that material.

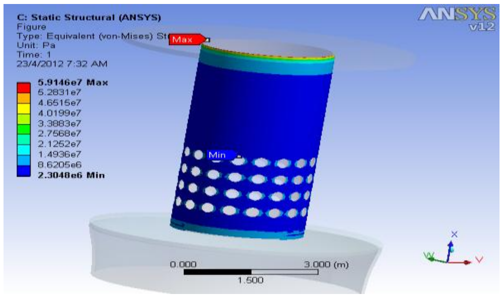

Figure 9.Von-Mises Stress Plot on Inner Reactant Column having rectangular pattern.

We are concentrated on inner reactant column of pressure vessel. From this analysis we can say that comparatively very low stress introduce on inner reactant column. Maximum von-mises stress is found on top portion inner reactant column as shown as red color contour plot above fig.9. This is also less than that of the yield point of that material.

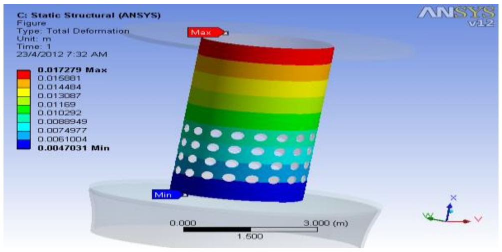

Figure 10. Total Deformation Plot on Inner Reactant Column Having Rectangular Pattern.

TABLE III. Analysis Result of Rectangular Pattern

Analysis No	No of Elements	Maximum von-mises Stress in Pa	Maximum Total Deformation in meter
1	102349	5.914e7	0.017279
2	95901	5.805e7	0.017297
3	82705	5.858e7	0.017315
4	75091	5.622e7	0.017237

10. NEW TRIANGULAR HOLE PATTERNS

As we know rate of reaction is directly controlled by the pressure in the column, as this indirectly control the mass flow rate. so we choose different holes pattern such a way that increasing the mass flow rate & also efficiency of process

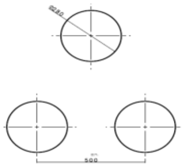

Figure 11.Triangular pattern holes

Now we select the triangular pattern which gives the maximum number of holes keeping the all dimensions same as in previous case. Now these new pattern gives total numbers of holes are 126.

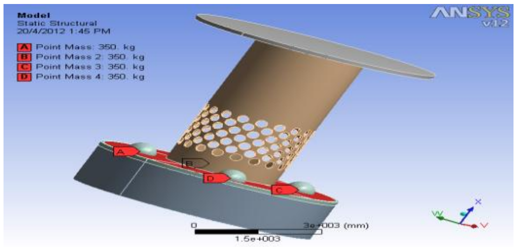

Figure 12.Reactant column with triangular holes pattern.This new triangular pattern is analyzed for the same operating conditions as in previous case and found out the results.

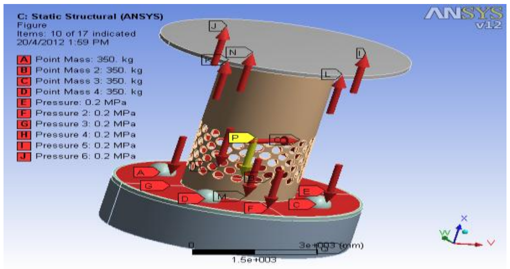

Figure 13.Reactant column with triangular hole patterns having boundary conditions

The maximum value of stress in this case is found out on the skirt support as shown in fig. It is also less than the yield strength of the material considering the factor of safety.

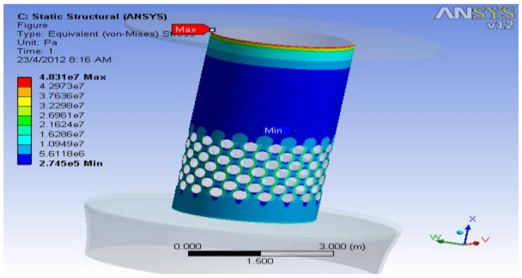

Figure 14.Von-Mises Stress Plot on Inner Reactant Column with new triangular hole patterns.

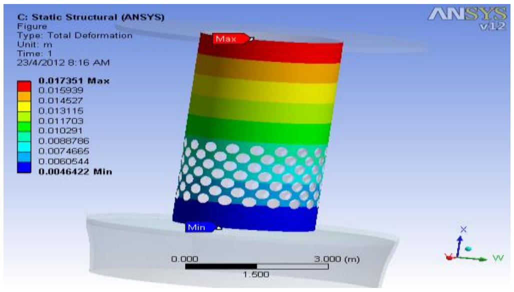

Figure 15.Total Deformation Plot On Inner Reactant Column with new triangular hole patterns.

TABLE IV. Analysis Result of Triangular Pattern

Analysis No	No of Elements	Maximum von-mises Stress in Pa	Maximum Total Deformation in meter
1	107453	5.955e7	0.017382
2	98077	6.070e7	0.017399
3	83282	5.974e7	0.017341
4	78179	6.058e7	0.017344

11. COMPARISON OF BASIC AND NEW PATTERN MODEL

Comparison of both the models from the above stress plots is decrypted in the table. From the above table some points are highlighted as below in table

TABLE V. Comparison of Basic and New Pattern Model

Parameters	**Previous Rectangular Holes Pattern Model.**	**New Triangular Holes Patterns Model.**
Number of Holes	72	126
Maximum Von- Mises Stress On Inner Reactant Column In Pa	5.914e7 (safe)	6.070e7 (safe)

Increase in number of holes increased the flow rate capacity of the process in the new triangular pattern model compare to basic model. Percentage increase in flow rate capacity is

$$\frac{126-72}{126} * 100 = 42.85\%$$

12. CONCLUSION AND FUTURE SCOPE

The analysis of the proposed reactant column assembly brought into light a number of inadequacies in design.

The first thing that was observed, the new hole pattern was selected, which, allowed 54 more number of holes which lead to increase flow rate capacity 42.85% Also Usage of Triangular pattern is more efficient for mass flow rate.

The new triangular holes pattern as the stresses became well distributed over the inner reactant column assembly due to more symmetrical distribution of reactant column assembly. Perspective and stresses are moderate which are lower than allowable stresses.

Future scope of this study is that currently only triangular pattern is simulated, we can perform similar analysis using other patterns. We can also vary the distance between the holes of the pattern and check effect on the stress increment.

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