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CFD ANALYSIS AND OPTIMIZATION OF AN INLET MANIFOLD FOR A LARGE TGU REACTOR

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ABSTRACT

This paper will discuss the use of Computational Fluid Dynamics (CFD) to study the flow characteristics of inlet manifolds into a large TGU reactor. The design parameters for the operation of the reactor required a very minimal system pressure drop, outside of the pressure drop across the reactor bed. For this reason several alternative designs were considered for the inlet manifolds and distribution into the reactor. Detailed CFD models were constructed of each proposed variant and analyzed to determine their pressure drop and distribution characteristics. The results of these analyses were then used to choose the best candidate for optimization as well as in providing guidance in system changes that would improve pressure drop and flow distribution characteristics. A discussion of how the results' guidance was used in optimizing the flow path will be provided. The paper will conclude with a brief overview of other considerations in the complete analysis of the reactor system.

INTRODUCTION

A tail gas unit (TGU) reactor is used in several industries to implement a hydrogenation reaction on the byproducts from a Claus sulfur recovery unit, used to reduce the amount of H_2S present in the gas stream (reference). The TGU is typically a horizontal bed reactor with several inlets located on the top of the vessel, an open space to allow for flow distribution into the reactor bed and an open space under the bed to allow distribution to the outlet nozzles located on the bottom of the reactor.

There are several important parameters in the operation of the reactor. To minimize compression requirements the reactor and its associated piping must present a minimal pressure loss (outside of the loss allowed for in the reactor bed). To optimize reactor performance the flow should be as evenly distributed into the bed as possible, and the amount of flow bypassing the bed near the walls should be minimized.

It was decided to perform Computational Fluid Dynamic (CFD) analyses to quantify the performance of a reactor under development. A primary purpose of the CFD analyses was to determine the best layout for the inlet piping to the reactor to minimize pressure drop and to provide optimal distribution into the reactor. A second purpose of the analysis was to quantify the distribution into the bed to ensure that there was even flow distribution into bed, and minimal flow bypass.

INLET PIPING ANALYSIS

Originally 2 models were developed of proposed inlet piping configurations. One configuration consisted of a 3 inlet piping system and one of a 4 inlet piping system. The geometry of each system is shown below.

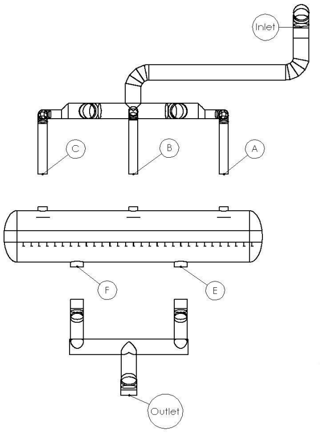

Figure 1 – Geometric layout of 3 inlet system

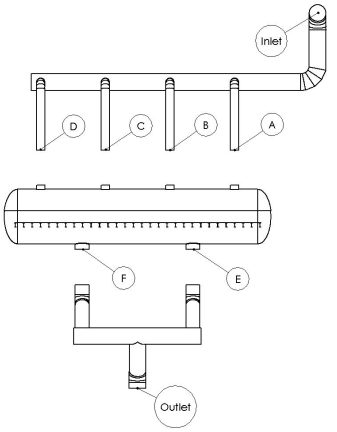

Figure 2 – Geometric layout of 4 inlet system

Flow variables such as pressure drop and mass flow rate were measured at the locations detailed in each figure above.

To perform the analyses, CFD models were developed of each configuration in Star-CCM+. The models were developed using the package's automeshing feature, with polyhedral cells and wall prism layers used. Initially, mesh density studies were performed to determine a mesh density that would not affect the results. As pressure drop through the piping was a primary variable under examination the mesh was refined until the wall y+ values were between 30 and 100. These values were chosen to provide good boundary layer resolution with the k-ε renormalization of groups (RNG) turbulence model selected for the analysis (reference).

The analysis was performed as a steady-state analysis with a mass flow inlet boundary condition and a pressure outlet boundary condition. The reactor bed was initially modeled using a porous media with the porous media parameters selected to reproduce the bed pressure loss predicted by the Ergun equation, which provides a good estimate of the pressure loss through a packed bed (reference).

Both piping systems were found to have nearly identical pressure losses into the reactor. It was found that the flow distribution of the piping systems was very different, as can be seen in the figures below.

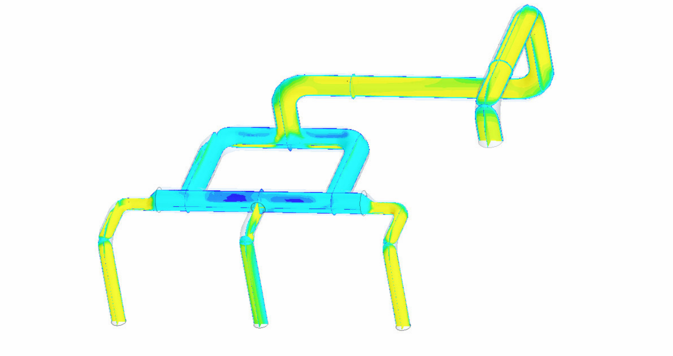

Figure 3 – Velocity profiles for 3 inlet piping system

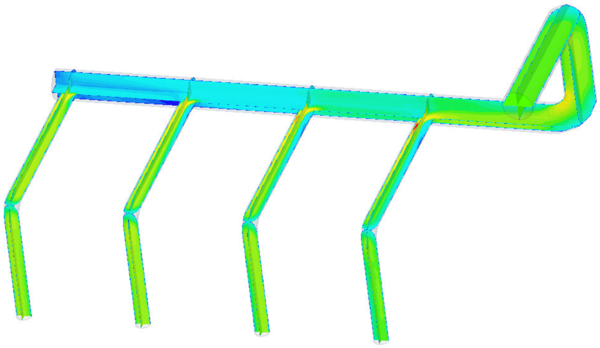

Figure 4 – Velocity profiles for 4 inlet piping system

As can be seen from the figures above, the 3 inlet piping system showed a strong bias towards the inlet pipes located on the sides, while the 4 inlet piping system showed even distribution through all of the pipes. For this reason the 4 inlet system was chosen for optimization.

The initial analyses also indicated that the flow distribution above the reactor bad was significantly biased towards the edge of the bed, as shown in the surface plot below.

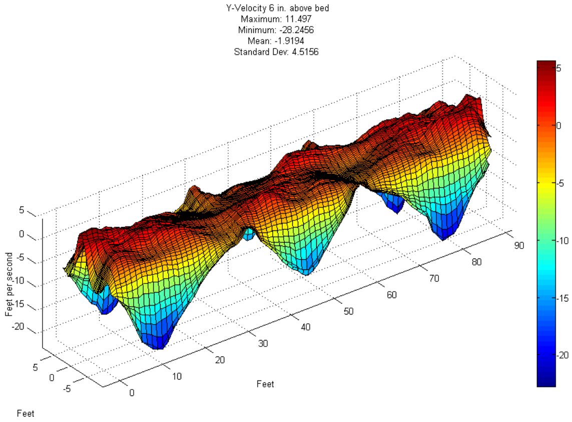

Figure 5 – Surface plot of vertical velocities above the bed

As can be seen in the figure above there is significant recirculation occurring in the center of the bed as the flow impinges on the outside of the bed and is forced to turn. This maldistribution of flow results in non-optimal bed performance, as the catalyst near the bed walls is exposed to a greater percentage of the flow. This will result in the catalyst near the walls degrading quicker than the catalyst in the center of the bed, causing increased operational costs due to increased bed catalyst changes. This established a goal for the system's optimization to improve the distribution of the flow into the bed, without significantly affecting the system's pressure drop.

BED DISTRIBUTION OPTIMIZATION

To perform optimization of the system to improve the distribution of the flow into the bed a series of 2 dimensional models were used to study the use of differing diffuser geometries at the inlet to the vessel. The use of the 2D models allowed for a wide variety of variants (approximately 20) to be studied quickly. After inlet geometry was selected the reactor model was updated and another analysis of the complete system was conducted to validate the performance of the geometry. As can be seen from the figure below an inlet geometry was found that concentrated most of the inlet flow towards the center of the bed.

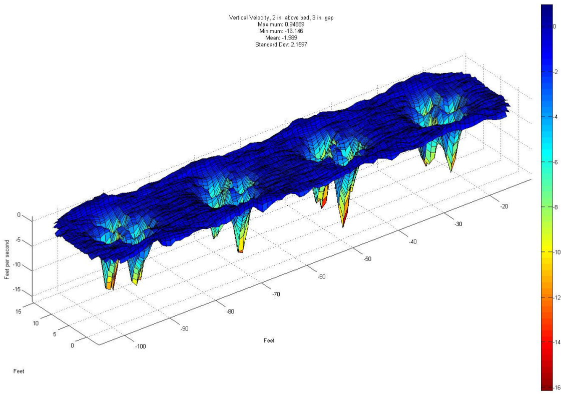

Figure 6 – Surface plot of velocities above bed after optimization

BED BYPASS QUANTIFICATION

The effect of solid walls on the flow through packed beds is to increase the porosity of the bed in the near wall region. This is due to the reduced packing that occurs at the bed-to-wall interface. The reduction in packing is highly dependent on the packed geometry of the bed, as is discussed below. This fact introduced a further goal for the analyses, to quantify the amount of flow that could be expected to bypass the bed.

Zong and Talbot [1] postulate that the zone of influence near the wall for a randomly packed bed lies between 4 and 6 sphere diameters of the wall. Past this distance, the bed can be assumed to reach a randomized packing, and the bulk bed void fraction can be used to characterize the bed.

Bear and Bachmat [2] introduced the concept of tortuosity of the flow structure near the no-slip wall. Tortuosity is defined as “a dimensionless parameter that accounts for the fact that the flow path is in general not straight”. The value of the tortuosity can be determined using vector calculus for a designed porous media, but has typically been measured in randomly packed beds. P. Cheng has written several papers that provide estimates for the tortuosity and modified void fraction near the wall.

Bear and Bachmat also provide a mathematical basis for performing numerical modeling with a change in porosity at the wall. It is known that the value of the void fraction will vary continuously as the wall is approached. Yet techniques using discretized regions to model the flow domain do not allow for this continuous variation to be accounted for during solution. In these cases, it has been found acceptable to model the change in porosity using step changes, as long as the flow characteristics at the step interface are not controlling.

As it was determined that the flow characteristics at the step change were not controlling in estimating the amount of bypass occurring with the bed the following procedures were used to estimate the amount of bypass occurring:

- The bed was separated into two domains, a near wall domain and a bulk bed domain. This was accomplished through the use of two models, one with the interface at 4 sphere diameters from the wall and one at 6 diameters.

- The bulk bed was modeled through the use of the pressure drop calculated by the Ergun equation for the bed’s nominal packing fraction.

- A geometric model was developed of the packing near the wall assuming face centered cubic (FCC) packing. This model was then used to estimate the change in packing fraction at the near wall location.

- The near-wall bed’s porosity was modified to represent the higher void fraction at the wall based on the Ergun estimated pressure drop for the increased porosity.

The models were then analyzed to determine the amount of bypass occurring at the near wall location. Both models indicated nearly identical bypass flows, which had been postulated by Zong and Talbot. Additionally, the amount of bypass flow was found to be almost 300% higher than the theoretical flow based on the exposed face area of the bed, which will result in decreased bed efficiency.

ADDITIONAL CONSIDERATIONS

An additional consideration in the performance of the reactor bed and the flow distribution through the bed is the bed support system. In this case the bed was supported by structural steel members that were periodically placed underneath the bed. Interrogation of the analysis results indicated that these supports provided a significant flow blockage as shown in the figure below.

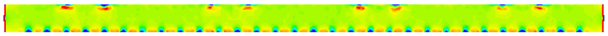

Figure 7 – Vertical velocities through the packed bed

As can be seen in the image above there are very large stagnant regions over the support members. These stagnant regions will result in reduced bed efficiency. Additionally, as the flow has to be accelerated through the bed to reach the open outlet area the pressure loss in the bed will be increased.

An additional consideration for the analysis was whether the horizontal scrubbing velocities on the bed's top face would be great enough to cause the packed spheres to move. To perform this qualification the maximum vector velocity above the bed was queried from the analysis. This velocity was then used to calculate the maximum lift and drag forces that could occur on a sphere located on the top of the bed. A free body diagram, shown below, was then developed for a 2 ball system to determine if rolling could occur.

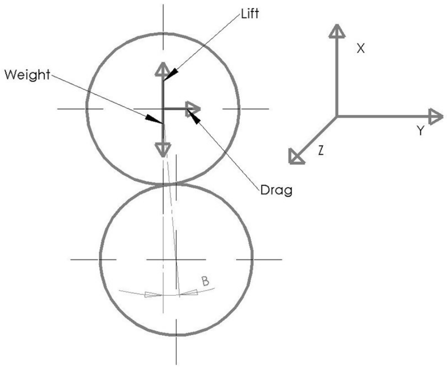

Figure 8 – Free body diagram of sphere system

Using a static analysis an angle B was determined for when the ball would move in the Y-direction, rather than down in the X-direction (stable falling into the bed). It was determined that the magnitude of this angle was very small, indicating that the system was stable at the scrubbing velocities occurring in the reactor.

CONCLUSIONS

A series of analyses were performed to determine the best configuration for a TGU reactor. These analyses were able to demonstrate the best inlet piping configuration for the reactor. The analyses also showed that there could be modifications made within the reactor to improve the flow distribution into the bed. A separate series of analyses was then able to determine the amount of bypass due to near wall effects would occur in the reactor; the amount of this bypass was shown to be significant, and independent of the modeling technique used. Additionally, the results of the analyses demonstrated areas where additional performance improvements could be achieved if additional bed support methods were studied. Finally, the information supplied by the analyses was able to be used to determine if there was a high probability of bed scouring occurring.

REFERENCES

1. Zong, C. and Talbot, J. Sphere Packings, Springer, August, 1999
2. Bear, J. and Bachmat, Y. Introduction to Modeling of Transport Phenomena in Porous Media, Kluwer Academic Publishers, 1991