CFD Modelling of Adsorption Behaviour in AGN Tank with Polyethylene Terephthalate Plastic Waste Based Activated Carbon

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Abstract. Indonesia imports fuel (fuel oil) in large quantities. Indonesia has reserves of methane gas in the form of natural gas in large numbers but has obstacles in the process of storage. To produce a storage tank to a safe condition then proclaimed to use ANG (Adsorbed Natural Gas) technology. Manufacture of activated PET based activated carbon for storage of natural gas where technology has been widely studied, but still has some shortcomings. Therefore to predict the performance of ANG technology, modeling of ANG tank with Fluent CFD program is done so the condition inside the ANG tank can be known and can be used to increased the performance of ANG technology. Therefore, in this experiment natural gas storage test is done at the ANG tank model using Fluent CFD program. This experiment is begin with preparation tools and material by characterize the natural gas and activated carbon followed by create the mesh and model of ANG tank. The next process is state the characteristic of activated carbon and fluid in this experiment. The last process is run the simulation using the condition that already been stated which is at 27°C and 35 bar during 15 minutes. The result is at adsorption contour we can see that adsorption is higher at the top of the tank because the input of the adsorbent is at the top of the ANG tank so the adsorbate distribution is uneven that cause the adsorbate concentration at the top of the ANG tank is higher than the bottom tank.

Keywords: Activated Carbon, PET, Methane Storage, ANG

1. Introduction

Indonesia imports BBM (Bahan Bakar Minyak) in a large scale. Badan Pusat Statistik (BPS) recorded that in February 2014, Indonesia imports BBM around 1,06 million tone or around US$ 1,13 billion. This is because BBM is the main fuel that been used by Indonesia people for transportation. We can see in year 2012, the number of vehicle already reach 94,373,324. The usage of BBM in Indonesia is increasing due to the fast growth of vehicle industries around 5-6% each year [1]. Natural gas have a big potential to substitute BBM because Indonesia have big gas reserves and Indonesia is at rank 14 worldwide with reserves around 103,3 trillion cubic feet, where natural gas is the main ingredient of methane gas production [2]. The main problem from this natural gas is in the storage and distribution process because in normal condition, natural gas is in gas phase so the storage capacity become small and not efficient to be used. The technology that generally used is CNG and LNG. However, CNG needs high pressure around >3500 psi or 25000 kpa (250 bar) and LNG needs low temperature (-161°C) that can harm the surrounding area. To solve this problem we need innovation to store natural gas such as storing in a cylinder tube with ANG (Adsorbed Natural Gas) and activated carbon as the adsorbent which make natural gas can be stored in low pressure around 500 psig (3447,37 kpa) and high storage capacity [3].

This activated carbon is made from PET plastic waste as raw material because the big availability in Indonesia which is the number is around 26500 ton each day based on Ministry of Environment of...
Indonesia. Furthermore activated carbon that made from PET has highest surface area compared with PVC and tires [4].

ANG technology generally has not been applied in vehicle even this technology has more benefit compared to CNG. One of the factor is the low adsorbent performance to adsorbed natural gas compared with CNG technology in the same tube. Because of that to predict the performance of ANG technology modeling of ANG tank is done that can be used for increasing the performance of ANG technology. This kind of experiment is already done at adsorption of hydrogen gas at activated carbon experiment which look at temperature and adsorption contour. Because of that in this experiment natural gas storage test is done at CFD model of ANG tank that will produce natural gas storage capacity, temperature and pressure contour data inside ANG tank.

2. Methodology
   2.1. Geometry Making
Simulation process is begin with geometry making at GAMBIT, this process is included in preprocessing process. At the geometry making there are 4 type of geometry which are vertex which is geometry making using dot, edge which is geometry making using line, face which is geometry making using area and the last is volume which is geometry making using volume or 3D. For area making, dot geometry making has to be done before, dot geometry making using coordinate, and than link the dot become line with edge and area making with face.

2.2. Mash Making
After geometry finish, followed with mash making. The purpose of mash making is to decide the iteration result accuracy at Fluent, The bigger the mesh than the iteration accuracy is better. At the meshing menu there are 3 type of mesh which are mesh edge which is mash making on line, mash face which is mash making on area and mash volume which is mash making on volume. Make mash on area isn’t same with geometry making that have to start from dot first, on mash area making can use mash face directly. At mash face making there are mesh type option, type of mash and amount of mash.

2.3. Boundary Condition
After making a complete mesh subsequent determination of the boundary conditions. These boundary conditions will be read on the Fluent therefore better define the desired boundary conditions beforehand though the boundary conditions there are not clear because when the boundary conditions specified in GAMBIT it can be replaced at Fluent, but if the boundary conditions. In the specific boundary conditions there is a choice that serves to select the type of boundary conditions that we want on a particular line such as inlet pressure, discharge pressure, and other boundary conditions that have been provided by GAMBIT.

2.4. Running Simulation
Simulations performed with axis-symmetric 2D model so modeling tube only half. Used a triangular meshing with Pave type and the interval count 450 At Fluent, menu-read file can have read the case, read data and read case and data. When the initial preparation to do is read the case, read the case and the data can be done when an existing file data that has been made. Then read case on file that has been exported from the .msh GAMBIT. Make a check on the grid, grid-check of the menu, the menu grid can also do scale to the size of a dimension that has been made. Then specify the conditions to be desired on the menu define, in this menu there are conditions of a model that can be adapted to the conditions of research, there is a material that serves to define the desired material, there is a boundary condition that serves to define the boundary conditions are desirable and also user -defined which serves to insert the UDF. Once it can be done save data by file-write-case or file write-case and the data, these two types differ only in the data. After his return to the menu solve, workmanship solve next-animate that serves to show the contours or the other on the window so that after iteration is completed we can play back, then do iterations.
2.5. Flow Diagram

![Flow Diagram](image)

Figure 1. Flow diagram

3. Result And Discussion

3.1 Activated Carbon

In this experiment PET based activated carbon is used that produce by Alristo Sanal at year 2015 for thesis. Characteristic from activated carbon is used for analysis. The following is the result of activated carbon characteristic.

| Activated Carbon Characteristic Data | PET   |
|-------------------------------------|-------|
| Surface area (Bil Iod) (m²/g)       | 1591.72 |
| Pore volume (cc/g)                  | 0.176  |
| Micropore volume (cc/g)             | 0.136  |
| Pore diameter (Å)                   | 15.2   |
3.2 Natural Gas Composition

In this experiment, adsorbate that is used for ANG test is natural gas from SPBG Pertamina JL.Raya Bogor. In this experiment gas composition test is done that become adsorbate in this experiment. This is done because adsorbate composition is needed in the adsorption calculation. Gas composition test is done in Lab Intensifikasi Proses Departemen Teknik Kimia Universitas Indonesia using Gas Cromatography (GC). The following is the result of gas composition from adsorbate that will be used:

| No | Name     | Time | Quality (%Area) | Height (µV)  | Area (µV.Min) | Area % |
|----|----------|------|-----------------|--------------|---------------|--------|
| 1  | CH₄      | 1.65 | 87.76           | 693,512.5    | 14,392.7      | 87.76  |
| 2  | N₂       | 1.73 | 4.70            | 38,002.3     | 770.5         | 4.698  |
| 3  | C₂H₆     | 1.94 | 3.78            | 29,539.4     | 620.0         | 3.781  |
| 4  | CO₂      | 2.19 | 2.26            | 10,349.3     | 370.6         | 2.260  |
| 5  | C₃H₈     | 2.92 | 1.28            | 5,394.5      | 209.6         | 1.278  |
| 6  | C₄H₁₀    | 6.68 | 0.22            | 321.8        | 36.3          | 0.222  |
|    | Total    |      | 100             | 777,119.8    | 16,399.7      | 100    |

3.3 CFD Simulation

In this study conducted simulations using CFD program which aims to observe the adsorption process that occurs in the tube ANG. By knowing the adsorption process that occurs in the tube ANG we can predict the performance of the ANG technology. Results of the program are the CFD pressure contour, contour and contour absorption temperature on the tube ANG. Simulations use 2d field by using only half of the tube ANG, because on the other half of the tube ANG will have the same result. In this simulation gas will enter from the top of the tube and flows to the bottom of the tube.

![Figure 2. Pressure contour of ANG tank](image-url)
Figure 3. Temperature contour of ANG tank

Figure 4. Storage capacity contour of ANG tank
Contours of pressure can be seen in Figure 2 where the pressure in the tube is at a pressure of 35 bar is uniformly distributed on the tube ANG. Contour temperature can be seen in Figure 3 where it can be seen the color difference where the color red is at the top of the tube. This indicates that conditions at the top of the tube has a higher temperature is due to the input of the adsorbent is at the top so that the distribution adsorbat uneven which causes the concentration of adsorbate the top of the tube is greater than the bottom of the tube in which the reaction of adsorption is exothermic so take off heat to the environment with greater concentration it will produce greater heat [4].

Contour absorption can be seen in Figure 4 where it can be seen the color difference where the color red is at the top of the tube. This indicates the absorption was more pronounced at the top of the tube marked with the colors redder than tube sections more because of the input from the adsorbent is at the top so that the distribution adsorbat uneven which causes the concentration of adsorbate the top of the tube is greater than the bottom of the tube. With a greater concentration it will produce greater absorption. When compared with the research conducted Nouh where research simulations using CFD program on ANG technology obtained similar results which were obtained by the distribution of storage capacity less prevalent. Incoming gas flow rate can be reduced so that natural gas can be absorbed and distributed better [4].

4. Conclusion
We can conclude from this experiment “CFD Modeling of Adsorption Behavior in ANG Tank with Polyethylene Terephthalate Plastic Waste Based Activated Carbon” that:
1. In CFD simulation we can get that the highest storage capacity is at the top of the tube which is the highest concentration of adsorbate is occur.
2. In CFD simulation we can get that the temperature is at the top of the tube which is the highest concentration of adsorbate is occur.
3. In CFD simulation we can get that the pressure is spread evenly at the ANG tank

5. Reference
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