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COMPUTATIONAL ANALYSIS FOR UNIFORMIZING FLOW AT THE OUTLET OF METHANOL STEAM REFORMER

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Abstract: *Methanol is a liquid fuel and good material for hydrogen production for fuel cells. The operating temperature of methanol steam reformer is lower than that of ordinary methane reformer, so it is being studied to transfer heat to convection heat transfer after fully utilizing heat inside the system rather than directly supplying combustion heat generated by the combustion engine. In this study, we want to observe the flow of cylinder multi-tube methanol in accordance with the shape of the outlet of reformed gas.*

Ansys Fluent® was used to simulate shape-based products mixture flow. The cases for height and diameter of the reformer outlet were selected through the computerized analysis and the corresponding streamline, static pressure were compared to correlate with the recirculation area. Also, using the most smooth flow distribution case, Fillet was added to the outlet and the corresponding flow effects were compared.

Keywords: *Computational Analysis; Reformer; Steam Reforming; Methanol; Mixture; Recirculation zone.*

NOMENCLATURE:

Greek letters

D Diameter of Outlet
H Height of Pressure vessel
R Radius of Fillet
x Axial coordinate
p Static pressure
$\bar{\bar{\tau}}$ Stress tensor

Subscripts

G_k Generation of turbulence kinetic energy due to the mean velocity gradients
G_b Generation of turbulence kinetic energy due to buoyancy
Y_M Fluctuating dilatation
$C_{1\varepsilon}, C_{2\varepsilon}, C_{3\varepsilon}$ Constant determined from experiments
σ_k, σ_ε Prandtl numbers

I. INTRODUCTION

Fuel cells are power generators that generate electricity directly by using the electrochemical reaction and have the advantages of being able to replace fossil energy that has problems such as air pollution and global warming [1,2,3].

Many types of fuel cells use hydrogen as fuel [4], which is plentiful resources because it can be obtained from water and has the advantage that combustion products are not related to environmental pollution, and it can store and transport energy [5]. However, since it can not be obtained directly from nature, hydrogen producing facility was required. The reformer is a reactor to produce hydrogen from fossil fuel that is studied widely using methane, methanol, ethanol, benzene, etc [6]. Due to low operating temperature, methanol steam reformer (MSR) has the advantage of being able to supply heat using waste heat generated inside the system due to their low operating temperature of 200 to 300℃ [7], so they do not need an independent burner. Additionally, they do not take up much volume when storing fuel due to their high energy density, and generate additional hydrogen through the water gas shift reaction [8,9].

Methanol conversion method consists of three elementary reactions: Steam Reforming, Methanol Decomposition and Water gas shift. The principal reaction, Steam Reforming, is an endothermic reaction [10], which absorbs the heat around it and result in a reaction, which requires additional supply of heat.

In this study, we would like to compare the flow characteristics of MSR multi-tube in the form of hollow tubes, where the heat was supplied to the outer tubes using superheated steam and methanol reaction takes place in the inner tubes. The simulation variables are diameter of a single outlet, the height of the pressure vessel, and the size of the fillet to compare with the reference case. The streamline and the static pressure were compared after mesh convergence test to find the optimized geometry to reduce the recirculating area in terms of the geometry change.

II. MATERIAL AND METHODS

2.1. Geometry of MSR

Ansys Fluent® was used to create geometry, mesh, and interpret 3D simulation, assuming a steady state. The MSR geometry and mesh profile were shown in Fig 1. The MSR has a total of 19 hollow tubes, through which they combined on an elliptical pressure vessel and exit through a single outlet. Parameters and boundary conditions for the geometry were shown in Table 1.

2.2. Mesh

Mesh was formed based on a geometry of 22mm in diameter and 50mm in height without fillet, which is a Reference case (Case 1) and inflation was formed to detail flow on the wall. Area weighted average velocity of outlet by mesh size was compared for mesh convergence test. As a result, mesh size was set to 3mm that has 2,318,462 elements.

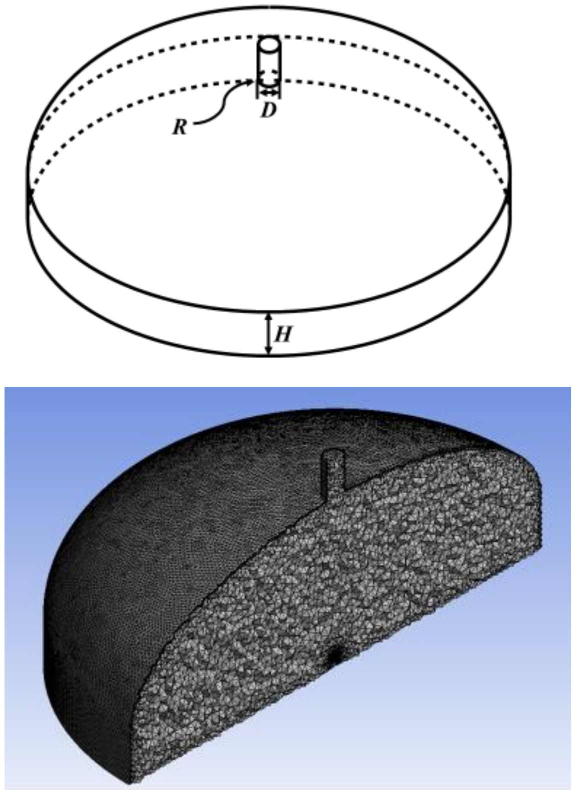

Figure 1. Geometry and mesh profile of MSR

Table 1. Geometry parameter and boundary condition

Parameter	Unit	Value
Diameter	mm	450
Inlet diameter	mm	4.55
Inlet velocity	m/s	1.94
Temperature	K	553.14
Pressure	kPa	2,980
Reynolds number	-	3,860

2.3. Cases of the Geometry

Table 2 shows the cases of the pressure vessel. Based on Case 1, the diameter of a single outlet was determined with specification of KS steel pipe. The height was varied to see the effect of height within given diameter. In addition, the variable size of the fillet is also investigated to understand flow recirculation with flow curvature.

Table 1. Cases of MSR

Parameter	Unit	Case1	Case2	Case3	Case4	Case5	Case6	Case7	Case8
Diameter	mm	22	22	27.5	27.5	36.2	36.2	36.2	36.2
Height	mm	50	100	50	100	50	100	100	100
Radius	mm	0	0	0	0	0	0	5	10

2.4. Solver

The general turbulence model of Standard k-epsilon was chosen to simulate MSR internal flow. In addition, Coupled scheme was selected and the volumetric changes in velocity, pressure and temperature were carried out through Hybrid Initialization until the Residual fell below 10^{-6}.

2.5. Governing equations

The governing equation was as follows [11].

Continuity equation

$$\nabla \cdot (\rho \vec{v}) = 0 \tag{1}$$

Momentum equation

$$\nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho \vec{g} \tag{2}$$

Energy balance equation

$$\nabla \cdot \left(\vec{v}(\rho E + p)\right) = \nabla \cdot (k_{eff}\nabla T - \sum h_j \vec{J_j}) + S_h \tag{3}$$

Turbulence model equations

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M + S_k \tag{4}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\epsilon}{k}(G_k + C_{3\varepsilon}G_b) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_\varepsilon \tag{5}$$

III. RESULTS AND DISCUSSION

3.1. Comparison of changes according to the diameter of Outlet and height of Pressure vessel

The analysis was conducted according to the change in the diameter of outlet and the height of pressure vessel without fillet. As a result, the velocity decreased as the diameter of the outlet increased. But there was not much difference in the streamline. In cases of Case 1, 3 and 5, which were height 50mm, can be seen that the flow phenomenon from different inlets moves irregularly after hitting the top of elliptical pressure vessel. On the other hand, Case 2, 4, and 6 with a height of 100mm can be seen that the mixture from different inlets recirculates without significantly affecting the behavior of the different compounds. They were clearly indicate that kinetic energy of the mixture flowing at 1.94m/s decreases under the influence of gravity as the height increases, hitting the top of pressure vessel and recirculating without affecting the flow of others.

When the diameter was same, the pressure difference depending on the height increases but the range was negligible at a maximum of 1Pa. However, as the diameter increased, the difference between the previous values was reduced. The pressure difference was a very small number compared to the operating pressure, but it was one of the important factors in the design as negative pressure occurs in the contraction pipe, resulting in additional recirculation zones.

The negative pressure in the pressure vessel appears at the entrance of the outlet of the pressure vessel. The pressure difference was greater at the outlet than at the inlets, and the stagnation zone was formed by the negative pressure. It can be problems such as recirculation, corrosion, cavitation, etc.

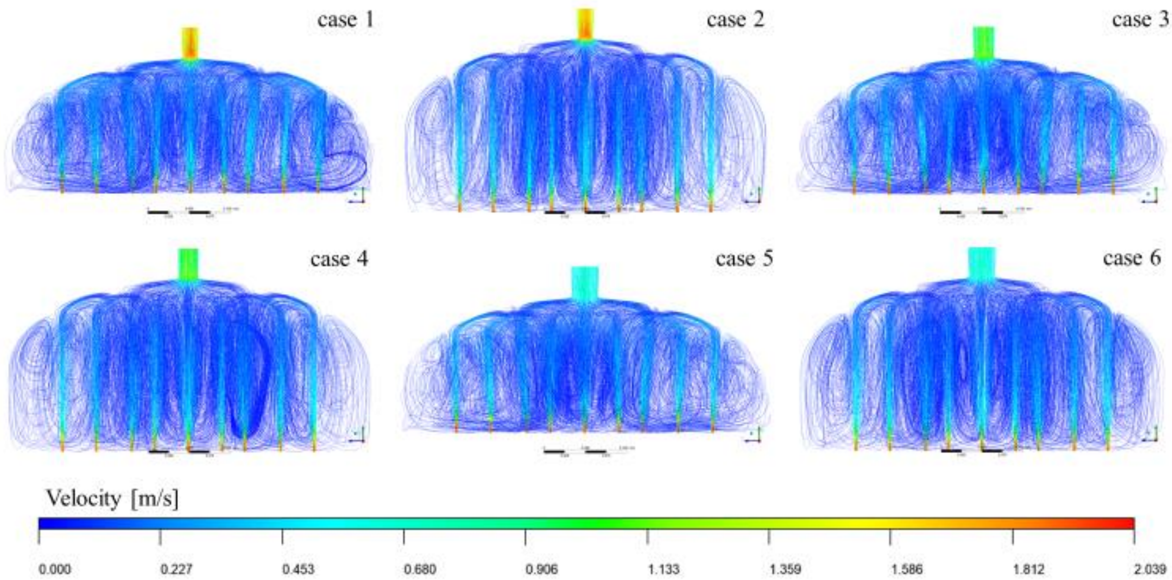

Figure 2. Velocity streamlines without fillet

3.2. Comparison of fillet effects

Optimized geometry was selected to compare the effect of fillet presence and absence. The size of the fillet was compared by varying the size of the fillet based on Case 6. When the size of the fillet was increased to 5mm and 10mm based on Case 6, the pressure difference was reduced compared to the previous value.

However, the difference between Case 7 and Case 8 was very small compared to the difference between Case 6 and Case 7. Thus, adding fillets reduces the size of negative pressure, but as the size of the fillet increases, the amount of reduction in negative pressure size with the previous value decreases.

IV. CONCLUSIONS

The analysis of the internal flow of MSR according to changes of variables has been carried out. The results of this study were as follows:

1) The streamline inside the pressure vessel was related to the height of the pressure vessel rather than the diameter of the single outlet. As the height increases, the kinetic energy of the flow decreases due to gravity, thus reducing the interference of the flow.

2) As the diameter of outlet increases, the size of the negative pressure generated at the entrance of the outlet decreases, and the pressure difference decreases.

3) When adding fillet geometry to the entrance of the outlet, it was effective in reducing the size of negative pressure. However, even as the size of the fillet increases, the amount of reduction in negative pressure size with the previous value decreases.

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