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3D Simulation of Hydrogen Production from Methanol Steam Reforming reactor

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***Abstract*— This work is a 3D numerical study, by the software Fluent, in this paper we are interesting to study the transfer phenomena (heat and mass) inside a methanol steam reforming reactor, the goals of work is to show the distributions of temperature field and the chemical species distribution, the reactor capacity, and influence of metal foam inside this reformer. The results show that the beside walls active there are a great thermic gradients and mass transfer because of reaction, in further we founded that the efficiency of this reformer is equal 43%. And insertion of metal foam increases their efficiency by 38%.**

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***Keywords*— 3D numerical study, methanol vapo-reformer, transfer phenomena heat and mass, metal foam**

I. INTRODUCTION

The procedure of methanol vapo-reforming is reaction to hydrogen production, this hydrogen supplies the combustible battery to produce electrical energy, currently, and this subject is a great project world in the field of renewables energies, so for that it has attracting the attention of researchers of world. Among these researchers, we are going to represent the following:

Hassan S.P et al. [1] were studying the hydrogen production from methanol steam reforming, in the catalyst $Cu/ZnO/Al_2O_3/CeO_2/ZrO_2$.,by the varying operational temperature [230-270 °C]. The results established that the methanol conversion depends strongly on the reaction temperature, therefore the maximum conversion obtained at 270 C.

Hongfang Mr. et al. [2] presented a numerical study for the methanol steam reforming on the catalyst of $CuO/ZnO/Al_2O_3$. The goal of this work is to study the hydrogen production and the thermal behavior inside the reformer. The results show that the temperature distribution varies clearer than the chemical species concentration. Therefore, the hydrogen production has a positive relationship to the food ratio and reactor inlet temperature.

Reiyu C. et al. [3] were numerically studying the transfer of heat and hydrogen production rate for a methanol steam reformer. This reaction is characterized by the thermal energy consumption (endothermic). Their results present that the axial conduction heat flux by plays a big role in the heat transfer and hydrogen production efficiency. The thermal energy of feed ratio also increases reactor performance.

In the second work of Reiyu C. et Al [5], ware testing carried out on a methanol steam reformer. The experimental results indicate that reactor efficiency depends on the reaction temperature, and also on the food molar ratio (MeOH/water).

The last study of Rei-Yu C. et Al [6], they ware numerically treating the reformer performance, this reactor is feeding by thermal energy by two way: internal and external. They noted that there is not a difference on the results between the two types in heating.

Ching-Yi Hsueh and Al [7] presented a numerical study on the transfer phenomena and the hydrogen production of a reformer with a serpentine flow. They were interesting to study the influence of the wall temperature, the molar ratio (H_2O/MeOH) and the Reynolds number on this reactor efficiency. Their results give: the high walls temperature, the small Reynolds number and the increase in the molar ratio (H_2O /MeOH) increase the hydrogen production.

Currently, we are interesting to study the transfer phenomena (heat and mass) inside a methanol steam reformer, we going to use software Fluent, by three-dimensional simulations. The goal of work is to note the temperature field distributions and the chemical species concentrations, thus the reactor efficiency and metal foam influence inside this reformer.

II. DESCRIPTION OF METHANOL STEAM REFORMING REACTION

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A. REACTION KINETIC LAWS

Methanol steam reforming reaction (Eq. 1), is largely studied in Peppley literature et al. 1999 (a [8], b [9]), Purnama et al. [10], Gao et al. [11] and Sandra Sa et al. [12]) on a commercial catalyst of $CuO/ZnO/Al_2O_3$:

$$CH_3OH + H_2O \longrightarrow CO_2 + 3H_2 \quad (1)$$

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There is a great discussion about this reaction mechanism. On the one hand, Santacesaria and Carra [13] proposed that reaction of methanol steam reforming is a sequence two reactions; methanol decomposition, followed by the water gas shift:

$$CH_3OH \rightleftharpoons CO + 2H_2 \quad (2)$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \quad (3)$$

In addition, [14] Takahashi et al. (1982), Jiang et al. (a [15], b [16]) proposed a mechanism suggesting an intermediate product which is methyl formate:

$$2\,CH_3OH \longrightarrow CH_3OCHO + 2H_2 \quad (4)$$

$$CH_3OCHO + H_2O \longrightarrow CH_3OH + HCOOH \quad (5)$$

$$HCOOH \longrightarrow CO_2 + 2H_2 \quad (6)$$

B. THE REACTION RATE

According to the articles [15] and [16], we can calculate the reaction rate by the flowing formula:

$$r_{vrm} = k_0 \exp\left(\frac{-E}{RT}\right) P_{CH3OH}^{n_1} P_{H2O}^{n_2} \quad (7)$$

Such as:

- $n_1 = 0.26$.
- $n_2 = 0.03$.
- $E = 105.1$ [kJ.mol^{-1}]. (Activation energy)
- $k_0 = 2.85.10^9$[mole $_{CH3OH}$ $kg_{cat}^{-1}.s^{-1}.kPa^{-\Sigma ni}$]. (Pré-exponentiel factor).

III. PHYSICAL MODEL

Our physical model is shown on figure 1, which is defined like three-dimensional rectangular channel having a 10 mm length and a size of face 0.6 mm *0.6 mm [17]. The flow direction is along the x-axis and the upper wall is defined as the catalyst which is active wall of reactor, and the remains walls are defining adiabatic walls. Our choice is based on the conclusions of Omidbakhsh et al. [17].

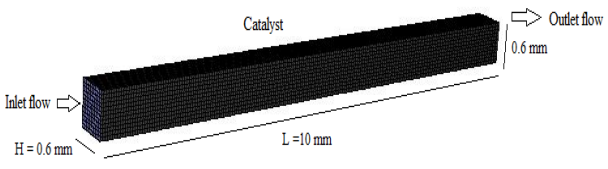

Fig. 1 our physical model for methanol steam reforming reactor

IV. THE SIMULATION HYPOTHESES

- The following assumptions are considered:
- The flow regime is laminar and stationary.
- Gases are considered perfect gases.
- Negligible load losses.
- The pressure drop is zero; the operating pressure considered is the atmospheric pressure.
- The gases physical characteristics are constant.
- The gases can be modeled as incompressible fluids (constant density). In microscopic and macroscopic calculations, this hypothesis is considered for pressure changes less than 20% of the operating pressure [18].

V. RESULTS DISCUSSIONS

A. VALIDATION :

Our work is compared with that of Jeong-Se Suh et al. [20]. The figure2 shows the evolution of the temperature curves. A great similarity between the two curves is observed especially in the first part or a rapid increase in temperature is observed. In the second part where we find a zero temperature gradient (the flow regime is established).

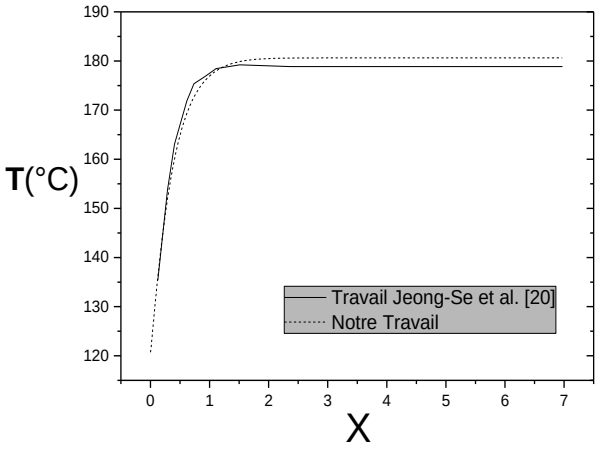

Fig.2 Comparison between the axial temperature distribution present work Vs [20].

B. SMOOTH CHANNEL (WITHOUT METAL FOAM):

1. TEMPERATURE FIELD:

Figure 3 shows the temperature filed inside the methanol steam reforming reactor; this picture watches the temperature distribution is defined by the inlet flow temperature °C 120 (393K), just the 10% first of dimensions channel, we have a

variation in distributions temperature, after that, the thermal field is maintained constant 453K in the rest of the channel, It is due primarily of the continuous and homogeneous provisioning applied by the hot wall.

2. CHEMICAL SPECIES DISTRIBUTION

The figures 4(a, b, c and d) are clearly shown, those pictures represent the molar fractions variation of the chemical species in function of along reactor lower wall. These figures indicate a reduction in reagents CH_3OH and H_2O accompanied by an increase in the products what are H_2 and CO_2, this evolution are logical because of the first two chemical species consumption and appear the two other species.
According to the figure 4.a, the efficiency of this reactor is defined by the methanol molar fraction consumption, which is calculated by the formula of [4]: $\eta = 43\ \%$.

C. CHANNEL WITH METAL FOAM

1. TEMPERATURE FIELD

Figure 5 shows the structure of the temperature profiles inside the reactor, if we are making compare between the two images, This case with that of pure fluid (fig.3), the insertion of the porous layer makes a thermal stability inside the reactor, there is no great difference in temperature between the active wall and the field, that means the temperature varied generally in the [453, 440 ° C].

2. CHEMICAL SPECIES DISTRIBUTION

Figure 6 (a, b, c and d) shows four images which give the molar fractions evolution of the four chemical species. We see that these images are similar to those that correspond to the smooth channel (fig.4.a, b, c and d). The difference between the two cases lies in the quantities of reagents and products which are more important in this second case. According to the figure 6.a, the reactor will be: $\eta = 81\%$.

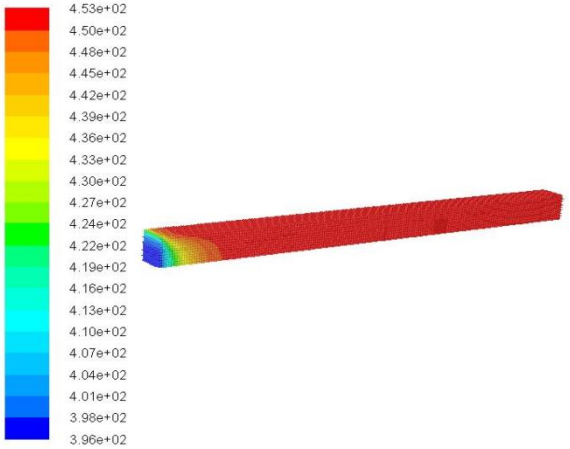

Fig.3: the temperature filed inside the rector (smooth channel case).

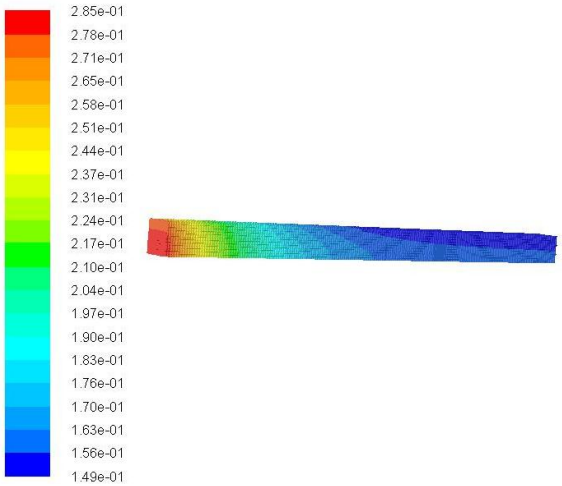

Fig. 4.a CH_3OH molar fraction distribution (smooth channel case)

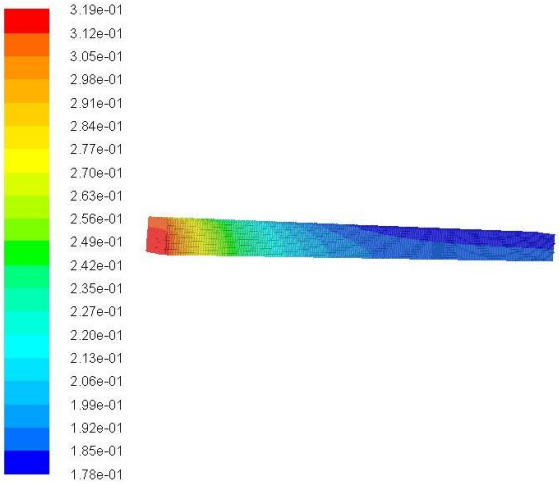

Fig. 4.b H_2O molar fraction distribution (smooth channel case)

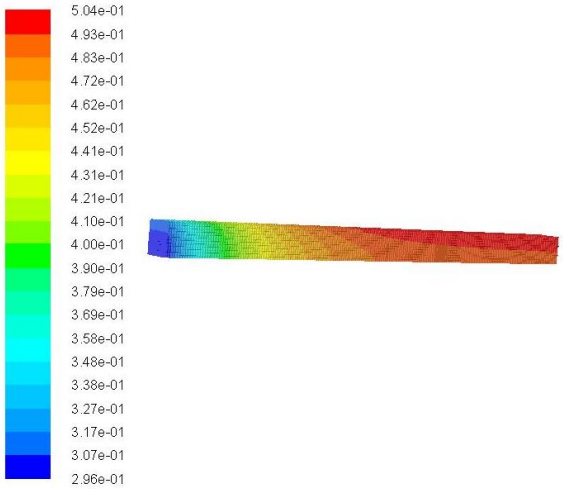

Fig. 4.c H_2 molar fraction distribution (smooth channel case)

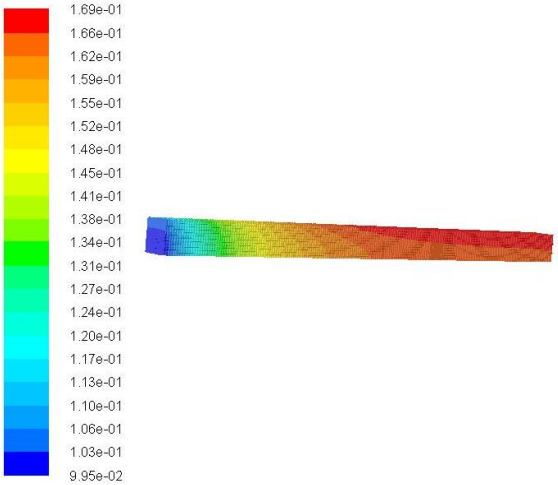

Fig. 4.d CO_2 molar fraction distribution (smooth channel case)

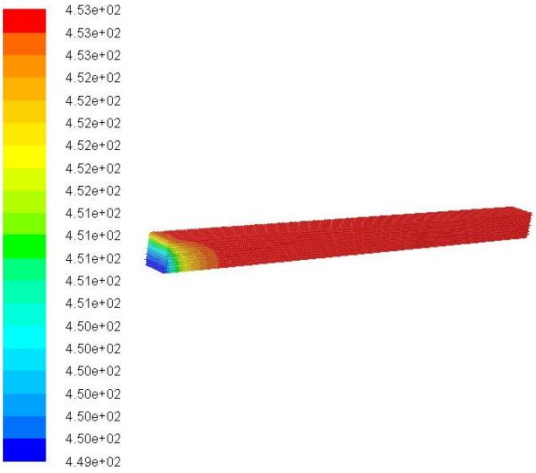

Fig. 5 the temperature filed inside the rector (channel with metal foam case).

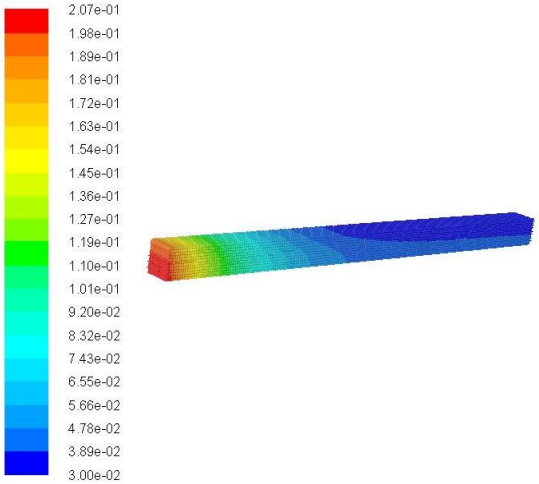

Fig. 6.a CH_3OH molar fraction distribution (channel with metal foam case)

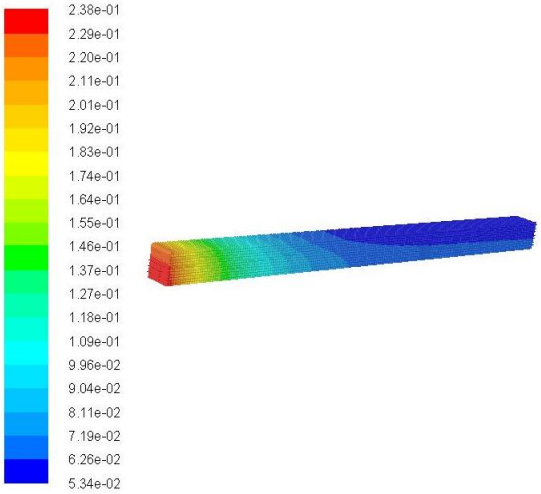

Fig. 6.b H_2O molar fraction distribution (channel with metal foam case)

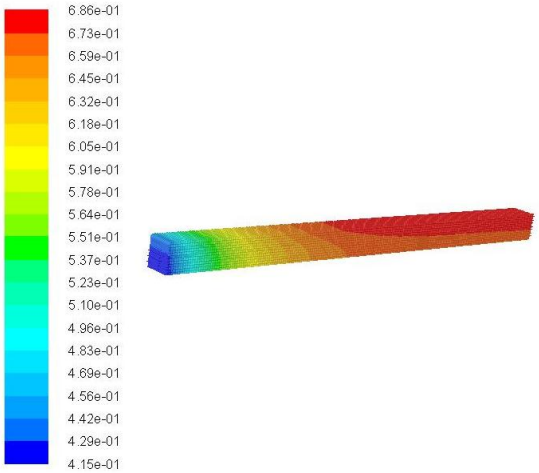

Fig. 6.c H_2 molar fraction distribution (channel with metal foam case)

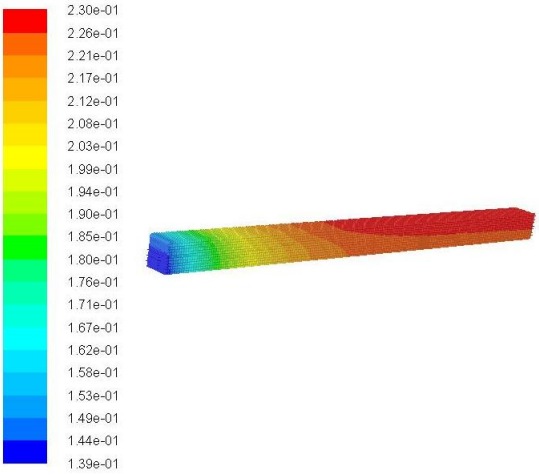

Fig. 6.d CO_2 molar fraction distribution (channel with metal foam case).

VI. CONCLUSIONS

In this work, we presented a 3D numerical study by Fluent, for hydrogen production from methanol steam reforming reactor; we represented this reaction and another part on the kinetic laws. The principal result of this work is the reformer efficiency is more than 43%, this capacity is acceptable because it is given in the literature [19], and (an output of 40%, with an error of 7%).

The insertion of a porous medium inside a reactor influences: on the mass transfer of mass by a greater consumption of the reagents and a greater production of hydrogen. The same effect thermal transfer, which is due to a good distribution of thermal energy inside the reactor and consequently greater thermal field stability. This gave a significant increase in reactor efficiency with a value greater than 38%, this increase in efficiency remains like results of simulation, while waiting to validate this value.

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