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Numerical investigation of Catalytic Combustion of Methane Using Wall Surface Reactions

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Abstract **–**Catalyzed combustion is a low-temperature, flameless process that emits less nitrogen oxide. It also specifies flammability limits and reactor design constraints. Catalyzed combustion's advantages determine its potential applications. We present a numerical analysis of the catalyzed combustion of a methane-air mixture on a heated platinum channel wall. The cylindrical channel is modeled with 2D axisymmetric solver. The modeling is based on the "Species transport. The finite volume calculation code Fluent was used to create the various numerical simulations. Interesting findings have been made regarding temperature and the mass fractions of the various species involved in combustion, including methane (CH4), carbon dioxide (CO2), water (H_2O), and nitrogen monoxide (NO) as sources of pollution issues.

Keywords – Catalyzed Combustion, Mass Fractions, Species Transport, Finite Volume, Carbon Dioxide.

I. INTRODUCTION

Catalyzed combustion is a flameless process that occurs at low temperatures, resulting in less nitrogen oxide. It also specifies reactor design constraints and flammability limits. These advantages determine the potential applications of catalyzed combustion. The catalytic oxidation of methane over noble-metal catalysts such as Pt, Pd, and Rh is of interest because it has a dual application for energy production (complete combustion) while emitting minimal pollutant emissions such as NOx.

Research on catalytic combustion is presently concentrated on, efficiency improvement, reactor design, and the quest in favor of better catalysts. Therefore, a deeper comprehension of the chemical and physical processes taking place on the catalytic surface and the interaction of the contiguous fluid domain is extremely important. Detailed models for catalytic combustion models have been developed, which include multistep heterogeneous surface reaction mechanisms. These models could serve as a guide for comprehension and optimizing catalytic combustion. This is particularly true of the behavior of the oxidation of hydrocarbons during ignition and extinction. [1-6].

In present work the impacts of heated wall on the combustion factors of a CH_4/air mixture under Platinum catalyst were numerically investigated.
A two-dimensional channel with longer l=60mm and d=0.9mm simulation is used to investigate the catalytic conversion of methane on platinum wall with various velocity and different ratio of CH_4 and H_2.

2. Modeling approach:

Our method of simulating catalytic combustion involves connecting fluid movement with chemical reactions occurring in the gas phase and at the gas-surface interface. The conservation equation and extra conservation equations for each chemical species, Navier-Stokes, and energy equation, all contribute to the description of fluid movement. The ideal gas law closes this set of equations. The fluid

flow is laminar in the circumstances examined in this research.

The current work used numerical analysis to examine the flow characters upon a catalytic platinum heated wall via a cylindrical channel using wall surface reactions.

3. Results and discussion:

3.1.Influence of velocity on methane conversion:

Fig.1 shows how inlet velocity affects methane conversion and shows that when inlet velocity increases in the channel, methane combustion drops noticeably. When the inlet velocity raises, the chemical reaction time when the fuel traverses the channel is so short that if the inlet velocity exceeds 1.7 m/s, the rate of combustion increases, resulting in unstable methane conversion.

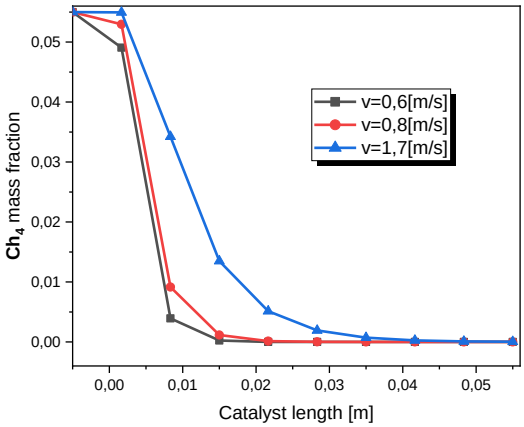


Fig.1 methane conversion as a function of various Velocity.

3.2. Influence of H_2 on methane reforming with CO_2:

Fig. 2 shows the remarkable Influence of H_2 on the methane conversion which the entire oxidation of methane initially produces H_2O and CO_2 then. Water is consumed as temperature rises as a result of the heat transformation reaction with the residual methane.

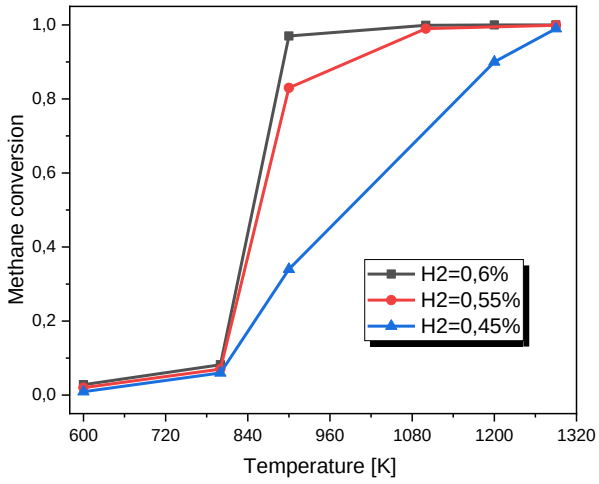


Fig.2 methane conversion as a function of temperature for various Values of H_2.

3.4. Influence of ch4 ratio on methane conversion:

Figure 3 depicts the significant influence of increasing the CH_4 ratio on the methane conversion with temperature; it can be seen that a low portion of methane causes the conversion to be delayed and requires a higher temperature than a ratio of CH_4=0.05.

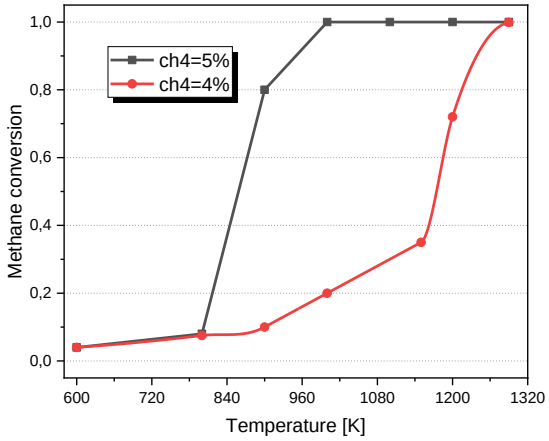


Fig.3 methane conversion as a function of temperature for two Values of Ch4

Fig. 4 clearly shows the distribution of Pt(s) surface coverage. For the two hydrogen values, it demonstrates that the surface coverage of Pt(s) goes up from the entry and then reaches its maximum before the outlet. The surface coverage of Pt(s) increases with lower hydrogen at 0.45%. While curves of Pt(s) surface coverage increase with decreasing H2, and achieve a maximum surface coverage of Pt (s).

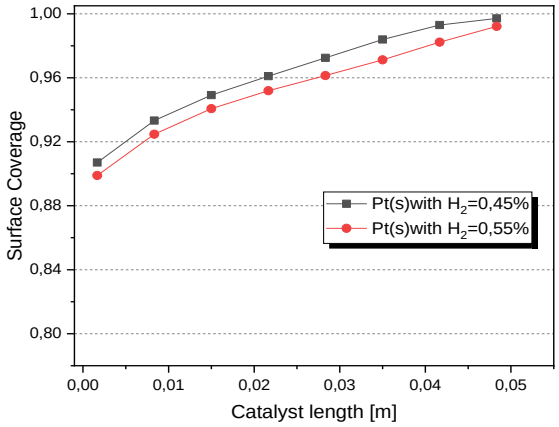


Fig.4 Simulated surface coverage on platinum versus catalyst length

The fig.5 shows the distribution of the concentration profiles of H(s), O(s), and C(s) along the catalyst length. Adsorbed oxygen reacts with C(s) to form CO(s) in the first part of the reactor, and complete oxidation of CO2. H(s) decreases gradually along the reaction axis to form H_2O. Therefore, fresh oxygen adsorbed produces CO(s). Water formation, on the other hand, continues along the catalytic reactor. We observed an increase in O(s) due to the little methane that is absorbed into the surface, the methane's slow chemical reaction rate, and the poor conversion rate.

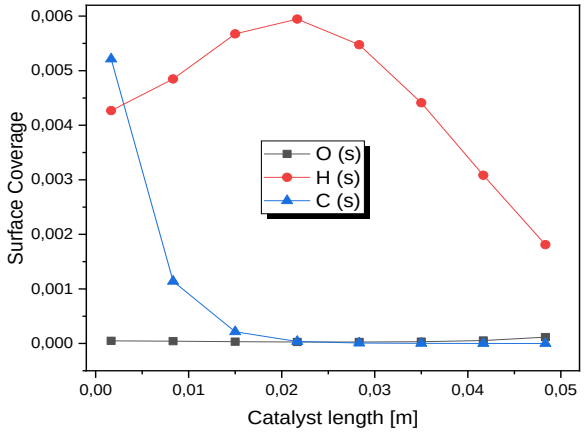


Fig.5 Simulated surface coverage of mainly products on platinum

Fig. 6 present a comparison between the simulated mole fraction of NO along the catalyst length in the presence of hydrogen with two values, the evolution of NO at the highest value of H_2=0.0055 does not occur because the platinum surface is obstructed by the high CO coverage. Furthermore, the reduction of nitrogen oxide by increasing hydrogen is clearly demonstrated. High carbon monoxide coverage increases the activation energy of this reaction. The presence of H_2 is more important than the concentration of the reducing agent in the lowering of nitrogen oxide.

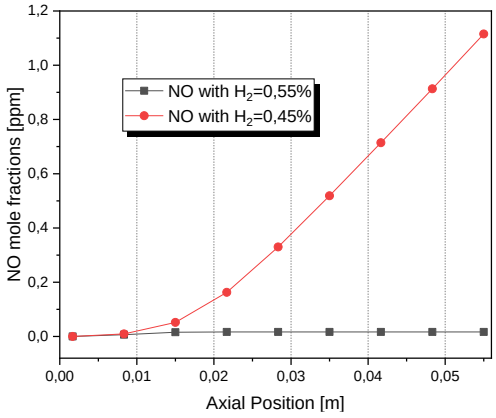
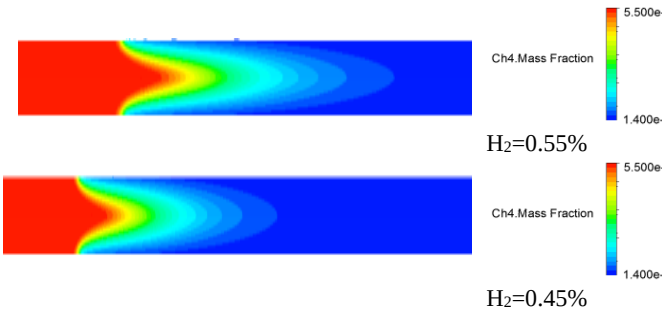


Fig 6 : Influence of H_2 concentration on the NO production

We use the simulation and modeling tools that have been developed. The two-dimensional species profiles of the reactants, methane, and all significant products in the catalyst channel are shown in Fig. 7. The operating temperatures for the computation of the profiles were 1290 K and ch_4=5.5% under isothermal circumstances. The addition of hydrogen to the initial mixture provides a way to catalyze the combustion of methane on platinum; the main effect of hydrogen addition is to provide enough heat to reach a catalyst temperature at which the methane oxidation process combusts. At two H_2 ratios, the qualitative reaction analysis reveals the effect of increasing H2 from 0.0045 to 0.0055.



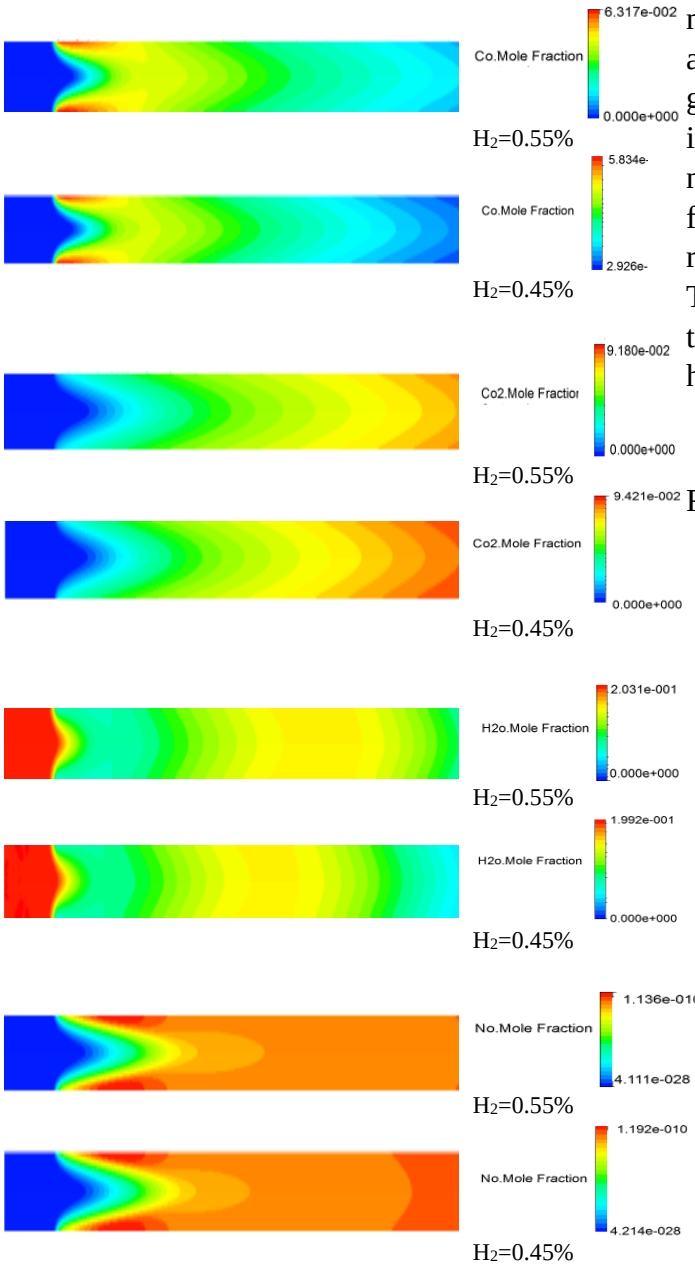


Figure .7:Numerically predicted profiles of mole fractions of reactants and major products along the catalyst for two different value of H2

Conclusion:

The performance of the heated platinum wall of cylindrical channel is numerically studied through a CFD Fluent code. The effect of inlet velocity, hydrogen addition, ch4 ratios, heated wall and surface coverage was investigated; the two-dimensional simulation reveals the interaction of mass and heat transport and surface chemistry. When it comes to the kinetic behavior of species that cannot be studied in experiments, modeling will be capable of explaining the findings. It has been revealed that as inlet velocity continuously rises, methane conversion decreases. Methane conversion and the reduction of pollutant gaseous emissions are greatly influenced by the addition of hydrogen. The influence of H_2 on the temperature of reforming methane is exposed to be more important at low fraction of H_2. The impact of H_2 on O(s) coverage is revealed to be more substantial at low fraction of H_2. The mole fraction of H, increases than decrease together with C(s) and O(s) respectively with hydrogen addition.

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