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Effects of Inlet Temperature and Channel Geometry on the Efficiency of a Catalytic Converter

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Abstract— **Environmental pollution is a problem of all civilized countries. Air pollution is a part of the problem and many researchers are working in the control of air pollution of various sources. One of these sources is vehicles. Some researchers are working on more efficient, less pollutant engines; some are working on developing the strategies and control techniques to satisfy the regulations about pollutants. During the cold start of an engine, the exhaust gas air pollutants are in high levels. Catalytic converter channels have square cross-sections. In this study, a catalytic converter channel was analyzed numerically by using a commercial CFD code. Inlet temperature of the channel was changed, and then the efficiency of a catalytic converter was calculated. All calculations of reduction of methane gas in the exhaust gas were modeled using twenty four equation surface reaction model. Every reaction is defined in the interface of the CFD code. Since the channel cross section was small enough, Reynolds number was less than 2300, the flow in the channel was considered to be laminar. SIMPLE algorithm is employed. The conversion efficiency of the catalytic converter was calculated on the reduction carbon monoxide and hydrocarbons, respectively, for each case. After the results were obtained for square cross-sectioned channel, the channel geometry was changed as triangular and oval cross-sectioned channel designs. The designs were constrained by same hydraulic diameter as square cross sectioned channel. The effects of inlet temperature and channel cross section on the conversion efficiency of a catalytic converter were investigated. The results are presented in terms of contours of species concentrations, velocity, pressure and temperature. It is seen that when the inlet temperature of the catalytic converter increased, the conversion efficiency increases as expected. In addition, the results were also compared with the results found in the literature, and observed that results are consistent with them.**

Keywords—Internal combustion engines; catalytic convertor; exhaust emissions; modeling; CFD

I. INTRODUCTION

Urban air pollution is a major problem of cities. Internal combustion engines are one of the major sources of air pollution for all seasons. The production of automobiles is growing every year. However, some hybrid and/or electric vehicles could be seen on the streets; reducing the emissions of conventional internal combustion engines is still important. One way to reduce emissions without any structural modifications on the engine is using the after treatment systems. One of these systems is catalytic converters. Catalytic converters are widely used in the automobile industry. Catalytic converters could be added to the old cars without catalytic converters, but that time these converters work as oxidation catalysts. In this study, a catalytic converter channel was analyzed numerically by using a commercial CFD code. In the analyses, inlet temperature of the exhaust gas was changed, and then the efficiency of a catalytic converter was calculated according to calculations in the channel of the catalytic converter.

There are numerous works on three-way catalytic converters. These studies can be divided into two: experimental and numerical studies. In this study we used numerical methods technique to determine the effects of inlet temperature and channel design on the conversion performance of a three way catalytic converter. Few of the literature including numerical methods are given.

A brief review of catalytic converters was given in Heck and Farrauto [1]. In this short brief the development and improvements of catalytic converters which are used in automobiles were discussed. In another study the same researchers, they reviewed the working principles of catalytic converters [2]. Aimard et al. [3] used mathematical model for catalytic converters. They presented one dimensional transient models with different numbers of variables. It is shown that, the medium complexity model, which they used in their study, can be utilized to study conversion efficiencies of CO, HC and NO_x emissions. Kishi et al. [4] described hybrid catalysts and electrical heated catalysts. Electrical heated catalyst was located downstream of hybrid catalyst before three way catalytic converter, by this way they had more efficient conversion of HC emissions after the start of the engine.

Tsinoglou et al. [5] used a commercial CFD software in their study. They modeled the whole catalytic converter as a one piece. They compared their results with other studies' results. They showed radial velocity component was consistent with experimental data. They introduced a new model FRM (Flow Resistance Modeling) method. This model was validated with CFD code results. The results were given in figures both CFD and FRM method together. They mentioned this new method can be coupled with transient

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chemical reaction models for catalytic converters. In another study, multi-scale analysis and strategy is searched to take a comprehensive view approaching catalyst design perspective and explained impacts of designs at different scales to a catalytic reaction process [6]. Santos and Costa [7] investigated the catalytic converter efficiency experimentally. They compared ceramic and metallic substrates. They concluded at low velocities ceramic substrate has higher conversion efficiency of CO and HC emissions than metallic one. On the other hand, metallic substrate has higher conversion efficiency at higher velocities [7]. For three channel geometry and 3 different dimensional modeling strategies are applied to three channel geometry by Mladenov et al. [8]. They compared 18 numerical models for modeling mass transfer. They investigated flow and mass transfer in the monolith channel in details using these models. They compared the results of numerical simulations with experimental data [8].

Kumar and Mazumder modeled a full scale catalytic converter using a CFD code. They added complex heterogeneous chemical reactions to solution. Steady state calculations were performed for a catalytic methane–air combustion process with 24 reaction steps and 19 species, and for a three-way catalytic conversion process with 61 reaction steps and 31 species for a monolith with 57 channels. Also, they took into account parallel computing [9]. In another study, the researchers Kumar et al. [10] proposed a new model of three-way catalytic converter. In their model, there are seven differential equations. They tested the model with real emissions data. They also proposed an aging model for catalytic converters [10]. Agrawal et al. [11] modeled a two dimensional catalytic converter with 21 channels. They solved chemical reactions. They used a commercial CFD code. They investigated flow, and calculated velocity and mass rates to show the effects of flow which is not equally distributed in the catalytic converter on the conversion efficiency. They showed their results in the graphics. Bertrand et al. [12] proposed a model based on lattice Boltzmann method –LBM, this method solves directly the Navier-Stokes equations and the method uses a fully implicit scheme. They modeled flow in an elliptical shaped honeycomb monolith reactor comprising a total of 7539 parallel channel. They presented velocity contours on some selected planes.

Hayes et al. [13] modeled a full size catalytic converter not a channel. They concluded that the monolith substrate configuration has a significant impact on the flow and temperature distributions, pressure drop, and on the resulting chemical reactions. Ling et al. [14] measured the concentrations of exhaust emissions, air-fuel ratio before and after the catalytic converter in which CeO_2 is the catalyst in the washcoat. They determined the dynamic behavior of this catalytic converter.

In our previous study we showed that more complex reaction models give better results [15].

II. Numerical Study

Computational fluid dynamics codes are widely used to model the fluid flow and heat transfer problems. These problems have the wide range from simple to complex physical problems. Also, combustion problems can be solved using computational fluid dynamics. However, in order to calculate the combustion, additional species transport equations should be solved. Also, the combustion reaction equation and model that predict combustion are widely. One of the limitations for these models are computational time. Models with complex and more equations need more computing time on a single processor. There are various algorithms and methods for modeling. In this study, three dimensional continuity, momentum, energy and species equations were solved together.

Continuity equation or in other words conservation of mass equation is given as

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0 \qquad (1)$$

Generalized momentum equation can be written as [16];

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu_{eff}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \sum \rho_s F_{si} \qquad (2)$$

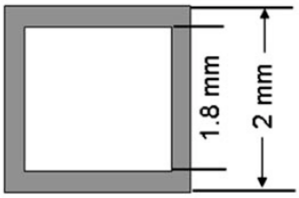
To determine the temperature distribution energy equation should be solved. Energy equation is given as

$$\rho \frac{De}{Dt} + p\frac{\partial u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) - \frac{\partial q_{rj}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\sum_s D\rho \frac{\partial Y_s}{\partial x_j} h_s\right) + \Phi + \sum_s \rho_s F_{si} V_{si} \qquad (3)$$

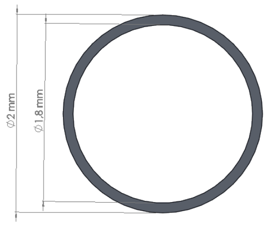
Species transport equation for solution of chemical reactions given as

$$\frac{\partial}{\partial t}(\rho Y_s) + \frac{\partial}{\partial x_j}(\rho Y_s u_j) = \frac{\partial}{\partial x_j}\left(D\rho \frac{\partial Y_s}{\partial x_j}\right) - w_s \qquad (4)$$

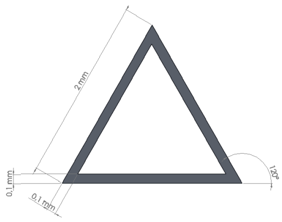
In order to determine the effect of channel design, three different channel geometry were selected as follows: square, circular and equilateral triangle cross-sections. The square cross-section was selected from [17]. The circular cross-section had the diameter of 2 mm, the equilateral triangle had 2 mm length per side. The porous medium inside all channels had 0.1 mm thickness. The length of the channel was selected as 127 mm. Results were given as contour graphics on the plane which passed through the center of the cross-section.



(a)



(b)



(c)

Fig. 1. Problem geometry (a) square cross-section [17], (b) circular cross-section, (c) equilateral triangle cross-section.

Methane was selected due to simple chemical structure. All investigation were conducted on methane gas. The equations used in this study were taken from [18]

In our analysis, Ansys Fluent 14.5 commercial CFD code was used. This commercial CFD software has ability to add species equations and then solve them. Inside the code there is 'Reaction Mechanism' window. Using that input window we select all equations which will involve in chemical and catalytic reactions. In the beginning densities of species were selected as 2.8×10^8 kgmol/m^2 and the washcoat precious metal value was selected as 1. Then, the surfaces were defined on which the surface reactions would take place. In the solutions the reaction equations were solved simultaneously inside the code.

Inlet and boundary conditions were given in Table 1. Wall temperature of the catalytic converter was 1000 K at constant value. Laminar flow condition was selected because inside the catalytic converter channel flow conditions are laminar, on the contrary inside exhaust pipe flow condition is turbulent [19].

Two layer mesh was created; therefore, the porous part was taken into account. The 'Skewness' and 'Orthogonal Quality' values were checked inside the CFD software to get more accurate results. Grid independency tests were done, and it was decided that the results for 78105 grids are accurate enough for square cross-sectioned channel (Fig.2).

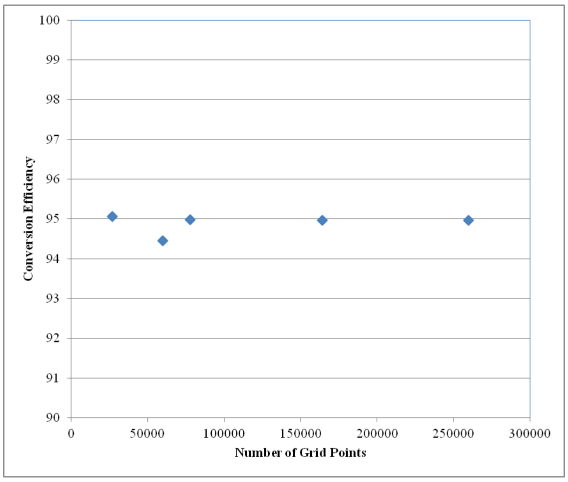


Fig. 2. Grid independency study results.

$$H_2 + Pt(s) + Pt(s) \rightarrow H(s) + H(s)$$

$$H + Pt(s) \rightarrow H(s)$$

$$O_2 + Pt(s) + Pt(s) \rightarrow O(s) + O(s)$$

$$CH_4 + Pt(s) + Pt(s) \rightarrow CH_3(s) + H(s)$$

$$O + Pt(s) \rightarrow O(s)$$

$$H_2O + Pt(s) + Pt(s) \rightarrow H_2O(s)$$

$$CO + Pt(s) \rightarrow CO(s)$$

$$OH + Pt(s) \rightarrow OH(s)$$

$$H(s) + H(s) \rightarrow Pt(s) + Pt(s) + H_2$$

$$O(s) + O(s) \rightarrow Pt(s) + Pt(s) + O_2$$

$$H_2O(s) \rightarrow H_2O + Pt(s)$$

$$OH(s) \rightarrow OH + Pt(s)$$

$$CO(s) \rightarrow CO + Pt(s)$$

$$CO_2(s) \rightarrow CO_2 + Pt(s)$$

$$O(s) + H(s) \rightarrow OH(s) + Pt(s)$$

$$H(s) + OH(s) \rightarrow H_2O(s) + Pt(s)$$

$$OH(s) + OH(s) \rightarrow H_2O(s) + Pt(s)$$

$$CO(s) + O(s) \rightarrow CO_2(s) + Pt(s)$$

$$C(s) + O(s) \rightarrow CO(s) + Pt(s)$$

$$CO(s) + Pt(s) \rightarrow C(s) + O(s)$$

$$CH_3(s) + Pt(s) \rightarrow CH_2(s) + H(s)$$

$$CH_2(s) + Pt(s) \rightarrow CH(s) + H(s)$$

$$CH(s) + Pt(s) \rightarrow C(s) + H(s)$$

III. Numerical Results

In order to see the effects of inlet temperature on catalytic converter conversion efficiency the inlet temperature was selected as 523 K, 623 K and 723 K, respectively. Reduction of methane is given in the figures. For simplicity the inlet and outlet parts of the channel were given in the figures. The species contours are given at the center of the cross-section. The inlet concentration was always same for all cases. To investigate the effects of inlet temperature, the concentration of CH_4, CO_2, O_2 concentrations along the channel were evaluated in this study; however, only variation of CH_4 concentration along the channel were presented in this manuscript.

The inlet concentration of square cross-sectioned channel can be seen from Fig. 3. Inlet concentration profile is similar but not exactly due to inlet temperature. The outlet methane concentrations of the channel were given in Fig. 4-6, with respect to inlet temperature values of 523 K, 623 K, and 723 K, respectively. For 523 K inlet temperature conversion of methane was not completed as seen from Fig. 4. There is no methane gas inside the channel when the inlet temperature was 623 K and 723 K. Increasing the inlet temperature reduces the length required to finish the catalytic process.

TABLE I. Inlet and Boundary Conditions

Flow Type	Laminar
Inlet velocity	5,5 m/s
Inlet temperature	523 K, 623 K, 723 K
Wall temperature	1000 K
CH_4 mass	0.05 % +0.05 %
O_2 mass	0.215 %

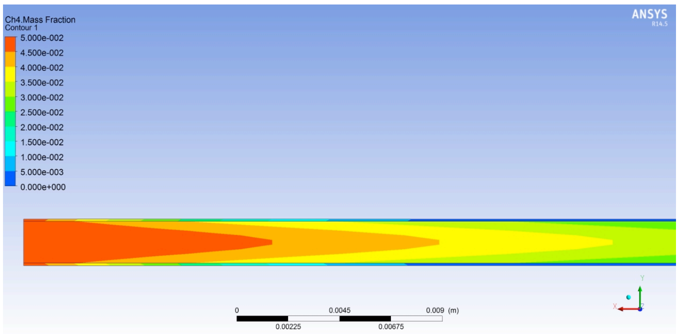


Fig. 3. Square channel inlet concentration 723 K.

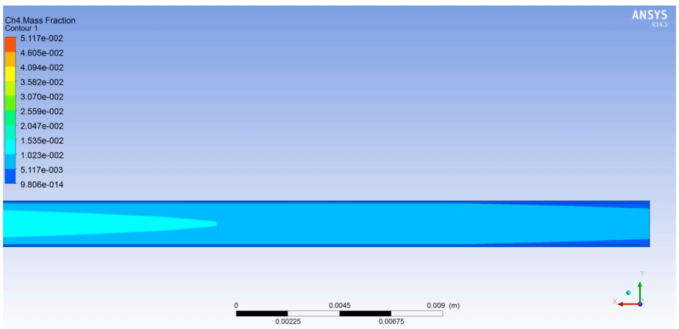


Fig. 4. Square channel outlet concentration 523 K.

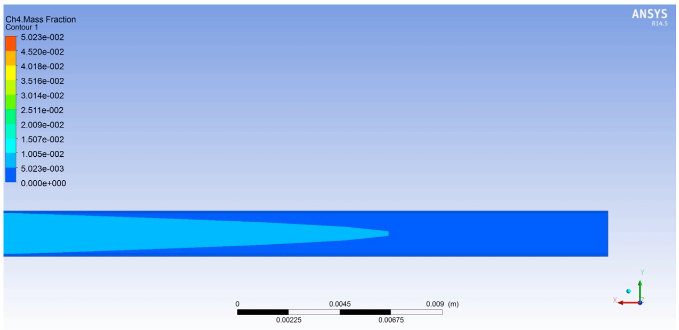


Fig. 5. Square channel outlet concentration 623 K.

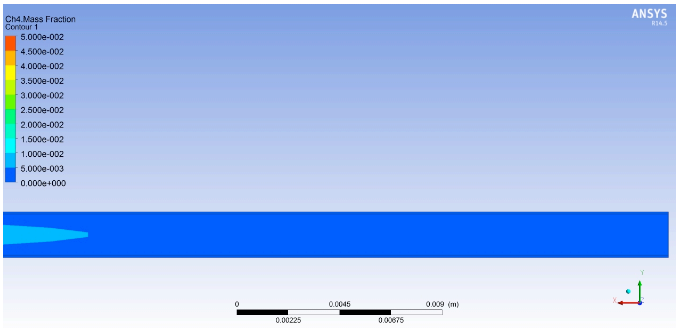


Fig. 6. Square channel inlet concentration 723 K.

If the channel design switched to circular design, the methane concentration reduces up to 10^{-13} values, i.e. nearly zero for 523 K (Fig. 8). On the other hand, for higher inlet temperatures methane gas concentration reduced to zero (Fig. 9, 10). The conversion completed nearly at the middle of the pipe for 723 K as seen from Fig. 10.

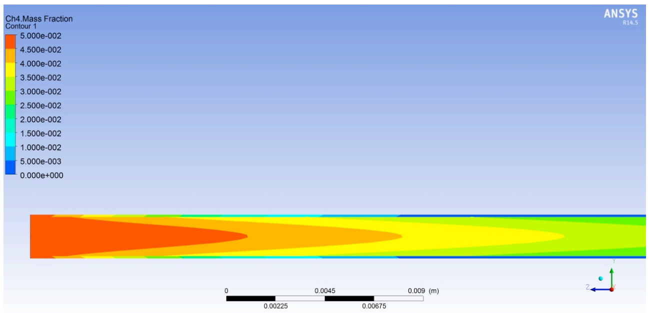


Fig. 7. Circular pipe inlet concentration 523 K.

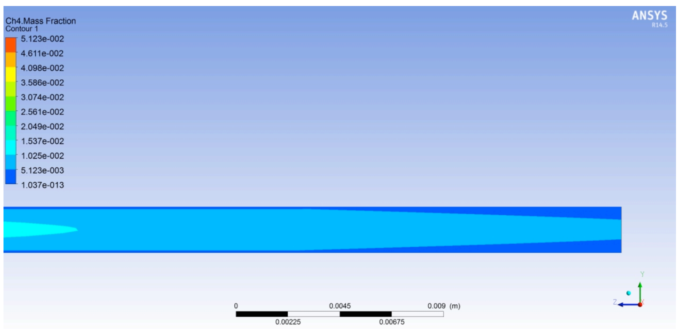


Fig. 8. Circular pipe outlet concentration 523 K.

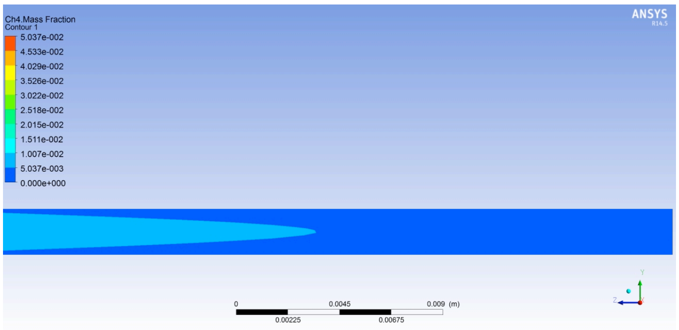


Fig. 9. Circular pipe outlet concentration 623 K.

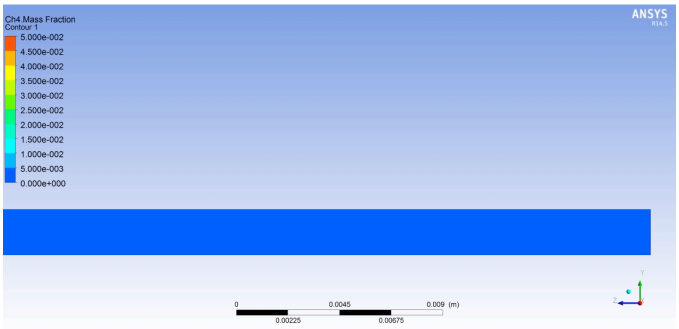


Fig. 10. Circular pipe outlet concentration 723 K.

When the equilateral triangle cross-sectioned channel was used, the methane converted quickly and there were no methane concentration at the exit of the catalytic converter. The equilateral triangular channel inlet concentration for 523 K was given in Fig. 11., and the full length channel concentration was presented in Fig. 12. It looked like the concentration contours were not symmetrical due to the plane which passes through the top of triangle to the base of the channel. Also, the thickness of porous medium can be seen at the top of the figure.

Recognizing the conversion efficiency it is not easy to follow the contour graphs. However, the conversion efficiency of three channels were given as charts. In Fig. 13 the catalytic converter efficiency is given for square channel with respect to inlet temperature. For 523 K conversion efficiency was less than 95 %, after the heated exhaust gas the efficiency rises to 98.4 %.

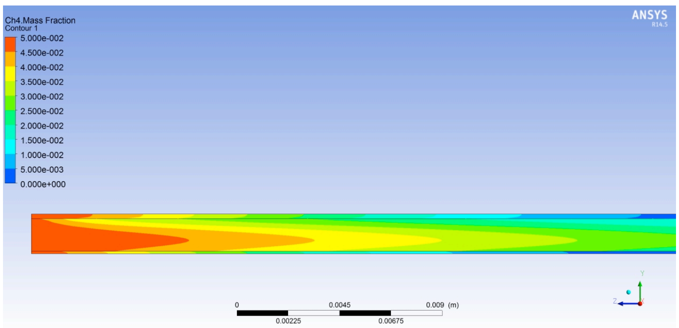


Fig. 11. Triangular channel inlet concentration 523 K.

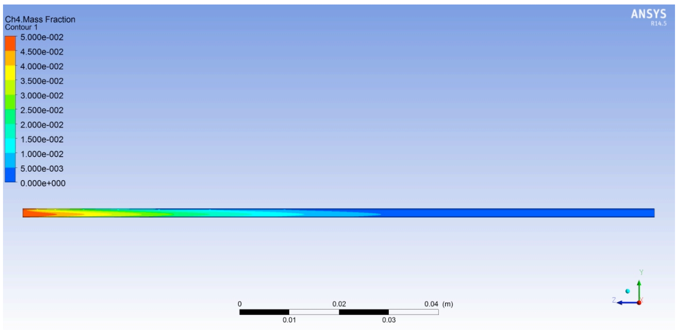


Fig. 12. Triangular channel full length concentration 523 K.

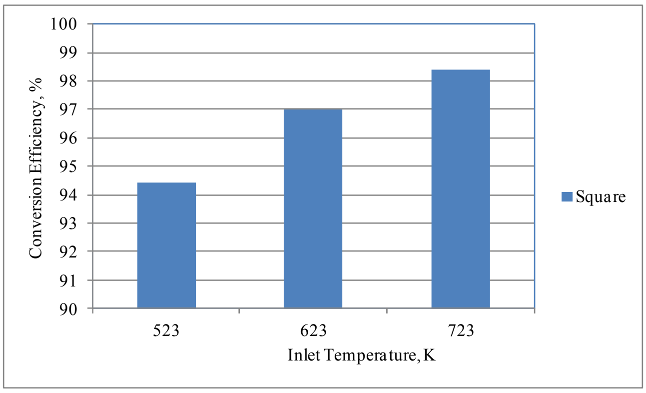


Fig. 13. Conversion efficiency of the square channel.

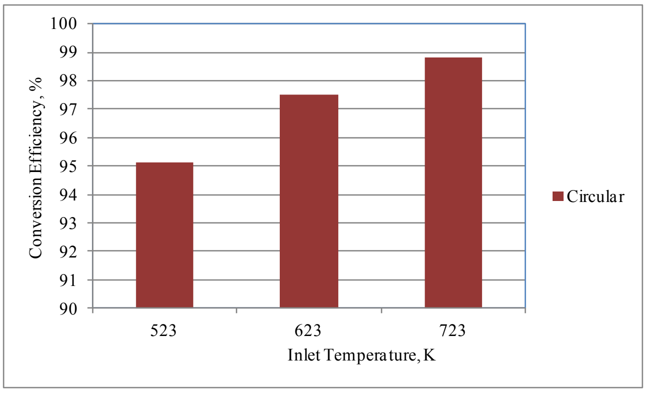


Fig. 14. Conversion efficiency of the circular channel.

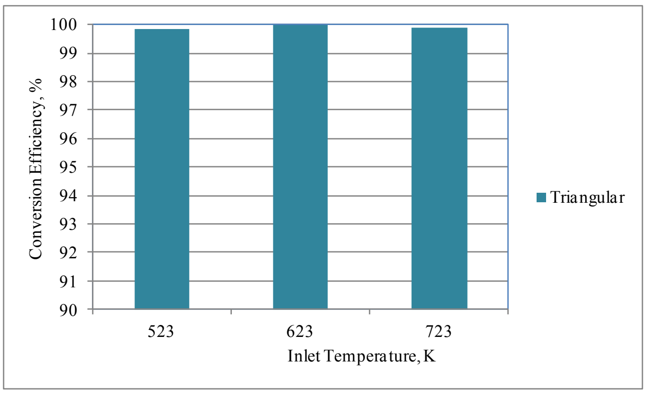


Fig. 15. Conversion efficiency of the circular channel.

For the circular channel the trend was similar to square channel (Fig. 14). However, for the equilateral triangular channel the conversion efficiency was very close to 100 % (Fig. 15). The reasons for this situation were thought as first the shape the cross section, because the angle between the sides was less than right angle. Second, the area of the triangle, because the area might be small compared with the other geometries. (The area decreases more than half for triangle cross-section compared to the area of square cross-section.) In the future work, the effects of the angle or shape of the triangle could be studied.

IV. CONCLUSION

The effects of inlet temperature and cross-section of channels were investigated: When the temperature was increased, the conversion efficiency increases. This is not correct for equilateral triangular cross-section. The conversion efficiency of the catalytic converter with triangular channels does not directly affected by the inlet temperature.

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