ANALYTICAL ANALYSIS OF CATALYTIC CONVERTER

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ABSTRACT

The automotive vehicles have been a significant contributor to air pollution on total mass basis. According to one survey it has been shown that transportation contributes about 44% (by wt.) of the major pollutants. Motor vehicles alone contribute about 40%. Transportation contributes about 55% of the man made hydrocarbons (HC), a little over 64% of the total carbon mono-oxide (CO) emission and about 40% of the nitrogen oxide (NOx).Major pollutants from automobiles are unburned hydrocarbon (UBHC), oxides of nitrogen, carbon monoxide, lead compounds, and oxides of sulphur. The air pollution due to these pollutants affects adversely materials, animals and human life. It reduces visibility to a large extent causing traffic hazards. The vegetarian and plants are affected badly by sulphur dioxide, photo chemical smog and lead. To evaluate the performance and design of catalytic converter in this work a mathematical model for catalytic converter is made which predicts the catalytic converter performance. We can optimize catalytic converter design by adjusting different parameters.

Keyword: *Catalytic converter, HC, CO, NO.*

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1. INTRODUCTION

Due to rapid increase in vehicles movement year by year, the automobile pollution control regulatory bodies tightened the emission level every year. Ultra low emission or zero emission vehicles are aimed and more preferred for future. So the researchers adopt multi dimensional approach for reducing emission level. Modification of fuels, Modification of engine design and operating parameters and Treatment of exhaust products of combustion are some of the major approaches. Many researchers are focusing on modification of fuels, and engine design, but very few researchers are concentrating on engine out emission reduction. Among various pollution control devices, Catalytic converter is being widely used. The significance of the catalytic converter is that it reduces harmful gases without any change in the design of the engine. Catalytic converter is a stainless steel container with a porous ceramic structure, mostly a single honey comb structure with many flow passages, through which the exhaust gas flows[Jan Kaspar et al [1], Vesna Tomasic et al[2]]. The flow passages are in many shapes viz., square, triangular, hexagonal and sinusoidal. In early times, loose granular ceramic were used with the gas passing between the packed spheres. However, later on ceramic monoliths were opted owing to its less volume, low mass and easy packaging facility. The monolith walls were coated with active catalyst layer, called washcoat, composed of porous, high surface area inorganic oxides such as gamma alumina, Ceria, Zirconia. Noble metal catalyst such as Platinum, Palladium and Rhodium are deposited on the surface and within the pores of the wash coat. When the exhaust gas flows in a catalytic converter it diffuses through the wash coat pore structure to the catalytic sites where heterogeneous chemical reactions occur, which varies depending on the type of catalyst installed [Ulrich G et al [3]]. Mostly vehicles running on gasoline are fitted with a three way converter, which converts the three main pollutants in automobile exhaust viz., carbon monoxide and unburned hydrocarbon undergo catalytic combustion and oxides of nitrogen are reduced back to nitrogen. The need for improvement of design and performance of catalytic converter has arisen due to prevailing stringent emission regulations. Efforts are being made for design improvement by reduction of emission during normal driving operations and cold start conditions. Some researchers have tried to reduce cold start emission by using chemically or electrically heated catalysts and thereby minimizing the catalyst warm up period during the cold engine start. Few others have made efforts to improve the performance of catalyst during post warm up period.

1.1 TYPES OF CATALYTIC CONVERTER

The catalytic converter is one of the most effective emission control devices available. Two types of catalytic converters are commonly used in automotive engines.

- **Two-way catalytic converters (Oxidation) -** used in diesel- fueled vehicles can reduce CO emission by 80% and a large portion of HC present in particulate matter emissions.
- **Three-way Catalytic Converters (Oxidation–Reduction)-** installed on gasoline fueled vehicles can reduce CO and HC emissions by about 90% and NO_X emission by 70% from uncontrolled levels.
- **Lean nitrogen-oxide Catalyst-** is a new type of catalytic converter which reduces NO_X emissions in lean conditions where a three-way catalyst is ineffective.

1.2 THREE-WAY CATALYTIC CONVERTERS (OXIDATION–REDUCTION)

Ensuring good quality air is essential for the protection of public health. Governments worldwide have adopted a range of increasingly demanding measures to curb air pollution with a particular focus on the emissions from motor vehicles. An important part of this strategy has been the development of the three-way catalytic converter to remove exhaust pollutants such as carbon monoxide, unburnt hydrocarbons and nitrogen oxides. This unit takes an in-depth look at the construction of this converter for petrol-driven vehicles and investigates the catalytic chemistry taking place at the molecular level.

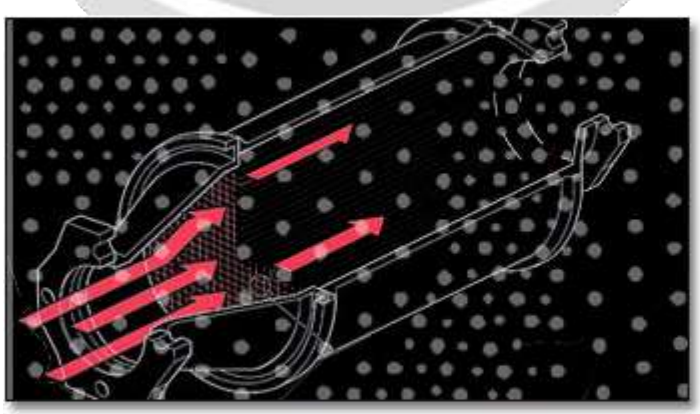


Fig.-1 The three-way catalytic converter

2 MATHEMATICAL MODELING

A mathematical model has been developed for a catalytic converter to predict the concentrations of carbon monoxide, unburned hydro carbons and nitric oxide at different positions of the converter. Although the performance of the catalytic converter could be assessed by conducting experiment on a test bed, but it involves expensive and time consuming engine testing. It has been well recognized that mathematical models often narrow down the range of required experimentation and reduce the required time and cost of optimization studies. In view of this, in the present study, a mathematical model has been used to the performance of a catalytic converter. It involves solution of a set of equations by numerical analysis and obtains the results for various parameters, such as diameter, length of converter, flow rate, specific heat of the catalyst etc. It has been observed that it is a good tool for the assessment of the performance under complex flow conditions.

The model predicts the bed temperature of the catalyst, gas temperature and concentrations of the species under the study along the length of the bed. It also predicts average catalyst temperature and conversion efficiency of each of the species, and helps in the design of converters and catalysts.

Based on the above assumptions, **the energy balance equation for gas phase** can be written as,

$$mf\,Cg\,\frac{\partial Tq}{\partial x} + hAcb\,(Tg - Tcb) + Acb\varepsilon\,\sigma\,(Tg^4 - Tcb^4) = 0 \qquad (1)$$

The first term on the left hand side represents the gas particle heat transfer while the second term on the same side indicates the convective heat transfer.

By considering chemical reactions due to the catalyst **the energy balance equation for the solid phase** is obtained as

$$\rho cb\,u\,Ccb\,\frac{\partial Tcb}{\partial t} = h\,Acb\,(Tg - Tcb) + K\,Acb\,(Tg - Tcb)/L - \blacktriangle HjRj\,\rho cb\,u \qquad (2)$$

The left hand side represents the transient heat transfer, while the first term on the right side denotes convection heat transfer and the last term gives heat of chemical reactions.

Neglecting the longitudinal and radial diffusion, **the material balance equation of 'j' the combustible species in a particle cell is given by,**

$$\underline{mf} \quad \underline{\partial Y_j} = Rj\,\rho cb\,(1-\varepsilon) \qquad (3)$$

Mg ∂x

2.1 COMPUTATION SCHEME

The literature available gives details of the schemes for cycle although the models are applicable to any cycle. In the present work the computation was restricted to an operating condition representing steady speed operation of the vehicle as cruising.

The solutions of basic energy and material balance equations are based on Euler's straight line method. The initial temperature of the gas and the catalyst bed are estimated from relations

$$T_{cb}(t,x) = T_{cb0}$$

$$T_g(t,O) = T_{go} \qquad t > 0$$

Initially, catalyst bed all along the length of the converter is assumed to be constant and equal to ambient temperature. Similarly, the gas temperature at any time at the entry to the converter has constant value for steady speed operation and is equal to Tgo.

At any point of the converter with respect to time. The conversion efficiency can be defined as,

$$\text{Conversation efficiency} = \frac{\text{Inlet concentration-exit concentration}}{\text{Inlet concentration}}$$

2.2 METHOD OF COMPUTATION

Successful predictions of a developed mathematical model would depend on the formulation of program to be run on a computer. In the catalytic converter model, the exhaust gas properties are used as input to the catalytic converter efficiency of carbon monoxide and nitric oxide.

As described above, the catalytic converter is designed on the basis of energy balance, heat balance and material balance equation. These are the basic equation for each of the species reduction. The step by step calculation is being made by modified Euler's method of iteration.

The input data includes the exhaust gas properties such as gas temperature, gas flow rate and specific heat, while the catalyst properties include specific heat, thermal conductivity and geometry of converter.

Programmes developed in C language shows the reduction of NO, CO & HC in the effluent and shows the converter calculation to predict gas temperature, solid temperature and conversion efficiency.

3 RESULT AND DISCUSSION

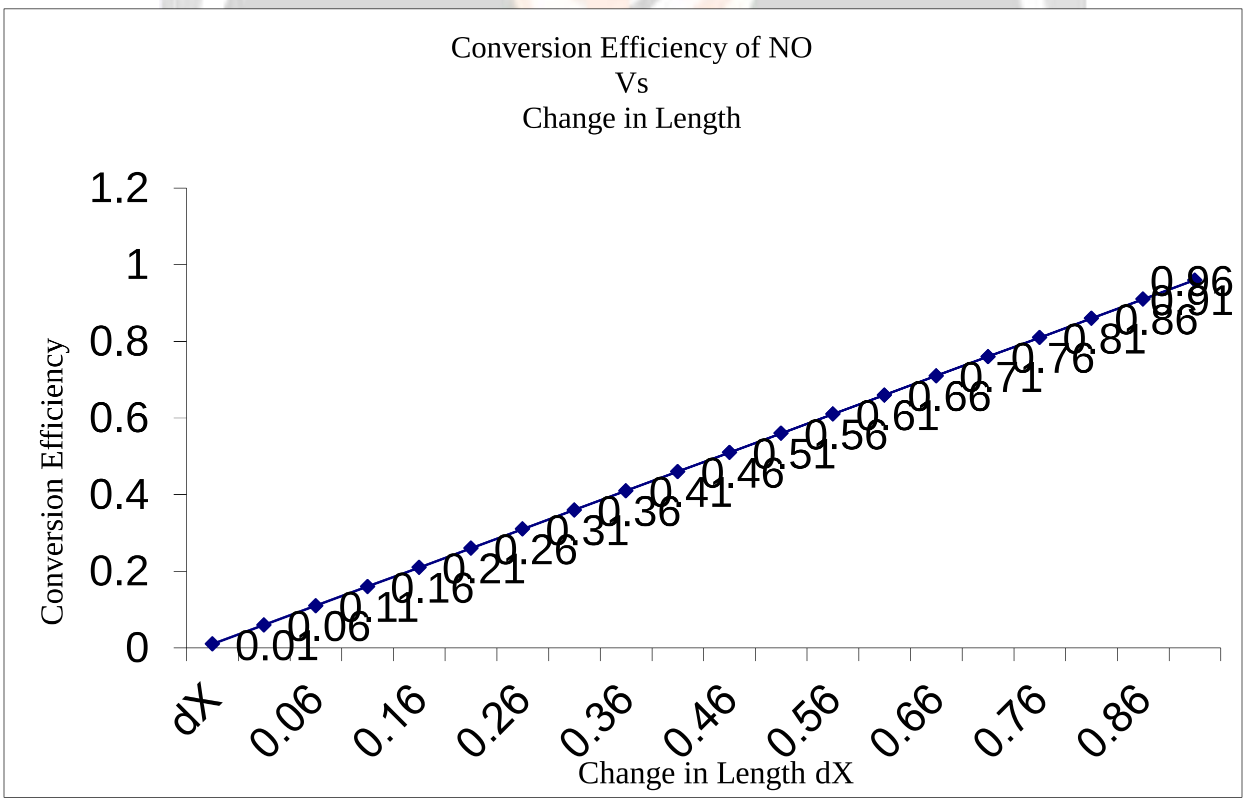
The mathematical model and its computer program in C language is a tool to evaluate the performance and design parameters. Optimization of the design parameters can be done for any catalytic converter depending on its input variable with the help of energy balance equation, heat balance equation and material balance equation we have evaluated the following different parameters;

(i) Variation of CO concentration from inlet to outlet to outside of catalytic converter.

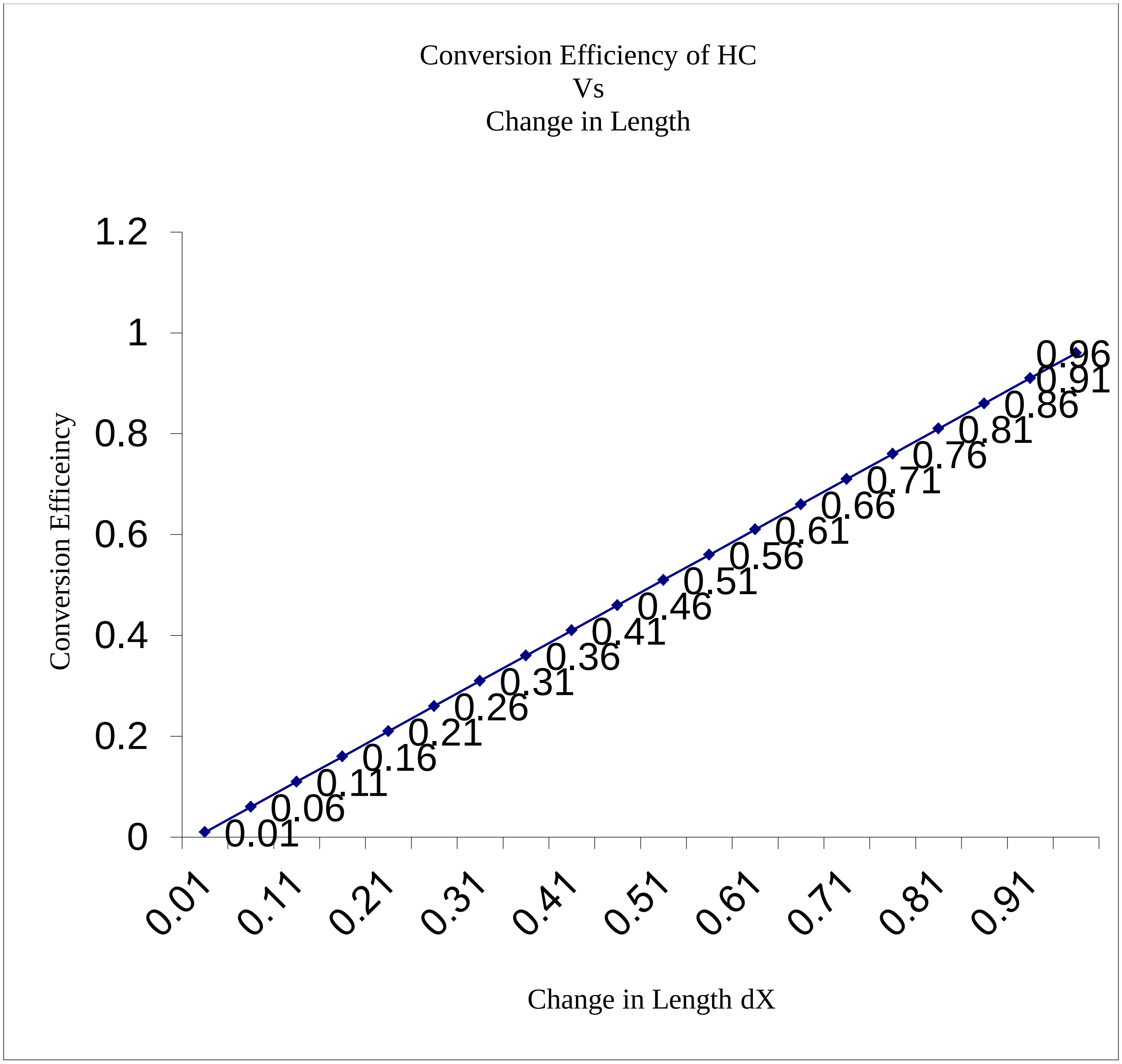
(ii) Variation of NO concentration from inlet to outlet to outside of catalytic converter.

(iii) Variation of HC concentration from inlet to outlet to outside of catalytic converter.

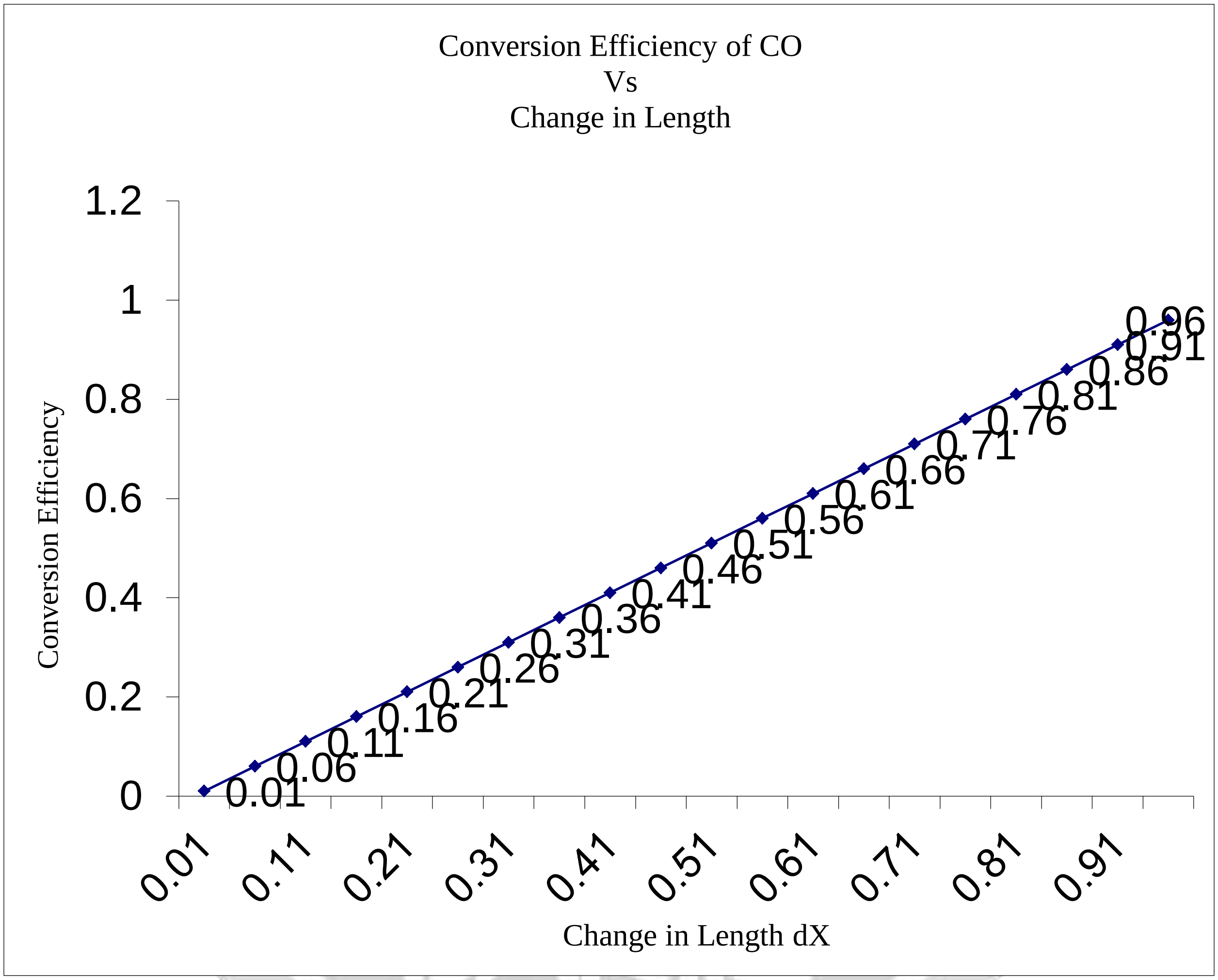
Graph of Conversion Efficiency of NO



Graph of Conversion Efficiency of HC



Graph of Conversion Efficiency of CO



4. CONCLUSION

Catalytic model's conversion efficiency depends on inlet gas temperature and mass flow rates. With higher inlet temperature, the conversion efficiency is higher for all the species in comparison with lower inlet gas temperature. The model also predicts that lower specific heat catalysts are better suited for the warm up rate is higher than the catalyst of higher specific heat.It has been found that catalytic converter of smaller diameter, takes less warm up time as compared to the converter of large size. For a converter of 12 cm diameter it takes about 30 seconds to reach a temperature of 850 K, where as a 22 cm diameter converter takes about the seconds. In case of rich mixtures supplied to the engine, it gives rise to higher concentrations of the CO and HC. Some additional air will have to supply to promote the oxidation reactions.It has been observed that the catalytic converter with sponge iron as catalyst offers less resistance to the flow of exhaust gases and hence there is little loss in engine power as compared with the other catalyst.

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