

# $\text{NO}_x$ Reduction and CO & HC Oxidation in a Dual Bed Catalytic Converter System

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## Abstract:-

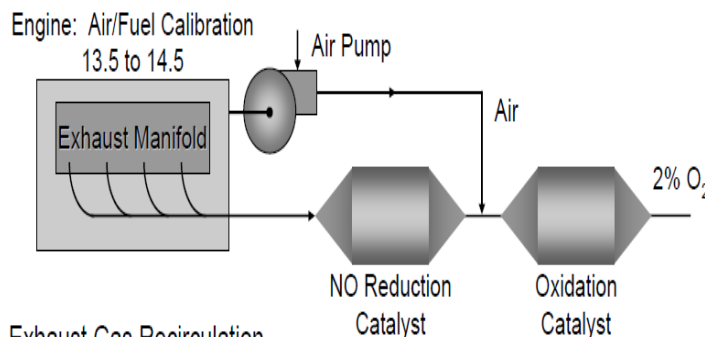
This paper illustrates the design of pollutant control system that is catalytic converter having dual bed with air injection for application in gasoline engine. High exhaust purification consisting of less harmful gases along with low sound waves moves out of the tail pipe.

**Keywords:** Catalytic converter, exhaust emission conversion, thermodynamic model

## INTRODUCTION

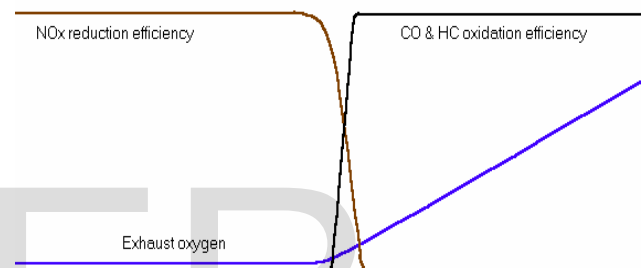
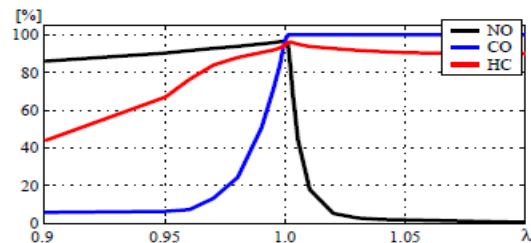
A dual bed catalyst has two separate chambers. Air can be injected in the middle of the catalyst to increase oxygen content in the back half of the converter. The engine can then be run slightly rich to improve NO<sub>x</sub> reduction in the front half of the converter. The air that is injected allows high efficiency oxidation of CO & HC in the back half of the converter. This type of converter can allow NO<sub>x</sub> reduction to occur in the front bed at maximum efficiency while CO and HC oxidation are occurring in the rear bed at maximum efficiency. It is the injection of air in front of the rear bed that allows both oxidation and reduction to occur at maximum efficiency. For the dual bed catalyst to operate at maximum efficiency, it must have very low oxygen levels in the exhaust entering the front bed. This only occurs when the engine is running slightly rich with no misfires or deposit problems. It must also have enough air injected in front of the rear bed to allow oxidation of the CO and HC. The front bed of a dual bed catalyst does also oxidize CO and HC. Even a rich mixture will leave some oxygen in the exhaust. The catalyst uses this small amount of oxygen to oxidize CO & HC into CO<sub>2</sub> & H<sub>2</sub>O. As NO<sub>x</sub> is reduced, oxygen from that NO<sub>x</sub> is freed up. If this extra oxygen was allowed to accumulate it would start to limit NO<sub>x</sub> reduction. But the oxygen from the NO<sub>x</sub> is used to oxidize CO and HC. This limits oxygen build-up in the front bed and keeps NO<sub>x</sub> reduction at maximum efficiency.

## Dual-Bed Catalytic Converter System:



## Exhaust Gas Recirculation

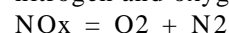
- Could Decrease NO<sub>x</sub> by About 30%
- Had a Negative Effect on Engine Performance



A dual bed catalyst depends on air injection to provide the oxygen to clean up CO & HC when the mixture is rich. Air is only injected into the rear bed. Many cars do not have air injection. Without air injection and a slightly rich mixture these cars must depend on something else to manage the oxygen in the catalytic converter.

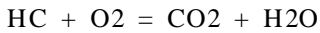
## THEORY OF DBAI

Hot exhaust gas along with sound waves generated at the end of exhaust stroke is sent to the exhaust manifold through the exhaust valve. Sound waves and exhaust gas pass from exhaust manifold to Catalytic converter through a pipe. Hot exhaust gases entering inside catalytic converter. Due to partial combustion the gases entering inside the catalytic converter consists of a mixture of carbon Monoxide (CO) Unburned Hydrocarbons (HC) and oxides of Nitrogen (NO<sub>x</sub>) which are harmful to the environment inside the catalytic converter there consists of two ceramic blocks with micro ducts consisting of platinum and rhodium in one block while platinum and palladium in the other block acting as catalysts. The toxic gas enter into the first ceramic block and heat up simultaneously. This causes the catalyst to react with the toxic gases. As the gas enters inside the nitrogen molecules are the first to react. The catalyst causes the oxides of nitrogen to reform into nitrogen and oxygen respectively.



The gas flows through the micro ducts of the second ceramic block where it react with the platinum and palladium. Inside the micro ducts of the second ceramic

block. Here the carbon monoxide reacts with oxygen molecules to form carbon dioxide (CO<sub>2</sub>)



The unburned hydrocarbons also react with oxygen to form water and carbon dioxide. The exhaust gas now becomes less toxic and comes out from catalytic converter having mixture of carbon dioxide (CO<sub>2</sub>) nitrogen (N<sub>2</sub>) and water vapours (H<sub>2</sub>O).

### **CONSTRUCTION**

The catalytic converter consists of following several components

#### **THE CORE OR SUBSTRATE**

The core is often a ceramic honeycomb in modern catalytic converters but stainless steel foil honeycombs are used too. The honey-comb surface increases the amount of surface area available to support the catalyst and therefore is often called a catalyst support.

#### **THE WASHCOAT**

A wash coat is used to make converters more efficient, often as a mixture of silica and alumina. The wash coat when added to the core forms a rough irregular surface which has a far greater surface area than the flat core surfaces do which then gives the converter core a larger surface area and therefore more places for active precious metal sites. The catalyst is added to the wash coat before being applied to the core.

#### **THE CATALYST**

The catalyst itself is a precious metal. Platinum is the most active catalyst and is widely used. It is not suitable for all applications however because of unwanted additional. Palladium and rhodium are two other precious metals used. Platinum and rhodium are used as a reduction catalyst while platinum and palladium are used as an oxidization catalyst

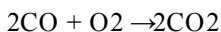
#### **TYPES OF CATALYTIC CONVERTER**

The two types of catalytic converter is discussed below:

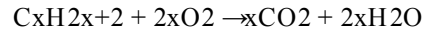
##### **TWO-WAY CATALYTIC CONVERTER**

A two-way catalytic converter has two simultaneous tasks

Oxidation of carbon monoxide to carbon dioxide:



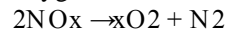
Oxidation of unburnt hydrocarbons (unburnt and partially-burnt fuel) to carbon dioxide and water



(combustion reaction) This type of catalytic converter is widely used on diesel engines to reduce hydrocarbon and carbon monoxide emissions.

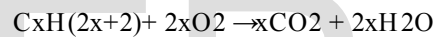
#### **THREE-WAY CATALYTIC CONVERTER**

A three-way catalytic converter has three simultaneous tasks: Reduction of nitrogen oxides to nitrogen and oxygen:



Oxidation of carbon monoxide to carbon dioxide:  $2\text{CO} + \text{O}_2 \rightarrow 2\text{CO}_2$

Oxidation of unburnt hydrocarbons (HC) to carbon dioxide and water:



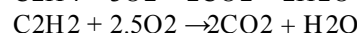
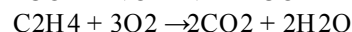
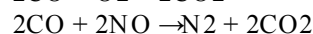
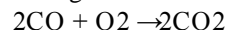
These three reactions occur most efficiently when the catalytic converter receives exhaust from an engine running slightly above the stoichiometric point. This is between 14.6 and 14.8 parts air to 1 part fuel by weight for gasoline. Generally engines fitted with 3-way catalytic converters are equipped with a computerized closed-loop feedback fuel injection system employing one or more oxygen sensors, though early in the deployment of 3-way converters, carburetors equipped for feedback mixture control were used. While a 3-way catalyst can be used in an open-loop system, NO<sub>x</sub> reduction efficiency is low. Within a narrow fuel/ air ratio band surrounding stoichiometry, conversion of all three pollutants is

#### **MODEL OF THREE-WAY CATALYTIC CONVERTER**

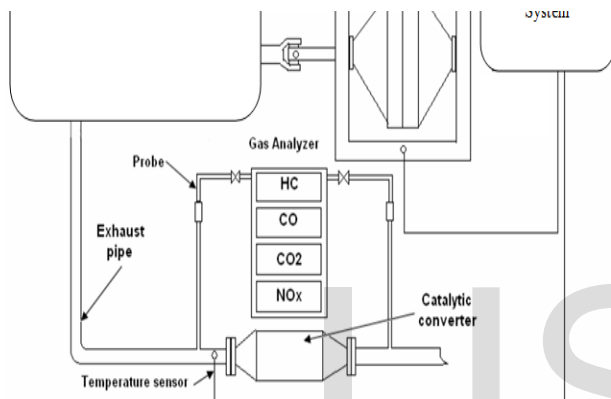
The mathematical model of a catalytic converter contains two elements. The first is the kinetic reaction model and the second is the transport equations for the mass, momentum and energy. We used a kinetic model based on the mechanistic steps. The transport model was based on the modeling of a single channel of the converter.

#### **THE KINETIC MODEL**

We consider a reaction scheme represented by a set of four global reactions:



## EXPERIMENTAL SET UP



## CALCULATION OF THE MASS EMISSIONS OF POLLUTANTS

The calculation procedures for the mass emission of pollutants and correction for humidity for oxides of nitrogen. The mass emission of pollutants are calculated by means of the following equation:

$$M_i = \frac{V_{mix} \times Q_i \times K_h \times C_i \times 10^{-6}}{d}$$

$M_i$  = Mass emission of the pollutant  $i$  in g/ km

$V_{mix}$  = Volume of the diluted exhaust gas expressed in m<sup>3</sup>/ test and corrected to standard conditions 293K and 101.33 kPa

$Q_i$  = Density of the pollutant  $i$  in kg/ m<sup>3</sup> at normal temperature and pressure (293 K and 101.33 kPa)

$K_h$  = Humidity correction factor used for the calculation of the mass emissions of oxides of nitrogen. There is no humidity correction for HC and CO.

$C_i$  = Concentration of the pollutant  $i$  in the diluted exhaust gas expressed in ppm and corrected by the amount of the pollutant  $i$  contained in the dilution air.

$d$  = distance covered in km

## VOLUME DETERMINATION

Calculation of the volume when a variable dilution device with constant flow control by orifice or venturi is used. Record continuously the parameters showing the volumetric flow and calculate the total volume for the duration of the test. Calculation of volume when a positive displacement pump is used The volume of

diluted exhaust gas in systems comprising a positive displacement pump is calculated with the following formula :

$$V = V_o \times N$$

where,

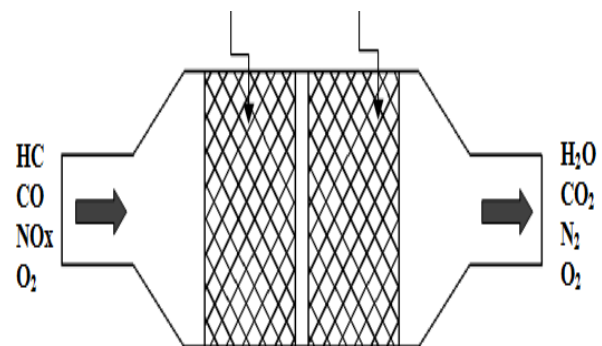
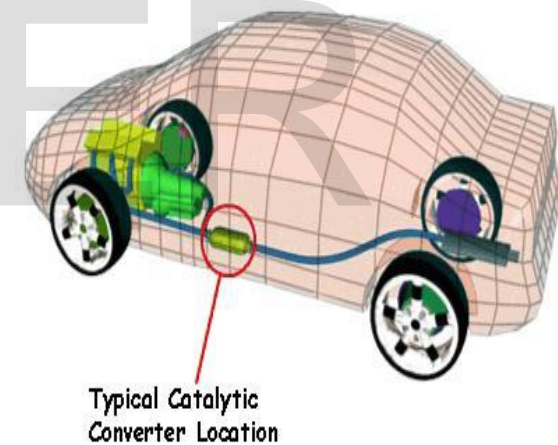
$V$  = Volume of diluted exhaust gas expressed in m<sup>3</sup>/ test (prior to correction)

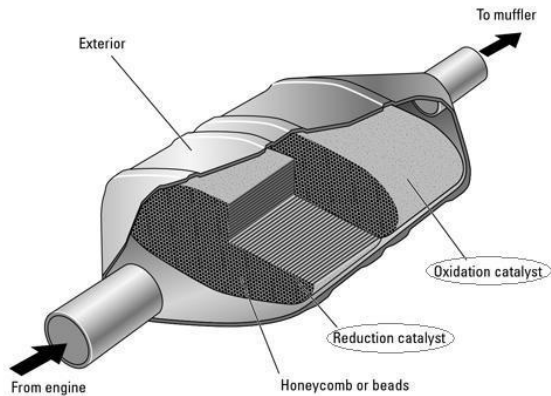
$V_o$  = Volume of gas delivered by the positive displacement pump on testing

Conditions, in m<sup>3</sup>/ rev.

$N$  = Number of revolutions per test.

## THERMODYNAMIC MODEL



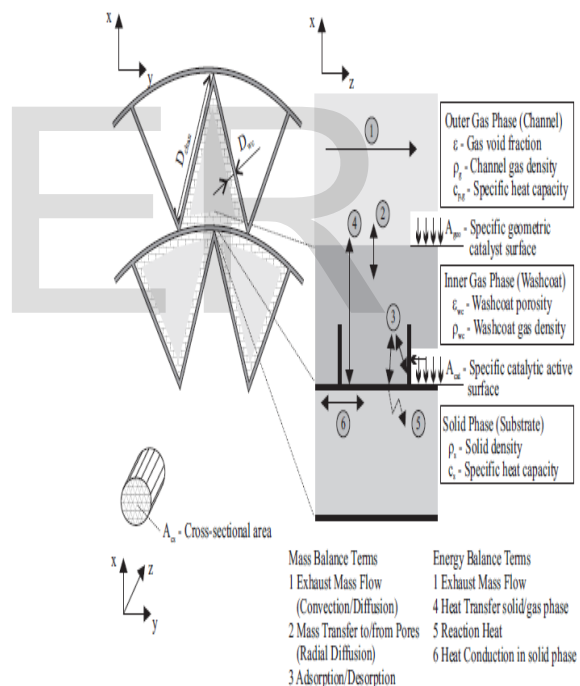


### PROCESS MODEL OF THE TWC

The TWC model presented in the following is referred to as the process model because its goal is to understand the most important dynamics as described above rather than the use in a control system. The model should be able to reproduce the dynamic input-output behavior of all measured species. The concentrations of NO, CO, HC, CO<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub> have been considered. Since only the total HC concentration could be measured. The cross sectional distributions of the flow velocity temperature and concentration profiles in the exhaust upstream of the TWC have been assumed to be uniform. In reality this is hardly the case. However the focus here is on the main dynamic phenomena rather than on the TWC's overall performance which can be significantly influenced by the flow velocity profile. Hence only one channel has been modeled using a one-dimensional approach. Geometry and material parameters such as storage capacities have been assumed to be constant along the flow axis. In reality ageing mechanisms close to the inlet are different from those close to the outlet of the TWC. At the inlet TWC deactivation occurs mainly because of poisoning. Towards the tail more thermal effects are dominant such as sintering. Additionally deactivation does not occur uniformly on the TWC cross section it is rather dependent on the exhaust gas flow velocity profile at the inlet of the TWC. All phenomena eventually lead to a reduction of the oxygen storage capacity. The cross sectional flow velocity profile in one channel is not constant along.

### THERMODYNAMIC MODEL OF THE TWC

Figure shows a sketch of heat and mass transfer and cross sectional geometry of the TWC. Two gas phases and one solid phase have been consider additionally mass is exchanged with the second gas phase by means of radial diffusion. The inner (second) phase contains wash coat and boundary layers. Here no axial convection occurs. Mass is exchange in the radial direction with the outer gas phase on the one hand by means of diffusion and with the solid surface on the other hand by means of adsorption or desorption.



### GOVERNING EQUATIONS

The physical model of the catalytic converter under study is shown in Fig. where the stagnation-point flow geometry is used. A mixture of gases and air described by the mass concentrations and flows with a velocity gradient and temperature perpendicular to a platinum plate of finite thickness. The lower surface of the plate is kept to the same temperature.

The boundary layer governing equations for the assumed frozen gas-phase are the following

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0$$

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial y} \right) + \rho^\infty a^2 x$$

$$\rho u C_p \frac{\partial T}{\partial x} + \rho v C_p \frac{\partial T}{\partial y} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial y} \right)$$

Where  $u$  and  $v$  are the longitudinal and transversal components of velocity, respectively  $\rho$ ,  $\mu$ ,  $C_p$ ,  $\lambda$  and are the density, viscosity, specific heat at constant pressure, and thermal conductivity of the gas-phase mixture.  $D_i$  corresponds to the diffusion coefficient of species.

In Figure

$\epsilon$  = Gas void fraction

$\rho_g$  = Channel gas density

$C_{pg}$  = Specific heat capacity

$A_{geo}$  = Specific geometry catalyst surface

$E_{wc}$  = washcoat porosity

$\rho_{wc}$  = washcoat gas density

$A_{cat}$  = Specific catalytic active surface

$D_i$  = Radial mass transfer coefficient

Flow is laminar and constant sherwood number is

$$Sh_d = \frac{D_i \times D_{chan}}{D_{iN_2}} = 2.47$$

$D_{iN_2}$  = binary diffusion coefficient of the species  $i$  in  $N_2$ .

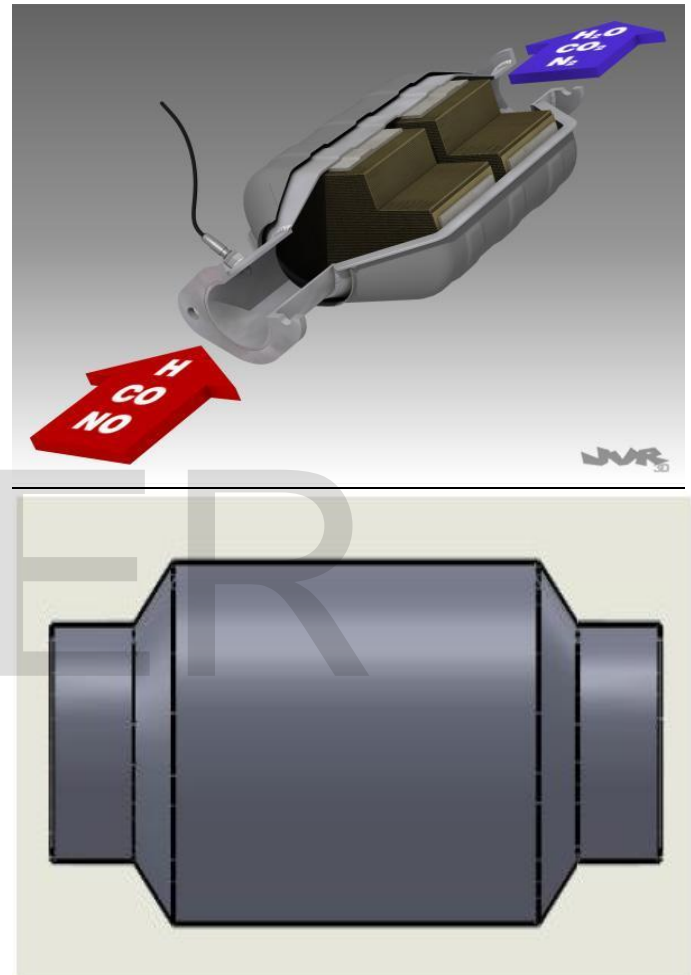
It was calculated by Fuller et.al. The mass balance for species  $i$  in the inner gas phase does not contain any convective or axial diffusion term only radial mass transport occurs. On the channel side mass is exchanged with the channel phase by mean of radial diffusion. On the solid surface side mass is exchanged by means of adsorption and desorption.

The mass balance for gas channel can be written as

$$\rho_g \epsilon \frac{\delta w_i}{\delta t} = \epsilon Deff \frac{\delta^2 w_i}{\delta^2 x} - \frac{m}{A_{cs}} \frac{\delta w_i}{\delta x}$$

$$- D_i A_{geo} (\rho_g \times w_i - \rho_{wc} \times v_i)$$

$$+ W_i \sum (D_i \times A_{geo} (\rho_g \times w_i - \rho_{wc} \times v_i))$$



## CONCLUSION

The numerical mathematical modeling of a catalytic converter is developed in this paper. The catalytic combustion model is for a mixture of  $CO$ ,  $NO$  and air, using the stagnation-point flow geometry. The proposed chemical reaction mechanism is able for reducing  $NO$  and oxidation of  $CO$ .

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