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Numerical Analysis Of Surface Reaction Of Catalytic Converter

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ABSTRACT

Pollution has become a major problem throughout the world. The automotive pollution is responsible highly for the global climatic changes since fifties increased concentration of pollutants in the vehicle emissions poses a serious health hazards to the public. Consequently, the air (prevention & control of pollution) act was passed in India in 1981, and its amendments and emissions control regulations became stringent step by step. Due to increasingly stringent government regulations on vehicle nitrogen oxides (NOx) emission levels the selective catalytic reduction (SCR) of NOx to N_2 by hydrocarbons has gained a great deal of attention. Catalytic converters for petrol driven passenger car have now become mandatory for new cars and SCR with ammonia water injection system is used to reduce the exhaust pollution.

The project work reports some result of investigations carried out on the operation of ammonia water injection system on exhaust carried out by simulation model to reduce the NOx formation. The present work was done on simulation model of catalytic converter on exhaust system using Comsol multiphysics software. This project report describes the use of catalytic converter and injected ammonia water to reduce the harmful exhaust gas.

Keywords: monolith reactor,NOx,NO,Ammonia

1.INTRODUCTION

The reduction of Automobile pollution using catalytic converter in the latest vehicle speaks in high volume towards its successes. The uses of catalytic converter are becoming compulsory for all the heavy vehicles in order to prevent global warming. The modelling of catalytic converter as well as its simulation of surface reaction is very important to determine the conversion rate or the amount of pollutants reduction in the core of catalytic converter of the flue gasses from the engines. The catalytic converter model is simulating for the implementation of new catalytic converter technology. For this aspect, the role of exhaust gas after treatment method for the catalytic converter components is playing a very vital across the world.Literature review reveals numerous publications on two-and three- dimensional computational fluid dynamic(CFD) modelling of a single channel of the monolith(Canu &Vecchi,2002;Chatterjee, Deutschamnn, & Warnatz, 2001; Deutschamnn, Maier,Riedel, Stroemann, & Dibble, 2000;Grimm & Mazumder,2008; Groppi, Belloli, Tronconi, &Forzatti, 1995; Holder, Bolliga,Anderson, &Hochmuth, 2006; Mantzaras, Appel, & Benz, 2000; Papadias, Zwinkels, Edsberg, & Bjormborg, 1999; Raja, Kee, Deutschmann, Warnatz, & Schmidt,2000; Sallamie &Koshkanab, 2003; Young & Finlayson, 1976, among many others).Recently, due to the shortage of better alternatives,the knowledge gained from the simulation of a single channel is extrapolated to the entire catalytic conveter.Since the channels are coupled to each other through heat transfer,and individual channels may encounter different flow rates,extrapolation of the results of a single channel to the entire converter is not always accurate,and may lead to flawed designs(Tischer,correa & duetschmann,2001).Shuai and wang (2004) modelled the monolithic reactor using a two dimensional model,in which the reactor was modelled as a porous medium and surface reactions were modelled using a two step mechanism.Kolaczkowski and Serbertsioglu(1996) performed analytical modelling of channel interactions in catalytic combustion reactors.The focus of their study was the effect of monolith material properties on heat dissipation.Chen,Alexio,Williams,Leprince,and Yong(2004)performed three dimensional CFD modelling of flow and heterogeneous reactions in catalytic converters.The pressure and velocity fields were calculated by modelling the monolith as a porous medium. The surface reaction model was then superimposed on the fluid flow results.Te objective of the present study is to demonstrate the effectiveness of a new implicit coupled for such large scale catalytic converter.

This paper describes how the modelling of catalytic converter has done using plug flow reactor to obtain its high efficiency while simulating the model, the characteristic graphs of various inlet

temperatures on what the changes in molar flow rate, selectivity parameters, temperature profiles etc.With the results this paper illustrates about the changes of different parameters of fluid like molar concentrations, temperature distributions, isosurface etc.which represents the conversions of pollutants like SOx and NOx in its monolithitic reacting surface made up of materials zeolite and kaoline.While on the designing the catalytic converter model the important issue is the impacts of scale up or scale down of the catalytic converter,that is what happens if the overall dimensions of the catalytic converter is going to increase or decrease,keeping the channel dimensions unchanged?This is a critical question which has to be answered by modelling and simulation in order to keep design cost low.

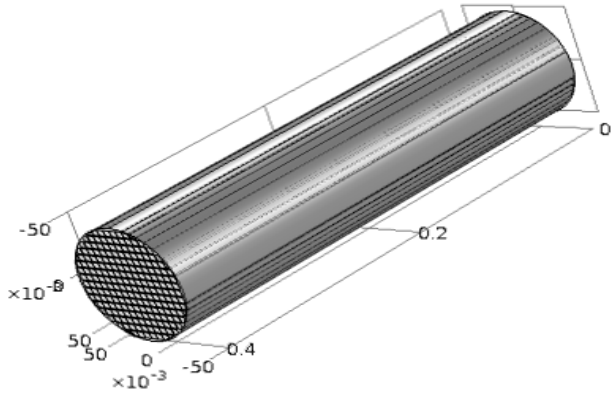


FIG: 1 SIMULATION MODEL FOR THE MULTI CHANNEL

2.COMPUTATIONAL METHOD

The modelling of catalytic converter is done here using comsol multiphysics software. The 3D model of the catalytic converter is drawn here with its inlet, outlet, inlet walls, outlet walls, reactor surface boundaries, and the domains like supporting walls &channel blocks. The 2D object of 100 mm dia circle with its channel blocks is extruded up to 470

mm to represent the 3D model of catalytic converter with its reactor surface. In the process of simulation It is used the 'standard SCR' reaction

$4NH_3+4NO+O_2 \rightarrow 4N_2+6H_2O$---------- (1)

In the absence of oxygen, to reduce NO a slower reaction also goes on, which is

$4NH_3 +6NO \rightarrow 5N_2+6H_2O$.---------- (2)

When the NO2/NO ratio is close to unity,a much higher rate reaction prevails, often known as 'fast SCR'

$2NH_3+NO+NO_2 \rightarrow 2N_2+3H_2O$.---------- (3)

Madia et al performed an investigation of the side reactions observed during the SCR process.Madia et al also investigated the effect of the increased NO2 fraction caused by an oxidation catalyst located upstream of the SCR converter, and concluded that increasing the NO2/NO fraction up to 1 enhances NOx conversion at low temperatures, due to the reaction with NO and NO2,which is significantly faster than reaction with NO and O2.In the numerical studies ,heterogeneous reactions mechanisms are used to describe surface reactions on catalytic plates,where the chemical species are absorbed,react with the surface plane of the catalyst,followed by the desorption.

The stationary plug flow is used In the simulation process, and the study 1 is computed to plot the graphs according to different temperatures.

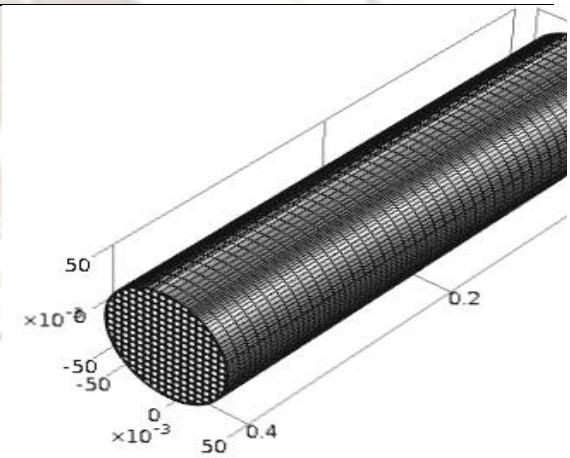


FIG:2 THE MESH OBJECT OF CATALYTIC CONVERTER

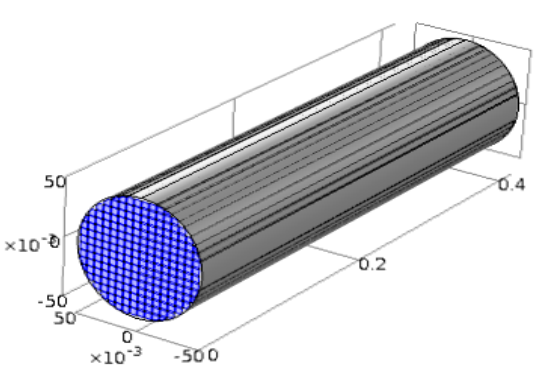


FIG:3 INLET

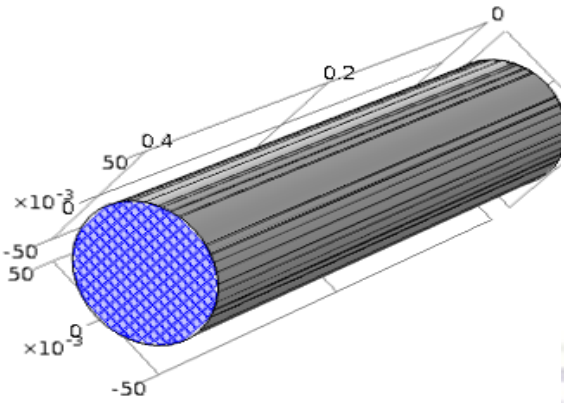


FIG:4 OUTLET

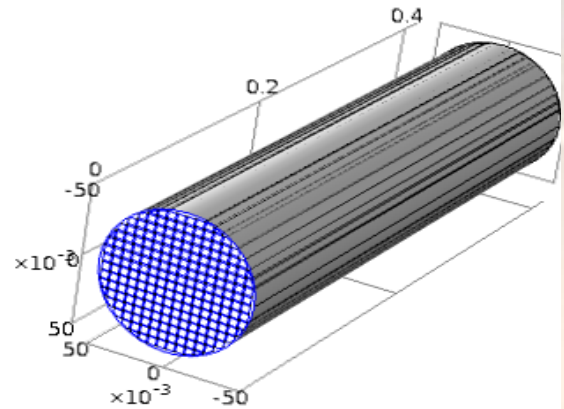


FIG:5 INLET WALLS

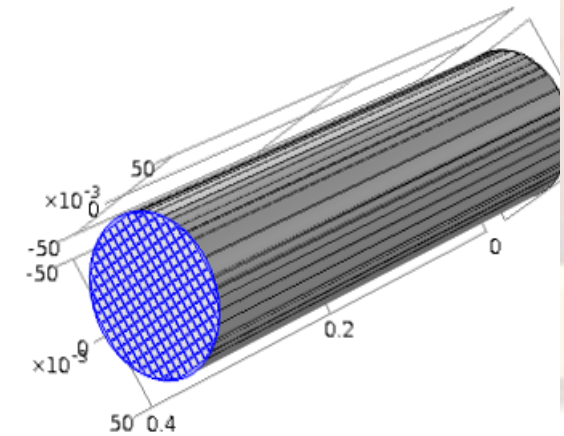


FIG:6 OUTLET WALLS

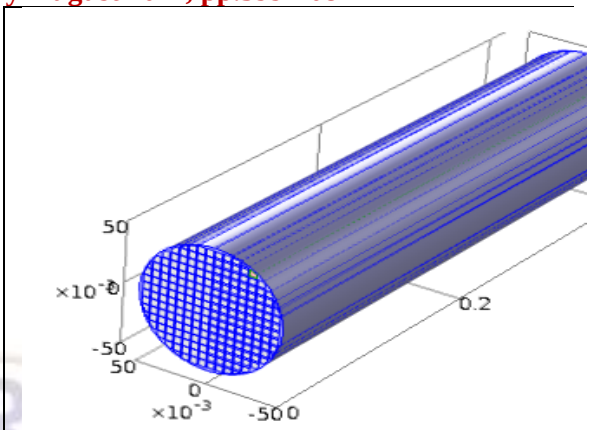


FIG:7 SUPPORTING WALLS

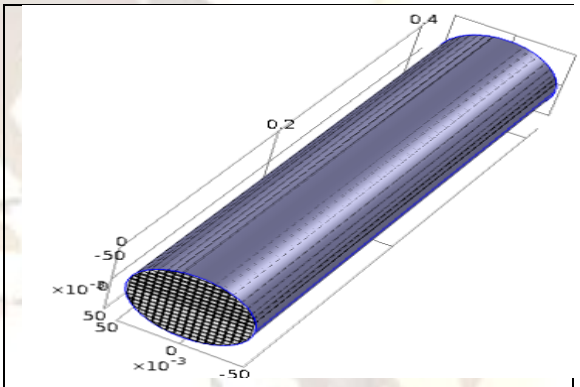


FIG:8 REACTION SURFACE

2.1 NO Reduction in a Monolithic Reactor

This is a modelling example of catalytic converter that removes nitrogen oxide from a car exhaust through the addition of ammonia. This example shows an application of the above described modelling strategy and demonstrates through a series of simulations how an understanding of this reactor and its system can be improved. To do this, it uses a number of the interfaces and features found in the Chemical Reaction Engineering Module.

This example illustrates the modelling of selective reduction of nitrogen oxide (NO) by a monolithic reactor in the exhaust system of an automobile. Exhaust gases from the engine pass through the channels of a monolithitic reactor filled with a porous catalyst, and by adding ammonia (NH_3) to this stream, the nitrogen monoxide can be selectively removed through a reduction reaction.

Yet, ammonia (NH_3) is also oxidised in a parallel reaction, and the rates of the two reactions are affected temperature as well as composition .This

means that the amount of added ammonia must exceed the expected amount of nitrogen oxide while not being so excessive as to release NH3 to the atmosphere.

The simulations are aimed at finding the optimal dosing of NH_3, and investigating some of the other operating parameters in order to gauge their effects. On defining the modelling strategy, first the selectivity aspects of the kinetics are studied my modelling initial reaction rates as function of temperature and relative reactant amounts. Information from these studies point to the general conditions required to attain the desired selectivity.

The reactor is then simplified and modelled as a non-isothermal plug flow reactor. This reveals the necessary (NH_3) dosing levels based on the working condition of catalytic converter and assumed flow rate of NO in the exhaust stream. A 3D model of catalytic converter is then set up and solved. This includes mass transfer, heat transport, and fluid flow and provides insight and information for optimizing the dosing levels and other operational parameters.

2.2 CHEMISTRY

Two parallel reactions occur in the zeolite/kaolin washcoat of the monolithic reactor .The desired reaction is NO reduction by ammonia:

$$4NO + 4NH_3 + O_2 \rightarrow 4N_2 + 6H_2O \quad \text{----------(1)}$$

However, ammonia can at the same time undergo oxidation:

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O \quad \text{----------(2)}$$

The heterogeneous catalytic conversion of NO to N_2 is described by an Eley-Rideal mechanism .A key reaction step involves the reaction of gas phase NO with surface adsorbed NH_3.The following rate equation (mol/(m^3s)) has been suggested in Ref.1 for Equatiion1:

$$r_1=k_1 c_{NO(} ac_{NH3/1+} ac_{NH3)} \quad \text{----------(3)}$$

Where

$$k1=A_1\exp(-\frac{E1}{RgT})$$

And

$$a=A_0 \exp(-\frac{Eo}{RgT})$$

For Equation2, the reaction rate (mol/(m^3s)) is given by

$$r_2=k_2 c_{NH3} \quad \text{----------(4)}$$

Where

$$k_2=A_2 \exp(-\frac{E2}{RgT})$$

2.3 THE PLUG FLOW REACTOR

To find the minimum level of (NH_3) required to reduce the NO present in the exhaust gas requires a reactor model accounting for changing reactant concentrations and system temperature. From a mass transfer point of view, channels of the reactor monolith can be considered to be uncoupled to one another. Therefore it is reasonable to perform initial simulations where a single reactive channel, modelled by nonisothermal plug flow equations represents the monolith reactor. This model is set up and solved using the Reaction Engineering interface.

2.4 MODEL EQUATION

Assuming steady state, the mass balance equation for a flow reactor is given by

$$\frac{dFi}{dV} = R_i$$

Where F is the species molar flow rate (mol/s) ,V represents the reactor volume(m^2)and is R, the species net reaction rate (mol/(m^2s)).the energy balance for the ideal reacting gas is:

$$\sum_i F_i C_{p,i}.\left(\frac{dT}{dV}\right) = Q_{ext} + Q \quad \text{----------(5)}$$

Where C_P is the species molar heat capacity (J/mol.k) and Q_{axt} is heat added to the system per unit volume (J/m^2s). Q denotes the heat due to chemical reaction (J/(m^2s)).

$Q= -\sum_j Hj\ rj$

Where h, the heat of reaction (j/mol) and, r the reaction rate (mol/m^3s)

The reactor equations are solved for a channel 0.36 m in length with a cross section area of 12.6 mm^2 .It is assumed that that exhaust gas containing 41.1 mmol/m^3 of NO at a temperature of 523K passes through the channel at 0.3m/s

2.5 THE 3D REACTOR

It is clear from the kinetic analysis as well as from the single channel model that temperature plays a central role in affecting the optimal dosing of NH_3.As the temperature distribution is likely to vary from the channel to channel in a catalytic converter, a full 3D reactor model is called for.

2.6 Model geometry

The monolithic reactor has a modular structure made up of monolith channel blocks and supporting solid walls. The reactor is 470 mm long and 50 mm in radius.

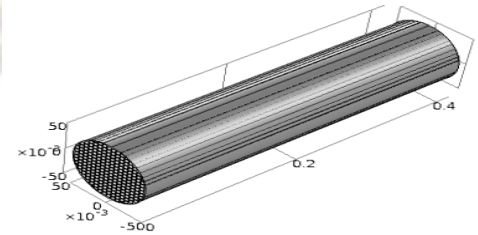


Fig:9 NO reduction chemistry takes place in the channel blocks. Supporting walls hold together the full reactor surface.

2.7 MODEL EQUATIONS AND ASSUMPTIONS

In the present example a pseudo homogeneous approach is used to model the hundreds of channels present in the monolith reactor. As no mass is exchanged between channels, each channel is described by 1D mass transport equations. Furthermore, fully developed laminar flow in the channels is assumed, such that the average flow field is proportional to the pressure difference across the reactor. The fluid flow transports mass and energy only in the channel direction. The energy equation describes the temperature of the reacting gas in the channels, as well as the conductive heat transfer in the monolith structure and the supporting walls. As the temperature affects not only the reaction kinetics but also the density and viscosity of the reacting gas, the energy equation is what really connects the channels in the reactor structure turning this into a 3D model.

2.8 Mass Transport

The mass balance describing transport and reaction in reacting channels are given by diffusion-convection equations at steady state:

$$\nabla.(-Di\nabla ci)+\mathbf{u}.\nabla ci = Ri \quad \text{----------(6)}$$

Here D_i denotes the diffusion coefficient (m^2/s), C_I is the species concentration (mol/m^3), and u equals the velocity (m/s). The term R ($mol/(m^3s)$) corresponds to the species rate expression.

Mass transport is only allowed in the direction of the channels, corresponding to direction of the x-axis in the 3D geometry used in this example. For the diffusive transport this is accomplished by setting the y and x components of the diffusivity matrix to zero. The pressure –driven flow in the monolith is also defined in the direction of the x-axis hereby restriction the convective mass transport to the channel direction as well. Each monolith channel thus behaves as a 1D plug-flow model with included diffusion. These separates channel models are connection though the heat - transfer equation for the reaction monolith.

2.9 Fluid Flow

Assuming fully developed laminar flow in channels, the average flow field is proportional to pressure difference across the reaction .The flow of reaction gas through the monolith can the be modelled using a Darcy's law interface with following governing equation;

$$\nabla.(p\,u)=0$$

$$\mathbf{u}=-\frac{k}{\mu}\nabla p$$

The monolith is treated as a porous matrix with the effective permeability $k(m^2)$.the density ,p(kg/m3),and viscosity,μ(Pa.s),represent properties of the reacting gas.

2.10 Heat Transfer

A single temperature equation describing the heat transfer in porous monolith reactor can be written as:

$$(pC_p)_{eq}\frac{\partial T}{\partial t}+p_f C_{pf}\,u\nabla T = \nabla.(k_{eq}\nabla T)+Q \quad \text{----------(7)}$$

For the stationary case this reduces to:

$$p_i C_{pf}\mathbf{u}.\nabla T=\nabla.(k_{eq}\nabla T)+Q \quad \text{----------(8)}$$

Where $p_i(kg/m^3)$ is the fluid density $C_p(J/kg.K)$ is The fluid heat capacity ,and k_{eq} (W/(m.k))is the equivalent thermal conductivity. Furthermore u(m/s) is the fluid velocity field, which in this model is calculated in the Darcy's law interface, and Q(W/m3) is the heat source, which is due to exothermic chemical reaction:

$$Q= Q_1 + Q_2 =-r_1H_1-r_2H_2$$

The equivalent conductivity of the solid –fluid system, keq is related to the conductivity of the solid k_{eq}, and to the conductive of the fluid, keq by:

$$K_{eq}=\Theta_P k_p+ \Theta_f k_f$$

Here Θp denotes the solid materials volume friction, here 0.25, which is related to the volume fraction of the fluid $\Theta_f$by:

$$\Theta_f+\Theta_p=1$$

model (equation8). the chemical reaction engineering module uses the following set polynomial as default expressions describing species thermodynamics properties

$$C_{p,\,i} =R_g\,(a_1+a_2T+a_3T^2+a_4T^3+a_5T^4) \quad \text{----------(9)}$$

$$h_i = R_g\left(a_1T+\frac{a_2T^2}{2}+\frac{a_3T3}{3}+\frac{a_4T4}{4}+\frac{a_5T5}{5}+a_6\right) \quad \text{----(10)}$$

$$s_i = R_g\left(a_1InT+a_2T+\frac{a_3T^2}{2}+\frac{a_4T^3}{3}+\frac{a_5}{4}T^4+a_7\right) \quad \text{--------(11)}$$

Equation (8) is the equation set up by heat transfer interface for a fluid domain. For the supporting in the reactor, only heat transfer by conduction applies:

$$-\nabla(k_8\nabla T)=0$$

Where k_8 (w/m-k) is the thermal conductivity for the solid walls

As mentioned, the temperature affects not only reaction kinetics but also the density and viscosity of the reacting gas. In this way the heat transfer equation connects channels in the reactor structure.

2.11 Thermodynamic and transport Properties

Accurate thermodynamic data is required as input to energy balance equation, both in the plug flow model (equation5) and the 3Dmonolith

Here C_p ,denotes the species heat capacity (J/mol k),T the temperature (K) and R_i the ideal gas constant ,8.314 (j/mol k) further ,h is the molar enthalpy (j/mol) and S_I represent its molar entropy (J/mol k).A set of seven coefficients per input for the polynomials. The coefficients a_1 through a_2 relate to the species heat capacity ,the coefficient a_3 is associated with the species enthalpy of formation (at 0 K) and the coefficient a_1 comes from the species entropy of formation (at 0 K).

The equation from outline by equqtion9 through equqtion11 is referred to as CHEMKIN or NASA format (ref 2) Database resources list the needed coefficients are for different temperature intervals (ref3).in the this exampl.

3 RESULT AND DISCUSSIONS

To model the injection of urea a typical catalytic converter is chosen whose dimension is 100 mm and length is 470 mm. It is necessary to inject urea as a liquid solution (called Ad blue solution) into the hot exhaust gas, which is normally between the temperatures of 423k to573k depending upon the load of the engine.

Urea injection process is modelled by Ad blue liquids (32.5% urea and 73.5%water), solid model is created and meshed in comsol multiphysics4.2 software.

3.1 SIMULATION PROCEDURE

For reacting gas mixtures the reaction engineering feature makes use of kinetic gas theory to set up expressions for transport properties such *as* diffusivities viscosity and thermal conductivity as function of temp ,pressure and composition .in this example ,the species diffusivities (m^3/ s) are calculated using the formula

$$D = 2.695.10^{-3} \cdot \sqrt{\frac{T^3 \left((M_A + M_B)/\left(2.10^3 M_A M_B\right)\right)}{P^\sigma A^\sigma B^\Omega D}}$$

---------(12)

Where Ω_D is a collision integral

$$\Omega_D = f\left(T, \sigma, \frac{\varepsilon}{k_b}, \mu\right)$$

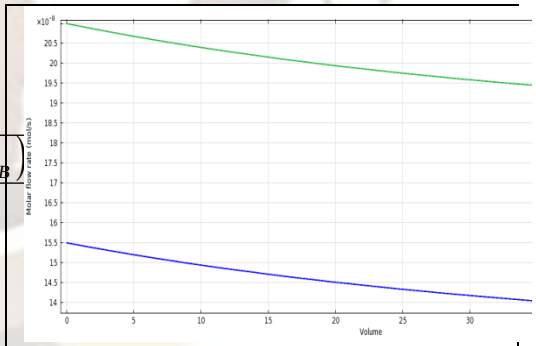
The chemical Reactions are modelled with chemical kinetic reaction mechanism. It is used to perform three different analyses concerning the reduction of NO in a monolithic reactor. the reactions modelled are:

1) Kinetic Analyses-to explore the system of competing reactions and learn what conditions that promote selectivity towards NO reduction
2) Plug Flow Reactor Model- to explore the coupled mass and energy balance equations in a single channel model, resulting in a first estimate of the NH_3 dosing level
3) 3D Reactor Model-testing the reactor operating conditions in a full 3D reactor representation, noting the space-dependent effect due to coupling between monolith channels.

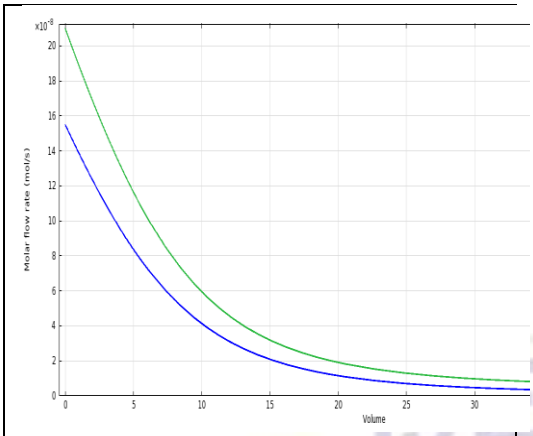
The surface reaction of NOx reduction will be effective only at certain temperatures. Hence to find out the range at which the reactions are effective, the simulations were conducted for four exits. The temperature profile came across corresponding the temperatures 423k, 523k, 623k,&723k with the changes in molar flow rate and temperatures.

The results are plotted below

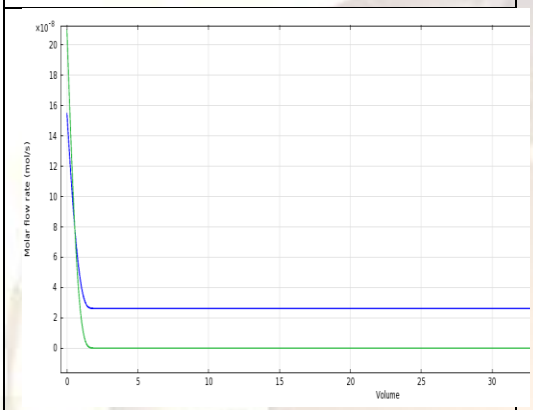
The graphs of molar flow rate are plotted below:



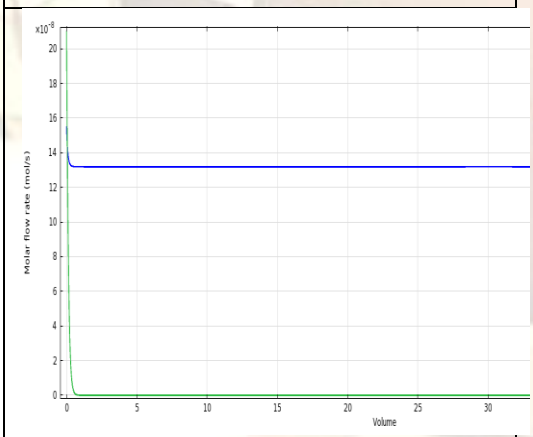
(a) Exhaust gas temperature 423k



b)Exhaust gas temperature 523k



c)Exhaust gas temperature 623k



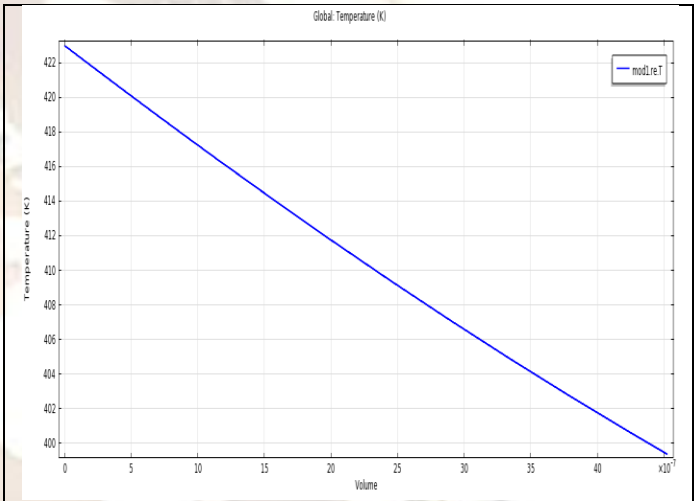
d) Exhaust temperature 723k

Fig:10 Spatial variation of flow rates of NH3 and NO for different temperatures with respect to volume of catalytic converter.

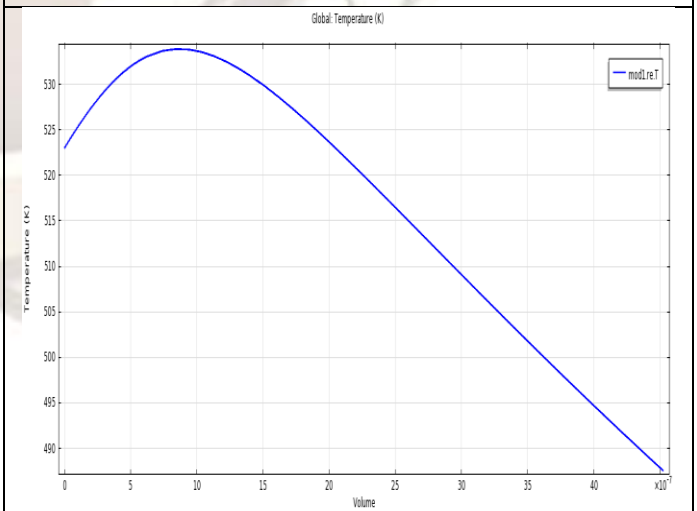
Various parameters like the reaction rates of reaction 1 and reaction 2, molar flow rates and temperature across the domain were calculated and measured. The measurements were done across the length of the catalytic converter.Fig:10 show the comparison of flow rates of ammonia and nitrogen oxide (NO) along the length wise direction. It is evident from the picture that, as the temperature of exhaust increases the reduction of NO is enhanced. For example at a volume of 15 units the NO level are147.5 and 2.0 moles /sec for the temperatures of 423k and 523k.Further increase in temperature does not enhance NO reduction as it can be seen for the figures 10 (b) and 10 (c).Analysing the figure it can be seen that the NO level is around 2.5 moles/sec. at a location of 15 volume units.

Hence it can be concluded that the optimum exhaust gas temperature for the NO reduction with ammonia for the given NO emission level is 523k.

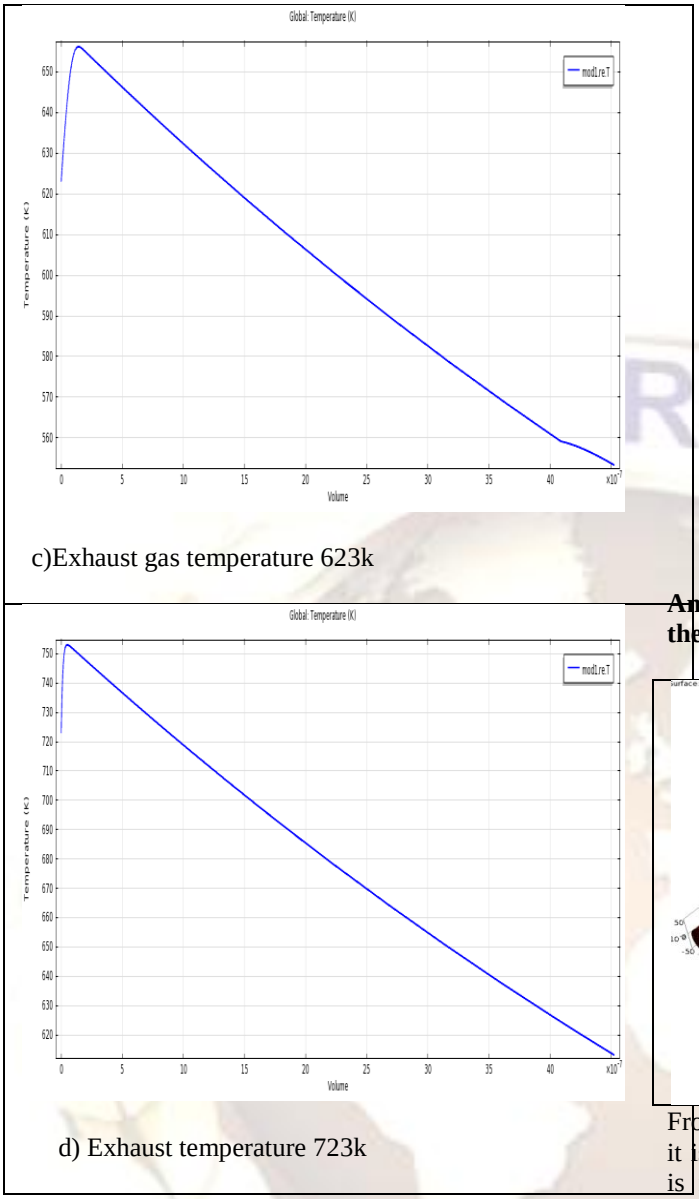
The graphs of temperature profile are given below;



(a) Exhaust gas temperature 423k



b)Exhaust gas temperature 523k



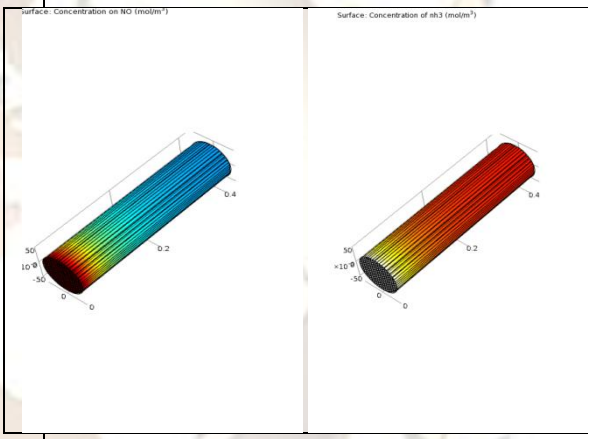
c)Exhaust gas temperature 623k

d) Exhaust temperature 723k

Fig: 11 Spatial variation of exhaust gas temperature for different exhaust conditions (inlet SCR condition).

From the fig: 11 a) temperature 423k,it shows that the temperature is very high (about 423k) at the zero volume (inlet) level of the SCR system, and it continuously reduces to about 402 k at the outlet of SCR system. It shows that there is apparently NO reaction induced temperature rise. The Fig: 11 b) temperature 523k represents that the temperature is 523 k at the zero unit volume of the SCR system and it suddenly goes high up to 530k at 10 unit of volume of the SCR system and then continuously decreases to below 490k at the outlet of SCR system. From the Fig:11 c)temperature 623k , it shows that the temperature graph rapidly increases from 623k temperature to above 650k temperature within 2 unit volume of the SCR system and then decreases to below 560k to the outlet of SCR system. The last Fig: 11 d) temperature 723k represents the temperature increasement from 723k to above 750k very fastly within the single unit volume of the SCR system and then continuously decreases to below 620k temperature at the outlet of the SCR system.

Ammonia (NH3) and nitrogen oxide (NO) for the surface concentration.

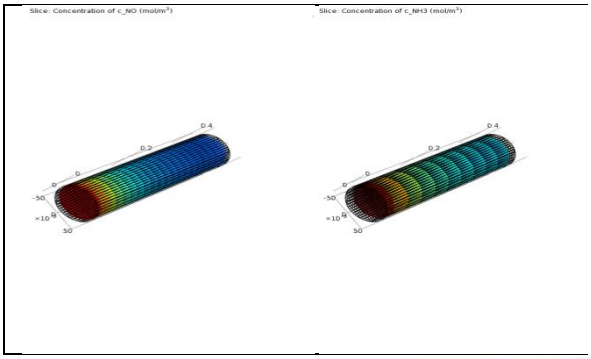


12 a. Concentration of NO 12 b. concentration of NH_3

Fig: 12 Surface concentrations of NO & NH_3 for a typical 3D volume

From the fig:12 concentration figure of NO & NH_3, it is shown that the surface concentration (mol/m^3) is maximum at inlet of the model, continuously decreasing towards the outlet of the model. This represents that the pollutants like NO,NH_3 are high in concentration at the inlet of the catalytic model and while passing through the catalytic core the pollutants get converted to some other elements by the chemical reaction inside the catalytic core. Which shows the lower concentration value of NO & NH_3 at the outlet of the model.

Ammonia (NH3) and nitrogen oxide (NO) for the slice concentration.

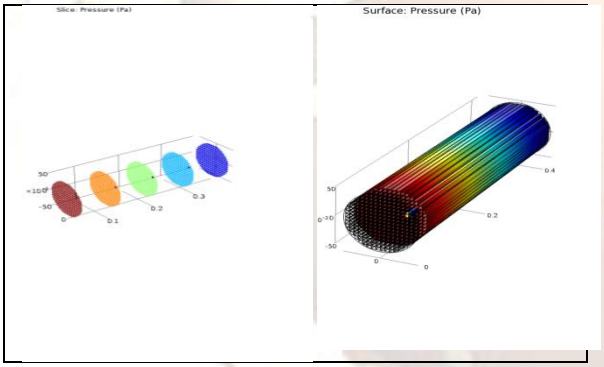


13 a concentration of NO 13 b. concentration of NH3

Fig: 13 slice concentration of NO & NH_3 for a typical 3D volume

The above figures shown the slice concentration (mol/m^3) of NO and NH_3 which is maximum at inlet and continuously decreasing towards the outlet. It refers the slice concentrations of NO & NH3 part by part how & by what value it is decreasing towards the outlet of the model. It represents that the surface reaction takes place from the inlet of the model and it is well finished before the outlet of the model.

Pressure on both the cases of slice and surface of the catalytic converter

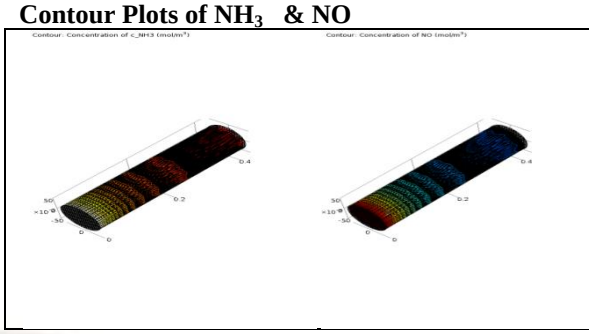


13 a Slice pressure 14 b surface pressure

Fig 14 Slice and Surface Pressure of Catalytic Converter model.

The figures show the pressure distribution through the catalytic converter model, which is having a higher pressure at the inlet and continuously decreasing pressure towards the outlet for both the slice and surface cases. This represents that at the inlet of the model due to the injected ad blue solution and entering exhaust gas from the engine the pressure is high, as the reaction takes place at the entrance of the catalytic core, the specific volume increases and hence the pressure increases. As the gas flows further downstream the reaction temperature reduces and hence the pressure too decreases.

Contour Plots of NH_3 & NO

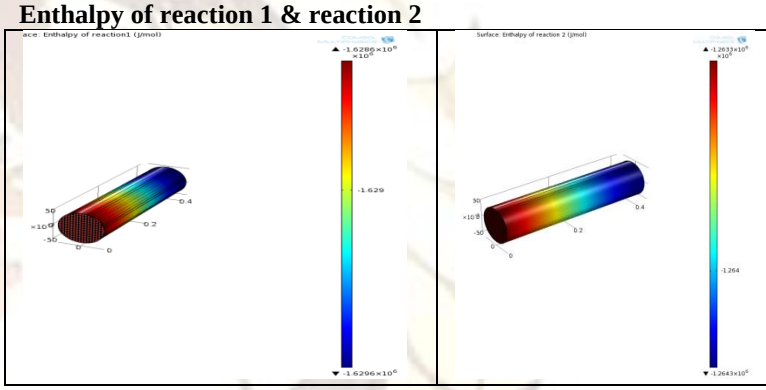


15 a Contour Plots of NH_3 15 b Contour Plots of NO

Fig 15 Contour Plots of NH_3 & NO

Contour plots of both the NH_3 and NO is higher at inlet and reduced to almost zero at the exit. Moreover the ammonia slippage is minimum in this case. Hence we can safely assume that health hazard due to ammonia is nil.

Enthalpy of reaction 1 & reaction 2

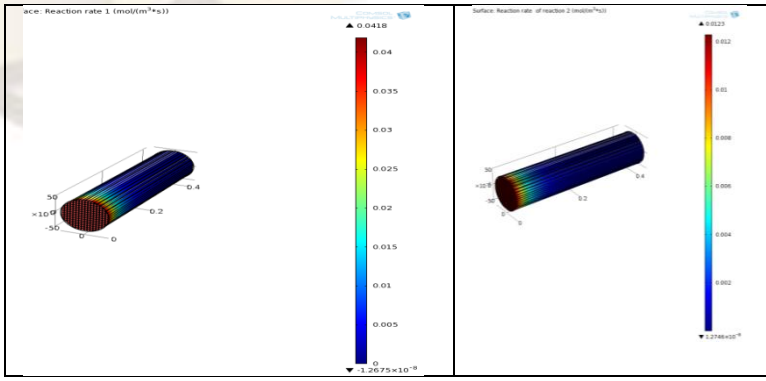


16 a Enthalpy of reaction 1 16 b Enthalpy of reaction 2

Fig 16 Enthalpy of reaction 1 and reaction 2

The Fig: 16, shows that the enthalpy is higher at the inlet portion and decreases to the outlet of the SCR system of both the cases of Reaction 1 & Reaction 2.This shows that by the time the exhaust stream enters the middle of the Catalytic core almost all the reactions have been completed. At the exit no reaction occurs at all.

Reaction rate of reaction 1 & reaction 2

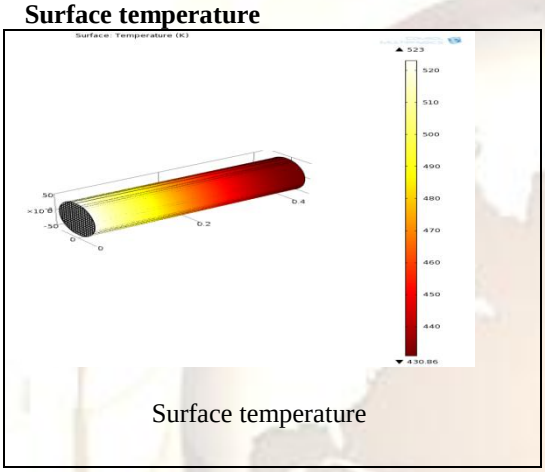


17 a. reaction rate of reaction 1 17 b. reaction rate of reaction 2

Fig 17 Reaction rates of reaction 1 and reaction 2

The Fig: 17 (A) shows that the reaction rate of reaction 1 is higher at the inlet of SCR system and continuously decreases to the outlet of the SCR system. The Fig: 6.6 (B) shows that the reaction rate of reaction 2 is also much higher at the inlet of SCR system and continuously decreases to the outlet of the SCR system. This represents that the chemical reaction started from the inlet of the SCR system and it is well finished before the outlet of the SCR system. The reaction is completed within the catalytic core.

Surface temperature



Surface temperature

Fig18. Surface temperature of the catalytic model

The surface temperature figure shows that the temperature variation is maximum at the inlet of the model which is approximately 523k and it decreases to the outlet where it seems to be less than 440k.This represents that the reaction has been occurred from the inlet of the SCR system and it is completed before the exit of the SCR system.

4. CONCLUSION

The SCR technology is a successful method of reducing the harmful gases such as NOx, HC, CO. The aim of the research work is to show the reaction of NO and NH3 in the monolith reactor of catalytic converter with varying temperatures by using COMSOL MULTIPHYSICS 4.2 software.

From the simulation study it was observed that the conversion of NO into N_2 is effective only in the middle range of temperature i.e. about 523k.

From the enthalpy picture it is seen that the internal energy is maximum at the inlet of the SCR system and decreases towards the outlet. This represents that the reaction is started from the inlet of SCR and finished well before the outlet of the SCR system. The reaction rate pictures of reaction 1 and reaction 2 also shows that the reaction rate is high at the inlet and decreases at the out let of the SCR system.

The concentration of NOx and NH_3 is also maximum in the inlet and reduced downstream of the SCR system .The pollutants like NO and NH_3 are higher in concentration (0.0557 mol/m^3) .The concentration of NO is reduced to a lowest value of flow at 0.005 mol/m^3 at the exit of the catalytic core. Whereas the NH3 concentration at exit is around 0.01 mol/m3.This clearly shows that the surface reaction occurs satisfactorily at the catalytic core.

Moreover it can be concluded that at 523k temperature the catalytic converter is highly effective and it reduces the pollutants to a very minimum level.

5. REFERENCE

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