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Numerical Simulation of Nitrous Oxide and Carbon Monoxide Abatement in the Catalytic Converter

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Abstract- Catalytic converters are one of the effective devices to reduce air pollution by motor vehicles by transforming nitrogen oxides and carbon monoxide in the exhaust to relatively harmless nitrogen and carbon dioxide respectively. However, due to the presence of precious group metals such as platinum, rhodium and palladium as catalysts, the cost of the catalytic converter is relatively high. Furthermore, the catalysts' activation and deactivation levels is highly dependent on temperature, hence the design of catalytic converter in the vehicle exhaust system is not easy. The objective of this study is to carry out simulation via CFD code FLUENT 6.0, on catalytic converter. CFD modeling module was conducted to predict the exhaust gas temperature at 10cm, 30cm, 50cm, 80cm and 110cm from the engine outlet to determine the best position of catalytic converter in the exhaust system. Another CFD modeling module was done to simulate the surface reactions on a single channel of a catalytic converter. The simulation result was then verified via experimental data published in the literature.

Keywords- Catalytic converter; Natural gas vehicle; Nitrogen monoxide; Carbon monoxide; Abatement; CFD.

1. Introduction

Fuel is combusted with controlled amount of air in internal combustion engine producing CO_2, H_2O and incomplete combustion products of CO and uHC. During the combustion process very high temperatures are reached due to diffusion burning of the fuel resulting in thermal fixation of the nitrogen in the air to form NO_x (Zeldovich, 1946). CO, NO_x and uHC in the exhaust undergo complex chemical reaction in catalytic converter to form CO_2, H_2O and N_2. In vehicle catalytic converter, the incoming gases are relatively cold when the vehicle has been dormant for an extended period of time, so the reaction rate is governed by the chemical kinetics of catalytic reactions. This presents worst case scenario for the catalytic converter. The catalyst surface heats up as a result of the heat gain from gas stream in addition to heat generated by the catalytic reactions. When the surface becomes sufficiently hot, the conversion rate will be determined by the chemical species mass transfer. Modelling and simulation works of catalytic converters has been done since 1970s. Early simulation works by Kuo et al. (1971), Heck et al. (1976), Young and Finlayson (1976), and Oh and Cavendish (1982) were in one-dimensional models. With computer development in the 1980s, Chen et al. (1988), Zygourakis (1989), Hayes et al. (1992) were among the pioneers to model catalytic converters in two-dimensional models. Empirical models done on catalytic converters simulation were in steady state models, transient models and light-off criteria on cold start engine. Now a day the solution of Navier-Stokes equations by numerical techniques has been made possible by the advent of powerful workstations, opening avenues towards the calculation of complicated flow fields in cyclone with relative ease via computational fluid dynamics software (CFD) codename FLUENT 6.0. The recent work in the catalytic converters modelling and simulation is summarised in Table 1.

All catalytic converter simulation and modeling works for steady state and cold start mentioned above were done for petrol engines emission abatement. There is no simulation work done for compressed natural gas vehicle emission abatement, neither in steady state nor cold start condition. Also, there is no modeling work on surface

reaction for catalytic converter using CFD FLUENT 6.0. This work was done to fill the knowledge gap in simulation and modeling for compressed natural gas vehicle emission abatement.

Table 1. Review on Recent Advances in the Catalytic Converter Modelling and Simulation

Researcher	Work description	Findings
Siemund et al. (1996)	Simulate one dimensional model of catalytic converter for temperature, air/fuel ratio and gas flow step changes and pulses on petrol injection engine. Simulations data are validated by experiments.	Despite the simplified assumption made, the agreement between simulation data and experimental data is satisfactory.
Hoebink & Marin (1997)	Develop kinetic modelling for catalytic converter based on theoretical condition.	Detailed kinetic modelling for model based control techniques is suitable to meet on-going demand for lower emissions.
Kirhner & Eigenberger (1997)	Simulate one dimensional two-phase model for catalytic converter during start-up and for heated up catalyst for petrol engine.	Hot-spot phenomena which cause deactivation is simulated.
Hoebink et al. (1999)	Study the major kinetic equations involving CO, NO and HC. Model predictions for light-off curves and compare quite well with experimental data for petrol engine.	Light-off is in the sequence of hydrogen, CO, propene. Catalysts capable of increasing the NO surface coverage or the NO dissociation or leading to a lower oxygen sticking coefficient would show a higher NO conversion rate.
Taylor (1999)	Use CFD modelling on catalytic converters to predict high temperature thermal behaviour under steady state, high load conditions. Areas of study are effect of heat transfer, oxidation reactions, heat generation and radiation heat transfer. Perform experiment to obtain actual data on petrol engine.	Excellent agreement between measured and computed temperatures, both inside the converter assembly and on outer shell.
Harmsen et al. (1999)	Study the transient oxidation of ethylene over catalytic converter under cold start condition. Elementary step model and rate parameters have been develop to descript the reactions. Experiment was done by feeding inlet gas conditioned to approximate an automotive exhaust gas.	Found two types of adsorbed species, - and di- -ethylene. -ethylene can be oxidised rapidly. Di- -ethylene is rather refractory and retards the reaction between adsorbed CO and oxygen adatom. Ceria has no significant effect on ethylene oxidation. Addition of CO to ethylene inhibits the ethylene oxidation.
Chan & Hoang (1999)	Predict the exhaust gas temperature along exhaust pipe and across catalyst monolith, including dew point and subsequent evaporation from start-up of a petrol engine. Simulate the CO, NO and HC conversion and validate with experiment data.	Wet surface heat transfer at catalyst monolith is important during engine warm-up, it prolong light-off time. Light-off point is at about 300^0C. Validation showed that predictive quality of model is acceptable.
Koltsakis & Stamatelos (1999)	Carried out study on oxygen storage and transient water-gas shift activity phenomena in catalytic converter and their computer modelling. Performed air/fuel scan test on the effect of CO, HC and NO reaction and emissions. The air/fuel oscillation scan effect is then simulated.	The air/fuel oscillation was beneficial for CO and HC at rich conditions, as well as NO for lean conditions. The results and the effect of oxygen storage and water-gas shift activity is successfully simulated by mathematic modelling.
Jeong & Kim (2002)	Study the effect of a flow maldistribution on thermal and conversion response of a monolithic catalytic converter.	The flow uniformities of cross-sectional area ratios below 0.25 are severely degraded. A steep radial temperature gradient during start-up caused by non-uniformed flow distribution caused low efficiency of the catalyst.
Mukadi & Hayes (2002)	Develop mathematical model of catalytic converter and modelling solution using Newton-Krylov method.	The Newton-Krylov with general minimal residual (GMRES) approach is feasible in the simulation of cold-start condition with importance of pre-condition choice. Parallel computing provide large degree of speed-up.
Harmsen et al. (2001)	Study the steady-state kinetics of acetylene oxidation over catalytic converter under cold start condition. Elementary step model and rate parameters have been develop to descript the reactions. Experiment was done by feeding inlet gas conditioned to	Partial reaction order is negative for acetylene and positive for oxygen. Increasing the temperature led to a higher conversion of acetylene and lower selectivity to CO. CO was found to be the only primary reaction product which may be oxidised to CO_2

	approximate an automotive exhaust gas.	consecutively. A reaction model for the partial oxidation of acetylene to CO has been developed.
Jirat et al. (2001)	Use own developed simulation program to model various reactor-adsorber arrangements.	HC conversion limiting factor is the heat capacity, not adsorption capacity. The simulation provides data on operating characteristic of different patented reactor-adsorber configurations.
Chatterjee et al. (2001)	Use CFD Fluent coupled with DETCHEM to simulate C_3H_6, CO and NO reaction in monolith catalytic converter in different temperature. Simulation data were validated with experimentally measured data. Experiment was done by feeding inlet gas conditioned to approximate an automotive exhaust gas.	Simulation data obtained were in good agreement with measured data. Chemistry module in DETCHEM provides better chemical reaction modelling in gas phase and surface reaction.
Koci et al. (2003)	Develop a multiphase (PT and PTRh catalysts), differentiated NO_x storage and reduction catalytic monolith converter. Experiment and simulation of periodic lean/rich operation of the low/high temperature and different converters are done on petrol engine.	Simulations results agree well with the experimental data. The mathematical model developed for prediction of dynamic behaviour can simulate the adsorber-reactor systems with adaptive control. The periodic lean/rich operation and the differentiation of washcoat can improve catalytic converter efficiency.
Akcayol & Cinar (2004)	Use artificial neural network to predict the catalyst temperature, HC emissions and CO emissions of a heated catalytic converter of a cold start gasoline engine. Experimental measurements are used for training data for artificial neural network.	The deviation coefficients of data obtained are less than 5%. The statistical coefficient of multiple determinations for investigated cases is about 0.9984 to 0.9997. The artificial neural network provides a feasible method in predicting the system parameter.

2. Methodology

The study involved the modelling and simulation of catalytic converter was done using CFD in two dimensional (2D). The CFD modelling and simulation are carried out via a commercial CFD code FLUENT 6.0. Separate simulation modules were created to study effect of positioning of the catalytic converter along exhaust pipe, and simulation of surface reaction on a single channel of catalytic converter. Figure 1 shows the overall steps in CFD analysis.

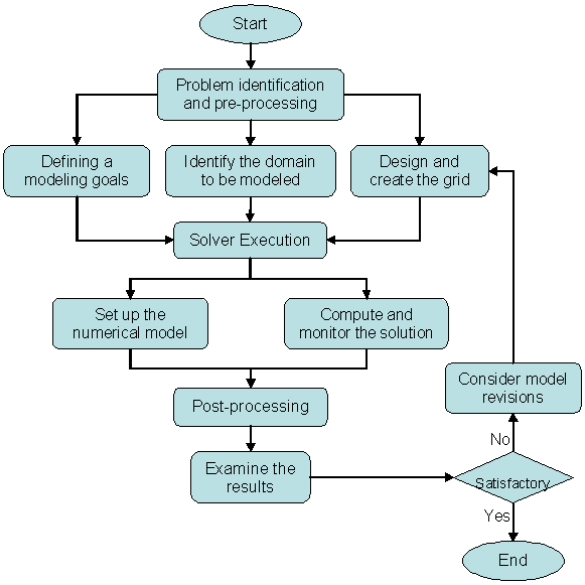


Figure 1. Steps on CFD Analysis

2.1 Module A: CFD Modelling of Temperature along Exhaust Pipe

2.1.1 Scope, Boundary Conditions and Assumptions

In the CFD modelling of temperature along exhaust pipe, the first step is a numerical grid creation (Figure 2). The exhaust pipe manifold modelled is 3mm in thickness. The quadrilateral computational grid was created using Gambit 2.0 with at least 618 nodes to yield a reasonable prediction. Since the 2-D exhaust pipe is rectangular in shape, simple quadrilateral grid was used. The second step is a solver execution in Fluent 6.0 in which the boundary condition, materials properties and calculation take place.

The gas density is assumed to be incompressible ideal gas condition with gas heat capacity abiding gas mixing law. Absolute pressure is at 1 atmosphere and air thermal conductivity is 0.0242 W/mK (Holman, 1989). The temperature of the exhaust gas flowing into the manifold from engine is at 920K (Chan and Hoang, 1999) and the gas velocity in the manifold is 0.5m/s. The diameter of the exhaust pipe modeled is 50mm as measured from a typical Proton Iswara Taxi. According to Holman (1989), exhaust pipe wall heat loss, the convection heat transfer coefficient is at 60 W/m^2K, external emissivity is 0.6 and the external temperature is fixed at 30^oC as per experiment condition by Chan and Hoang (1999). The boundary conditions for this simulation module are summarised as in Table 2.

Table 2. Boundary Conditions of the Exhaust Pipe Model

No	Zone	Type	Parameter
1	Fluid	Fluid	NGV exhaust
2	Inflow1	velocity-inlet	Velocity Magnitude : 0.5m/s Temperature : 920K
3	Wall	Wall	Temperature : 300K Convection Heat Transfer Coefficient: 60 W/m^{2}K Free stream Temperature : 300K External Emissivity: 0.6 External Radiation Temperature : 300K
4	Outflow1	Outflow	Flow rate weighting : 1

2.1.2 Solver

The simulation is then solved with a 2-D, segregated, laminar flow, unsteady state, first order implicit solver in FLUENT. Figure 3 shows a typical iteration residual plot for catalytic converter simulation. The iteration is carried out until the convergence is reached as shown in Figure 4. The convergence residuals for x-velocity, y-velocity and continuity were monitored to 1x10^{-3} convergence criterion whereas for energy was monitored to 1x10^{-6} convergence criterion.

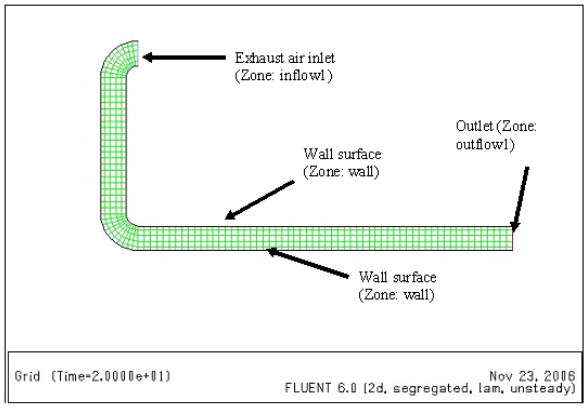


Figure 2. Computational grid creation

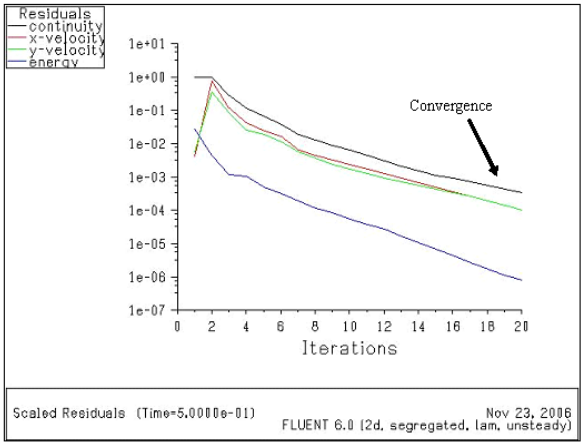


Figure 3. Iteration (Solver Execution)

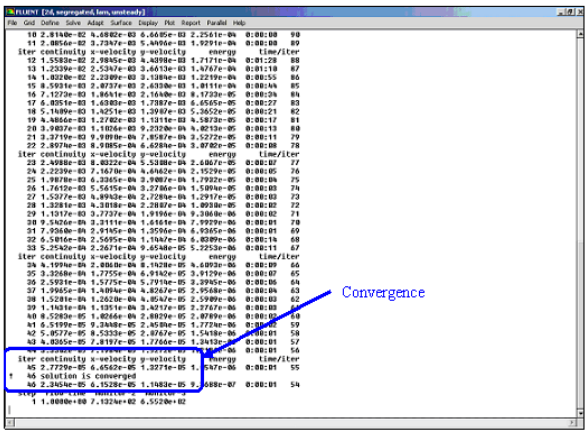


Figure 4. Convergence

After the iteration converged, the temperature contour along the exhaust pipe can be obtained. The iteration process until convergence took about 4 minutes.

2.2 Module B: CFD Modelling of Surface Reaction in Catalytic Converter

2.2.1 Scope, Boundary Conditions and Assumptions

In the CFD modelling of surface reaction in catalytic converter, the first step is a numerical grid creation (Figure 5). The quadrilateral computational grid was created using Gambit 2.0 with at least 25921 nodes to yield a reasonable prediction. Since the 2-D single channel is rectangular in shape, simple quadrilateral grid was used. The second step is a solver execution in Fluent 6.0 in which the boundary condition, materials properties and calculation are taken place.

The channel of catalytic converter chosen for the modelling work is 1.0mm in diameter which is similar to the catalytic converter used by Chatterjee et al. (2001) in their experiment. The catalysts modelled are PT and Rd. The exhaust gas is produced by gas engine under stoichiometric condition at cold start and assumed at 750K constant similar to data used by Chatterjee et al. (2001).

The gas density is assumed to be incompressible ideal gas condition with gas heat capacity abiding gas mixing law. Absolute pressure is at 1 atmosphere. The boundary conditions for this simulation module are summarised as in Table 3.

Table 3. Boundary Conditions of the Single Channel Model

No	Zone	Type	Parameter
1	Fluid	fluid	NGV exhaust
2	Inflow	velocity-inlet	Velocity Magnitude : 0.5m/s Temperature : 750K
3	Wall	wall	Temperature : 300K Free stream Temperature : 300K External Radiation Temperature : 300K
4	Outflow	Outflow	Flow rate weighting : 1

2.2.2 Chemical Reactions

The chemical reactions which based on Chatterjee et al. (2001) in Table 4 are keyed into the Fluent 6.0. CO_2<s>, O<s> and N<s> are surface species. The pre-exponential factor A_r value has to be multiple by factor of 10^{-15} input data for CO reaction and factor of 10^{-16} for NO reaction for FLUENT.

Table 4. Surface Reaction, Rate of Expression and Constant Input into Fluent

No	Reaction	Forward Rate Expression	A_r	β_r	E_r (J/kgmol)
1	$2CO + O_2 \rightarrow 2CO_2$<s>	$k_{f,r} = A_r T^{\beta r} \exp^{[-Er/RT]}$	3.7 x 10^5	0	1.08 x 10^8
2	NO → O<s> + N<s>	$k_{f,r} = A_r T^{\beta r} \exp^{[-Er/RT]}$	5.0 x 10^4	0	1.201 x 10^8
3	N<s> + N<s> → N_2	$k_{f,r} = A_r T^{\beta r} \exp^{[-Er/RT]}$	3.0 x 10^5	0	1.05 x 10^8
4	O<s> + O<s> → O_2	$k_{f,r} = A_r T^{\beta r} \exp^{[-Er/RT]}$	2.0 x 10^5	0	1.15 x 10^8
5	CO_2<s> → CO_2	$k_{f,r} = A_r T^{\beta r} \exp^{[-Er/RT]}$	0.01	2.4	1.70 x 10^8

2.2.3 Solver

The simulation is then solved with a 2-D, segregated, laminar flow, steady state solver and first order implicit in FLUENT to reach the convergence. Figure 6 shows a typical iteration residual plot for catalytic converter simulation. The iteration is carried out until the convergence is reached. The convergence residual for x-velocity, y-velocity, continuity and all species were monitored to $1x10^{-3}$ convergence criterion whereas for energy was monitored to $1x10^{-6}$ convergence criterion.

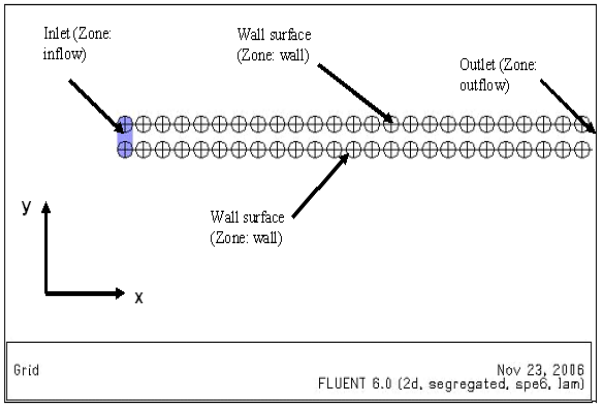


Figure 5. Computational Grid Creation

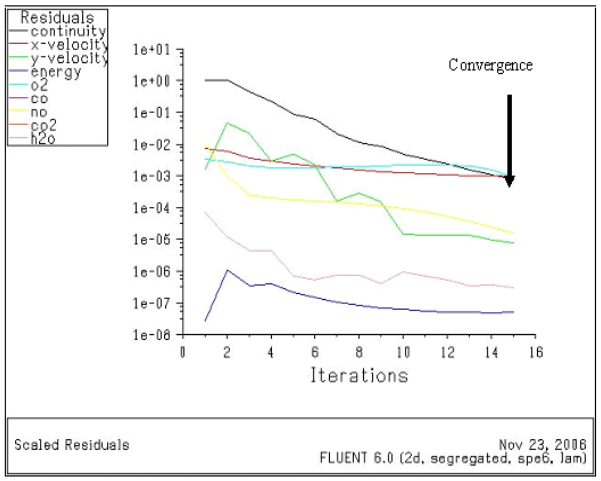


Figure 6. Iteration (Solver execution)

After the iteration converged, the mass fraction contour of NO and CO in the catalytic converter can be obtained. The iteration process until convergence took about 12 minutes.

3. Results and Discussion

3.1 Effect of Distance of Catalytic Converter from Manifold on Catalytic Converter Efficiency

3.1.1 Importance of Catalytic Converter Position along Exhaust Pipe

Determination of catalytic converter position along the exhaust pipe of automotive is critical in effective abatement of NO and CO. Placing the catalytic converter too near to the engine outlet is not favorable for the catalytic converter life time because extremely high temperature will cause deactivation of catalyst. Pt sintering occurs above 973K (Forzatti and Lietti, 1999) and start to deactivate at temperature above 1173K (Heck et al., 2002). Rd will start to react with alumina above 873K (Forzatti and Lietti, 1999) and deactivate at temperature above 1073K (Heck et al., 2002). Extreme high temperature will also causes

physical damages to catalytic converter. Placing the catalytic converter too far from the engine outlet will cause longer heat up time for catalytic converter due to heat loss and result a delayed and lower NO and CO conversion.

3.1.2 Prediction and Validation of Exhaust Gas Temperature at Inlet of Catalytic Converter

Module A uses CFD Fluent 6.0 to simulate the temperature profile along the exhaust pipe taking consideration of heat loss along the exhaust pipe wall. The outlet temperature from the engine is assumed at 920K constant as per work by Chan and Hoang (1999). The simulated temperature at the pre-determined position is assumed to be inlet temperature into the catalytic converter at the position. Figure 7 shows the temperature profile inside the exhaust pipe from 1s to 10s after the engine starts. CFD simulation result of the temperature profile of the inlet of catalytic converter positioned at 110 cm from engine and measured data by Chan and Hoang (1999) is shown in Figure 8. Comparing both data in Figure 8, it showed that the predicted temperature profile at the first 10s by CFD is in agreement with the experimental data from the work of Chan and Hoang (1999). After 10s, the simulated temperature increases in a rate quicker than the measured data by and remain consistent 556 K after 15s as shown in Figure 8.

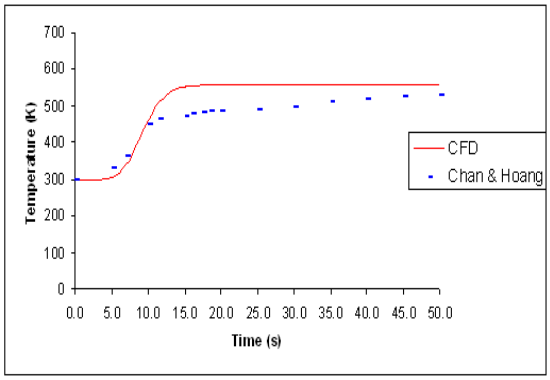
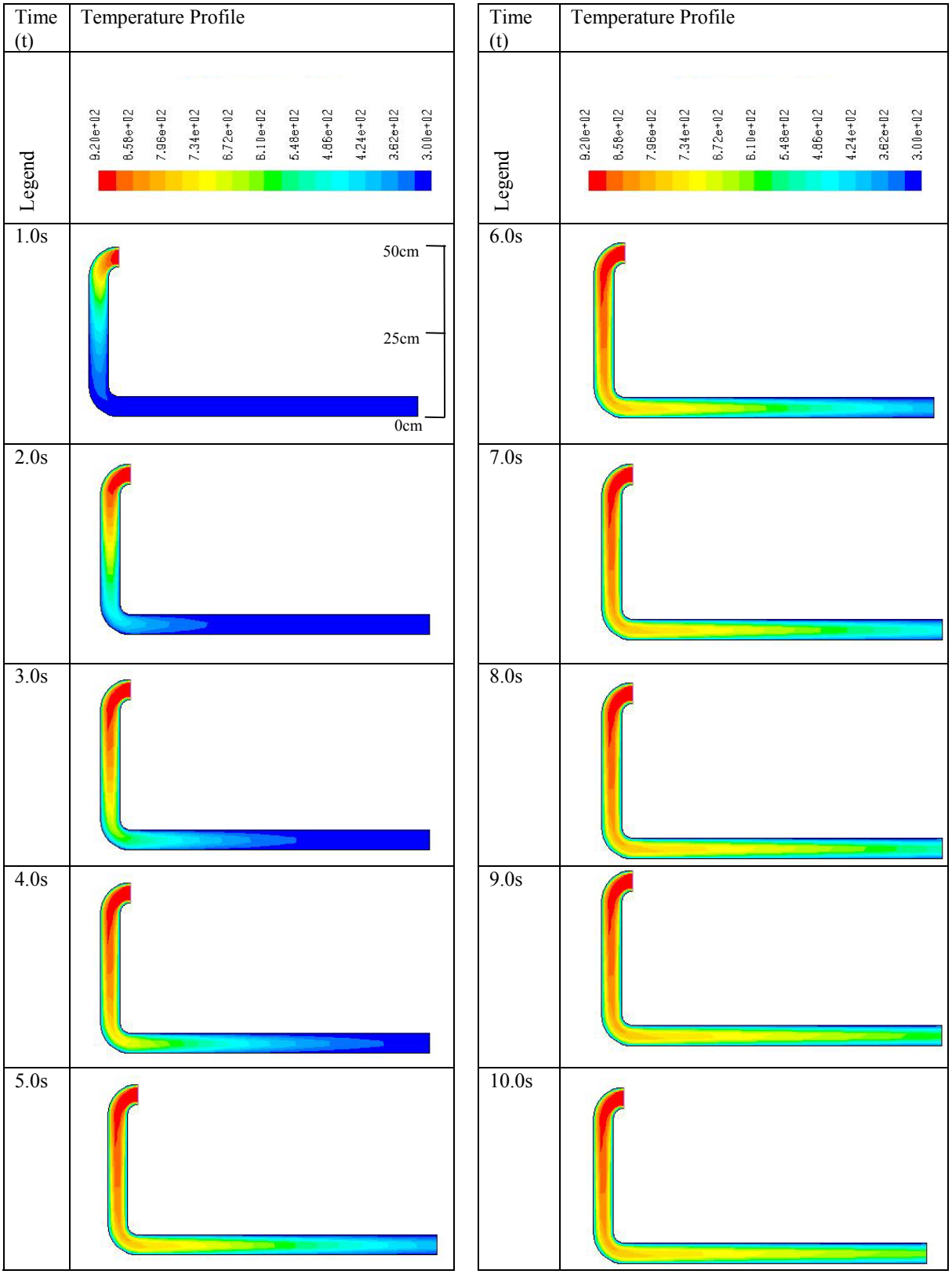


Figure 8. CFD Simulated Temperature Profile of the Upstream of Catalytic Converter at 110cm from Engine. Experimental data from Chan and Hoang (1999).

Figure 7. CFD Simulation of Temperature Contour of Exhaust Gas inside the Exhaust Pipe from 1s to 10s after Engine Started



3.1.3 Prediction of Exhaust Gas Temperature at Inlet of Catalytic Converter

Temperature profile at inlet of catalytic converter at position 10 cm, 30 cm, 50 cm, 80 cm and 110 cm from the engine respectively, are simulated by CFD using the assumption that the first 10s data is accurate as mentioned in 3.1.2. The results are shown in Figure 9.

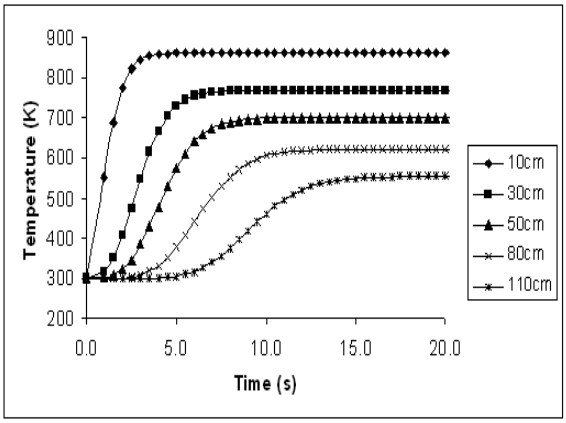


Figure 9. CFD Simulated Temperature Profile at Inlet of Catalytic Converter at Position 10 cm, 30 cm, 50 cm, 80 cm and 110 cm from Engine Outlet, respectively.

Based on the simulated temperature profiles, it is not advisable to put catalytic converter 10cm from the engine because the catalytic converter will experience sudden increment of an extremely high temperature to 800K in less than 5s where deactivation of catalyst will start to happen. From the interpolation, it can be concluded that installing catalytic converter below 25 cm from the engine is not suitable because the catalytic converter will be exposed to temperature above 780 K.

At distance of 50 cm from the engine, the inlet temperature is 700 K after 10 s, the monolith temperature will achieve CO light off temperature at about 90s (1.5 minutes) and NO light-off temperature at about 210s (3.5 minutes).

At distance of 80 cm from the engine, the inlet temperature is 623 K after 10s, the monolith temperature will achieve CO light off temperature at about 240s (4 minutes) and NO light-off temperature at about 600s (10 minutes) which is too long for effective NO and CO abatement in cold start engine.

3.1.4 Sectional Discussion

The temperature profiles of inlet of catalytic converter at different position showed that it is not suitable to install catalytic converter less than 25 cm from engine since the catalytic converter will subject to high temperature (>780 K) and causes deactivation of catalyst. It also showed that it is not suitable to install catalytic converter at distance more than 80cm from the engine due to long lag time in CO and NO abatement at cold start. It is more suitable to install at a range between 25 cm to 80 cm. A typical measurement done on car model Honda City manufactured in 2006 found that the distance between the catalytic converter inlet and the engine outlet is 55 cm.

3.2 Prediction of Catalytic Converter Surface Reaction Profile

CFD simulation done in Module B on NO and CO mass fraction at 750 K inside a channel of catalytic converter are shown in Figures 10 and 11 respectively.

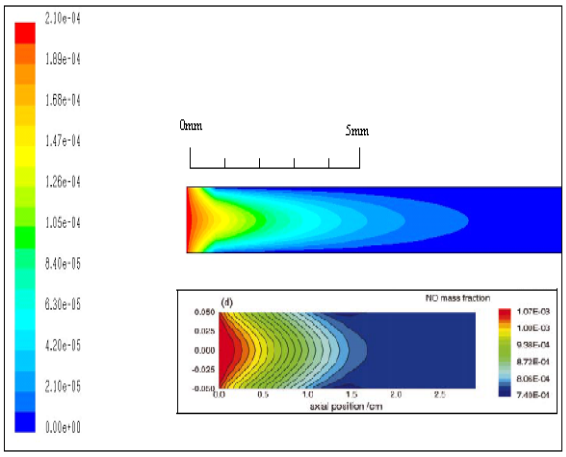


Figure 10: NO Mass Fraction Profile inside a Cell at 750K. Inserted diagram at lower right is data from Chatterjee et al. (2001)

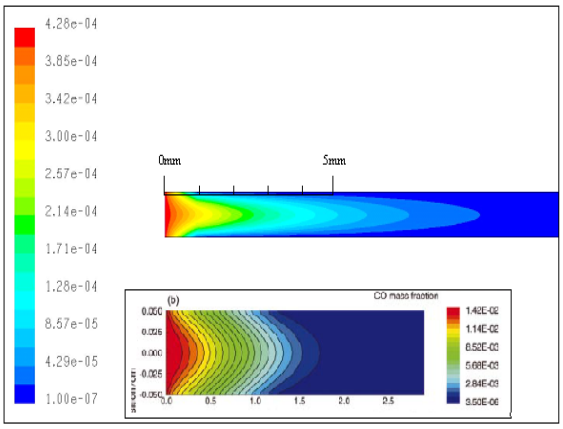


Figure 11: CO Mass Fraction Profile inside a Cell at 750K. Inserted diagram at lower right is data from Chatterjee et al. (2001)

The CFD simulations show NO and CO conversions happen within first centimeter and completely converted within two centimeters; which is agreeable with work by

Chatterjee et al.(2001). The NO surface reaction contour obtained showed a complete conversion.

The CO conversion simulation within a channel showed an almost complete conversion in axial distance which is very much agreed with work by Chatterjee et al. (2001). According to Chatterjee et al. (2001) this phenomena is explained by means of surface coverages. For the axial distance of 5 to 7 mm, the NO coverages varied strongly because of the decrease in CO concentration in the gas phase. During this transition the number of free catalysts site allow more NO to be adsorbed and disassociated (Chatterjee et al., 2001).

The CFD simulation of NO and CO mass fraction profile is similar to pattern simulated by Chatterjee et al. (2001). Surface chemical reactions input into the CFD Fluent 6.0 are much simplified compared to the DETCHEM chemistry module used by Chatterjee et al. (2001).

4. Conclusion

The simulation in CFD Fluent 6.0 to predict NO and CO emissions of a cold start CNGV with catalytic converter were done. The CFD model in prediction of exhaust gas temperature at inlet of catalytic converter showed that it is not advisable to place catalytic converter below 25 cm and above 80 cm from the engine outlet. Placing catalytic converter too near to the engine will subject catalytic converter to extreme heat as shown by the result of simulations. Eventually, the life span of the catalytic converter is shortened. Placing the catalytic converter too far from the engine outlet will cause longer heat up time for catalytic converter as simulated and result a delayed and lower efficiency of NO and CO conversion.

CFD Fluent 6.0 can used to model NO and CO surface reactions on a single channel of catalytic converter. However, due to limitation of functions to input catalysts surface coverage, other parameters such as Arrhenius constants have to be adjusted to produce satisfactory simulation results. In this simulation the A_k of literatures value has to be multiple by factor of 10^{-15} input data for CO reaction and factor of 10^{-16} for NO reaction for FLUENT.

5. Future Study

Results obtained from the computer modelling exercise have demonstrated that CFD FLUENT is capable of modelling the NO and CO abatement by catalytic converter in cold start condition. In the advancement of computational fluid dynamics and advent of a powerful workstation, there is still very wide scope of research of catalytic converter that could be done in the future. The suggested scope for future study includes simulation improvement on CO conversion in catalytic converter and simulation of HC abatement. Future study in combination of pollutants abatement and exhaust system temperature profile in a single modelling program will be useful. CFD FLUENT coupled with appropriate modules such as DETCHEM or FEMLAB should be done in the future to simulate more complex and new catalytic converter technology such as HC and NOx trap, preheated catalysts to achieve zero emission vehicles.

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