MODELING AND SIMULATION IN THE FIELD OF ENVIRONMENTAL AND AIR POLLUTION ABATEMENT;

SPECIAL EMPHASIS ON

CATALYTIC CONVERTERS

BY

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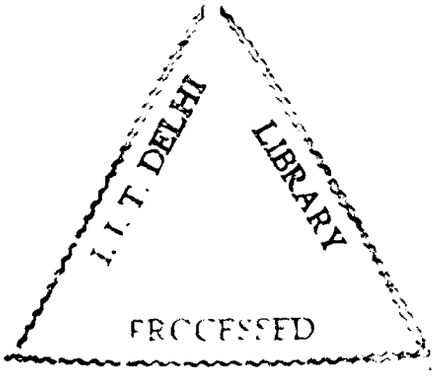

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CERTIFICATE

This to certify that the thesis entitled, "**Modeling and Simulation in the field of Environmental and Air Pollution Abatement; Special emphasis on Catalytic Converters**", being submitted by **Ms Sanchita Chauhan** to Indian Institute of Technology, New Delhi, for the award of degree of Doctor of Philosophy is a record of bonafide research work carried out by her. She has worked under my guidance and supervision and has fulfilled the requirements for the submission of this thesis, which to my knowledge has reached the requisite standard.

The results contained in the thesis have not been submitted, in part or full, to any other university or institute for the award of any degree or diploma.

18/06/03

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ABSTRACT

This thesis concerns Modeling of Automotive Catalysts for the purpose of controlling tail-pipe emissions. The work focuses on development of a model capable of simulating various components present in exhaust gas after-treatment system during cold start. The model developed was a simple model that could give fast and reasonably satisfactory results for species conversion and simulates both for the thermal transient and the steady state conversion for the desired species.

Keeping this as the objective a transient model to simulate for both thermal and conversion characteristics of adiabatic monolith converter operating under warm-up conditions was made. The transient response of the catalytic converter for hydrocarbon systems during cold-start period in the converter was analysed. During this warm-up period when the engine has just started, the catalyst is at the ambient temperature (i.e., has the same temperature as the surroundings), usually in the range of -20°C to 45°C depending upon the climatic conditions of the place.

For the reactions to get initiated on the catalyst surface the catalyst requires pre-heating to a temperature of about 250-300°C. During a normal operation the incoming hot exhaust gas pre-heats the catalyst till the later achieves its operational temperature commonly referred to as the light-off temperature (is a measure of activity and is normally defined as the temperature at which 50% conversion of pollutants is achieved). This catalyst warming-up process takes about 1-2 min and during this time as much as 60-80% of the total hydrocarbon emission occurs. Solution to this problem is still under development.

Improvement of design requires fundamental understanding of the complex processes taking place in the converter involving fluid flow, heat and mass transfer and chemical reactions. The design improvements also require in addition to experimental testing (which is very expensive), an ability to numerically simulate the models and predict the converter performance.

Hydrocarbon composition in the exhaust is a function of the engine temperature and operating conditions. With conventional analysers it is not possible to have time dependent information about the activity of different hydrocarbons present in the exhaust [Koltsakis et al., 1997]. So a rough approximation is made in such computations. Initially single fast oxidising hydrocarbon propylene was considered

representing the total hydrocarbons and later another relatively slow oxidising hydrocarbon propane was added to see the combined effect on the system. Both homogenous as well as catalytic reaction terms are accounted for in the mass and energy balance equations for the gas as well as the solid phase. The variations in gas concentration, gas temperature and solid temperature along the length of the converter with respect to time are determined.

For gas concentration and gas temperature the equations are ordinary differential equations of first order and for the catalyst temperature the equation is partial differential. All these equations are coupled, representing a quasi steady-state system and their solutions are interdependent. The ordinary differential equations are solved by Runge-Kutta method of fourth order and the partial differential equation is solved using Backward Implicit Scheme. Also the effect of changes in various parameters like inlet gas temperature, catalyst loading, cell density, initial solid temperature, and concentration of the reactant etc on conversion of the reactant gas was studied.

Comparison of modeling for two-gas system using a quasi steady-state system was made with results later derived for unsteady state system. In the former case as already stated a combination of three ordinary differential equations and one partial differential equation

represented the system and in the later case of unsteady state system four partial differential equations, representing the gas phase concentrations, temperature and solid temperature respectively was considered.

Nitrogen oxide engine-out emissions during cold start are not considered as it has been reported that these emissions are very low for engine operating at low loads. Also due to high hydrocarbon emission rates at cold start, the effect of carbon monoxide emissions is also neglected in the present work.

As only warm-up of the converter is being considered, model analysis providing exhaust gas composition averaged over distinct driving operation modes (idling, acceleration, constant speed and deceleration) is not taken into account for modeling purpose.

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