A Stochastic Reactor Based Virtual Engine Model employing Detailed Chemistry for Kinetic Studies of In-Cylinder Combustion and Exhaust Aftertreatment

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Introduction

The objective of this work is to demonstrate a Stochastic Reactor based Virtual Engine concept (SRVE) for study of chemistry in in-cylinder combustion, through piping, and in the catalyst. The SRVE is based on stochastic reactors, which take into account inhomogeneities and turbulent mixing. Due to the low number of computational cells in each submodel (~100 - 1000), the model is CPU efficient. In all models detailed or reduced chemistry is applied, to correctly account for chemical reactions. The model is used to study the effect of A/F oscillation frequency on tail-pipe emissions in an SI engine.

Stochastic Reactor Virtual Engine Model Description

The model is based on a stochastic reactor in-cylinder combustion model, earlier successfully applied for SI ([1]-[3]), Diesel (e.g. [4]-[6]), PPC ([7]) and HCCI ([8]) engine operation modes. In a stochastic reactor model the probability density function describing the state of the gas charge is discretized by a number of particles, each having different properties (composition, enthalpy). This makes it possible to incorporate detailed chemistry and to consider inhomogeneities. Since spatial information of the individual particles is not considered, the CPU time is kept affordable. For SI engine combustion the engine geometry is taken into account by the use of a turbulent flame propagation model [2]. Compared to simpler 0D models the SRM has the potential of emission prediction.

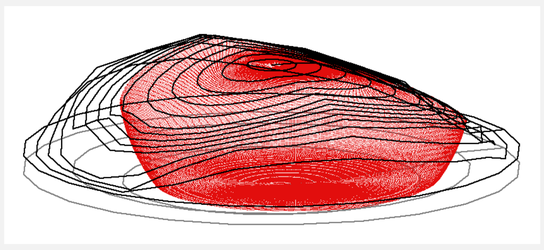

Fig. 1: The flame front at a given time.

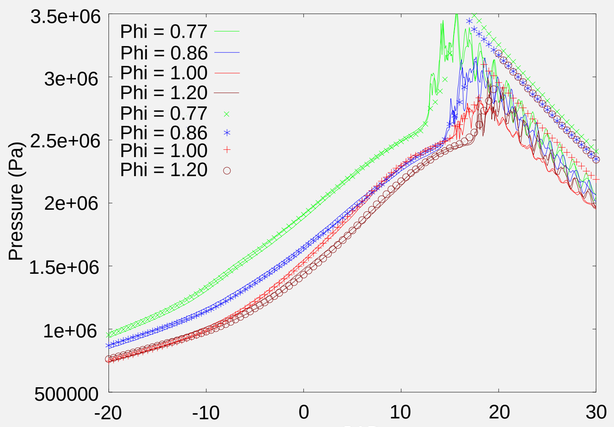

Fig. 2: Application of the In-Cylinder combustion model for knock prediction [2]. Lines are experiments, markers are calculations.

Chemical reactions in the exhaust pipes are modeled using a chain of stochastic Partially Stirred Reactors (PaSR). In each reactor the gas is discretized in a user defined number of particles.

Fig. 3: Graphical representation of the pipe model.

The catalyst brick is modeled with a representative channel transient 1D thin film layer model [9]. Heat and mass transport between bulk gas and thin film layer is modeled by the use of heat and mass transfer coefficients. In the thin film layer (washcoat) detailed or global surface chemistry is applied.

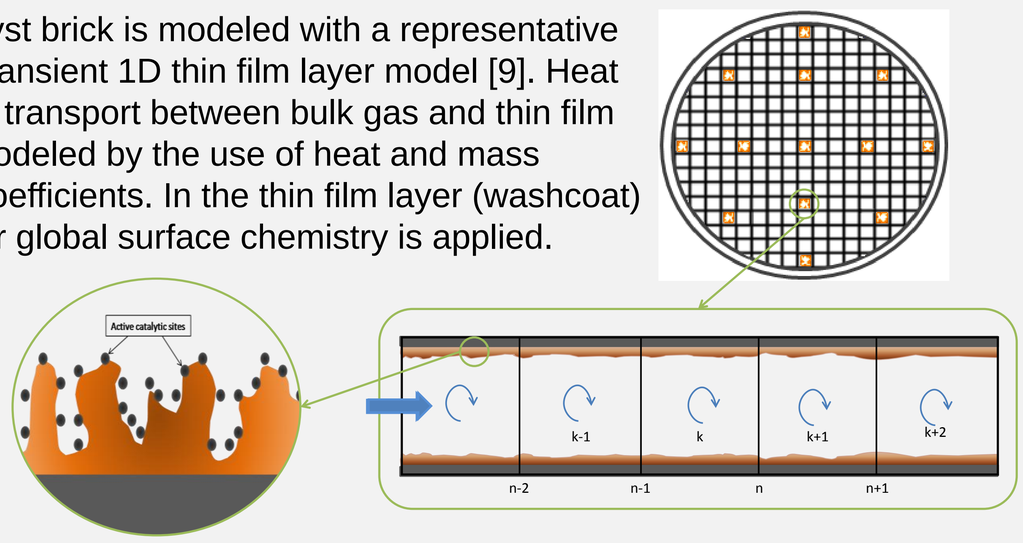

Fig. 4: Graphical representation of the catalyst model

In each part of the reactor network detailed or reduced chemistry is applied.

Conclusions

- *The λ oscillation frequency is shown to have high impact on TWC emission conversion.*
- *Important effects are caught when using chemical kinetics in in-cylinder combustion, exhaust pipes as well as catalyst models.*

Results and Discussion

The SRVE is applied to a hypothetical model of a typical passenger car SI engine. The effect of λ variation frequency on TWC conversion efficiency is studied

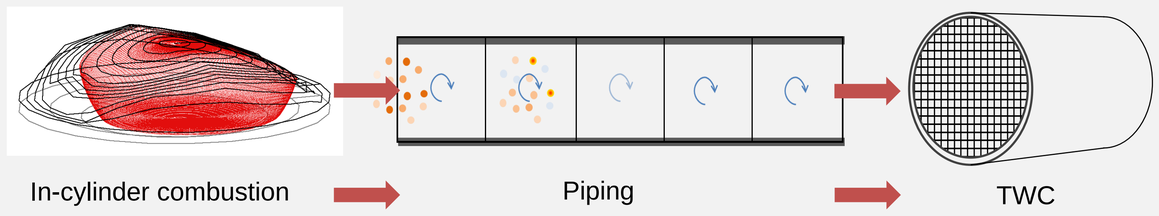

Fig. 5: Graphical representation of the reactor network used in the SRVE for this application.

In-cylinder combustion

In-cylinder combustion is simulated with the stochastic reactor two-zone model employing turbulent flame propagation [2]. A skeletal mechanism for PRF (iso-octane / n-heptane) blends [10] is applied for laminar flame speed, emissions and knock prediction. Calculations are performed at λ values of 0.98, 1.00 and 1.02, see fig. 6 for pressure traces. Note the kink in the pressure trace by the end of combustion. This kink is explained by a snapshot of the flame at this moment; at this moment the flame hits the cylinder walls in the squish area closest to the spark plug (placed a few mm from the centerline), resulting in a sudden decrease in burn rate.

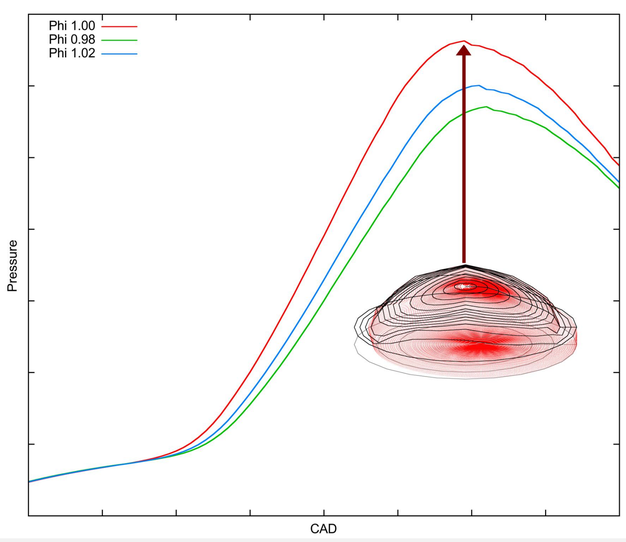

Fig. 6: Pressure trace for ϕ 0.98, 1.00 and 1.02.

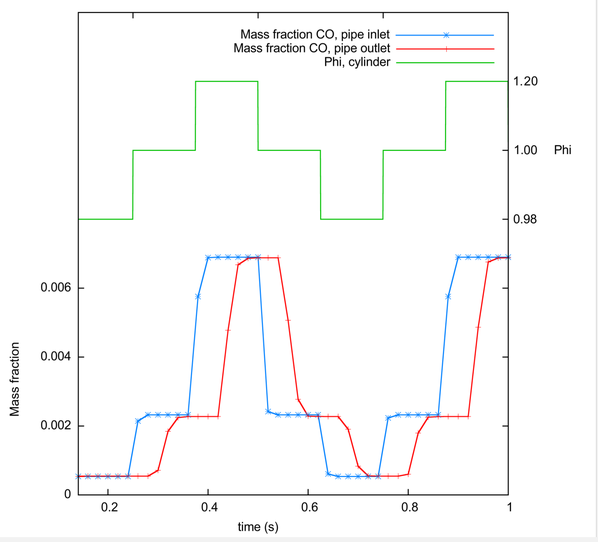

Fig. 7: ϕ oscillation (green line) and mass fraction CO, inlet and exhaust flow to/from the pipe, for ϕ oscillation of 2 Hz.

Exhaust pipes

The exhaust pipes between cylinder and TWC are simulated with a stochastic reactor pipe of 1 m. The exhaust gases from the in-cylinder calculations are injected into the exhaust pipe as a step function, see fig. 7 above. The skeletal PRF mechanism used for in-cylinder combustion is also used in the pipe. In fig. 7 it is seen that CO, as expected, attains the highest concentration during the fuel rich phase. CO conversion in the pipe is in principle zero. In table 1 inlet and exhaust maximum mass fractions of various species as well as conversion rates are given. It is seen that radicals such as OH are removed in the pipe system, whereas emission conversion is very low. It is interesting to note the high increase of NO_2 in the pipe; under fuel lean conditions NO is oxidized to NO2 in the exhaust pipe.

	Inlet	Exhaust	Conversion
CO	6.90E-03	6.88E-03	2.4 %
OH	4.48E-05	1.67E-08	99.96 %
NO	3.91E-03	3.89E-03	0.51 %
NO2	1.71E-05	4.75E-05	-177 %

Table 1: Maximum value of species mass fraction and conversion in pipe, 2Hz ϕ oscillation.

Three-Way Catalyst

The exhaust gas from the pipe is injected into the catalyst model. A global TWC chemistry with oxygen storage is used [11]. Unstable unburned hydrocarbons are lumped to the reference species C_3H_6 and stable hydrocarbons are lumped to the reference species C_3H_8.
The catalyst temperature is set to 850 K, and the exhaust gas temperature is 700 K.
The inlet and exhaust mass fractions of CO and NO are shown in fig. 8.
The outlet mass fractions of NO and CO are significantly different at different oscillation frequencies.
At 2 Hz equilibrium conversion rate is not reached, which smoothens the effect of λ oscillations. Thus the overall conversion rate for CO is 54 % higher at 2Hz. Table 2 gives the conversion rate for all emissions.

	1 Hz	2 Hz
CO	44 %	68 %
NO	49 %	49 %
HC	85 %	84 %

Table 2: Emission conversion in TWC.

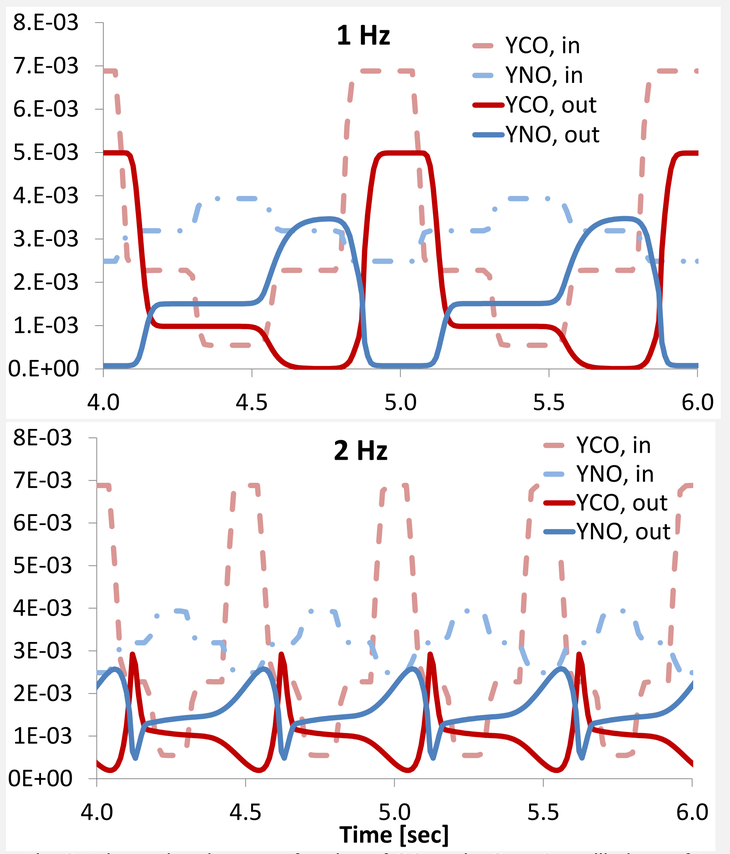

Fig. 8: Inlet and outlet mass fraction of CO and NO, at λ oscillations of 1 and 2 Hz

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