1D ENGINE MODELING WITH DETAILED REACTION KINETICS

Karin Fröjd[1], Cathleen Perlman[1], Adina Tunér[1*], Fabian Mauss[2]

[1]LOGE AB – Lund Combustion Engineering
Scheelevägen 17, Beta 2, 223 70
Lund
Sweden
kfrojd@loge.se
cperlman@loge.se
atuner@loge.se
Tel.: +46 46 286 2486
* corresponding author

[2]Brandenburg University of Technology Cottbus
Faculty of Environmental Sciences and Process Engineering
Konrad-Wachsmann-Allee 1, 03046
Cottbus
Germany
fmauss@tu-cottbus.de

ABSTRACT

Numerical investigations of the response of fuel consumption and exhaust emissions on internal-combustion engine parameters or transient-load cycles are needed for the analysis and optimization of the complete powertrain system. For this purpose, simple and numerically fast but still accurate models are needed for in-cylinder combustion and for exhaust after-treatment. The chemical processes must be represented in sufficient detail to predict emission levels of soot, NO_x, CO and unburned hydrocarbons. This work reports on a network of transient one-dimensional reactors invoking detailed chemistry for the accurate emission prediction throughout the engine powertrain.

Our approach is based on the stochastic reactor model (SRM) for the simulation of all in-cylinder processes. Stochastic reactor models assume statistical homogeneity of the gas charge. The SRM model is suitable to predict combustion and pollutant formation in SI and Diesel engines including unwanted combustion, such as engine knock. The network makes further use of stochastic perfectly stirred reactor models for pipe sections. This allows modeling inhomogeneities in the exhaust gas. Models for catalysts and for particulate filters are available, invoking detailed surface chemistry or simplified global chemistry.

Keywords: *1D engine simulation tool, internal-combustion engine, catalyst model, diesel particulate filter DPF model.*

1. INTRODUCTION

Typical 1-D engine simulation tools available nowadays offer a rather advanced description of the physical phenomena within engines' cylinders [1], [2]. However such models are limited when modeling the gas chemical composition, and/or the chemical processes within the engine. The inclusion of chemical information in one-dimensional flow calculations offers the prediction of autoignition or engine knock, and/or the formation of exhaust pollutants: NO_x, soot, HC, CO. It further facilitates calculation of the overall fuel consumption and thereby the CO_2 emission.

DARS (Digital Analysis of Reaction Systems) [3] has been built with the specific purpose of enabling detailed chemical analysis to engineering applications, with one particular focus on internal combustion engines. This tool handles gas phase chemistry, surface chemistry and particulate modelling via a suite of reactor models and reaction mechanisms. DARS includes homogeneous models (theoretical and engine based), stochastic reactor models (SRM) for HCCI, DICI, SI engines, flame models (premixed or counterflow), a reaction mechanism database for various fuels and tools for mechanism development, reduction, and export. DARS also allows for combining detailed chemistry investigations with one-dimensional commercial engine simulation tools (GT-Power and Ricardo Wave).

Recently the engine model was extended with a gas exchange model. For emission aftertreatment a catalyst model and a diesel particulate filter (DPF) model became available. The gas exchange model rounds off the SRM engine model [4]. The stochastic reactor model assumes statistical homogeneity instead of full homogeneity as in a zero-dimensional reactor model. The model includes direct injection, valve flow and combustion using detailed chemistry.

The one-dimensional catalyst model, briefly presented in this paper, is based on earlier research in the field and uses a representative channel model to simulate the catalyst behaviour. This model is fully described in reference [5]. A transient one-dimensional thin film layer model is used to calculate the evolution of gas phase as well as surface sites. In the thin film layer either global gas-phase chemistry or detailed surface chemistry can be considered. The latter facilitates simulating site blocking and poisoning of the catalyst.

The one-dimensional DPF model considers representative channel pairs to simulate the particulate filter behaviour. Soot deposition inside and on top of the filter wall is modelled by the spherical unit collector concept. Deposited soot is oxidized by molecular oxygen (O_2) and nitrogen dioxide (NO_2). In catalysed particulate filters nitrogen dioxide can be created from nitrogen oxide through catalytic reaction paths. Among others, the model predicts the soot cake thickness, porosity and permeability, and the influence of the soot cake on back pressure and gas velocities. The DPF model further predicts the gas phase emissions – for example NO_2.

This paper focuses on the newly developed engine cylinder gas exchange model, the catalyst model and the DPF model. The possibility of integrating these models into a 1D engine simulation tool is also discussed. The fully integrated model is under final refinement and therefore only preliminary results showing its capabilities have been included. Figure 1 displays the engine reactor network which can be facilitated with the tools presented in this paper. The network includes inlet/ exhaust/ distribution/ EGR

pipes, turbocharging, gas coolers (intercooler, EGR cooler), valves, catalyst and particulate filter.

2. MODEL

2.1 The stochastic reactor model for engine in-cylinder simulation

In this section we first present the stochastic reactor model for simulation of DICI engines during the closed cycle. The inclusion of the valve breathing model is discussed thereafter. Further information can be found in reference [4].

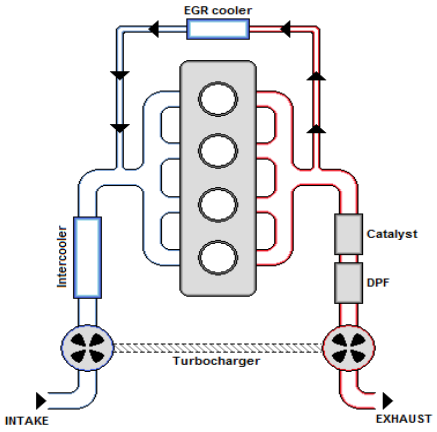

Figure 1: Illustration of the reactor network of an internal combustion engine that can be modelled with the 1D tool.

The Stochastic reactor model (SRM) is a PDF (Probability Density Function) based model for simulation of reactive systems. The SRM engine model was first developed for HCCI engines [6]. Since then the SRM based engine models have been further developed for DICI, and DISI engine applications. The inclusion of mixing effects at low computational costs is the strength of the SRM.

2.1.1 The PDF and the MDF

In a real engine or in a CFD model the chemical composition, temperature and mass, are spatially resolved. In the space dimensionless SRM the state variables are described by a probability density function (PDF).

The temperature and species PDFs exhibit skewed bell shapes with several peaks, due to phenomena such as auto-ignition and wall cooling. During a calculation with the SRM the shapes of the PDF as well as the range of the numerical values change with each time step. The PDF is discretized in a user defined number of "particles" or realizations by mass, representing the discretized mass density function (MDF).

2.1.2 The SRM for DICI

The DICI-SRM is an extension of the HCCI-SRM, described in [6], including the direct injection model. The model is intended to be computationally efficient and able to provide predictive information of engine performance and emissions. It is suitable for simulating diesel engines (CI) and p-HCCI.

In direct injection engines, such as diesel engines (CI) the combustion process is strongly influenced by the mixing processes [7], if the chemical processes are much faster than the physical processes. Nevertheless, the actual initiation of the combustion and the formation of pollutants is a chemically decided phenomenon. The SRM offers, using a detailed kinetic model together with a reasonable mixing model, to predict chemistry-flow interaction. It therefore predicts chemically slow processes such as auto-ignition or emission formation, such as soot, NO_x and CO formation. Comparisons of CFD and SRM predictions for a Diesel engine are reported in reference [8]. A VW DI engine was investigated in reference [9], by means of DICI-SRM calculations. Good agreement between experiments and calculations has been reported for the global engine

performance parameters BMEP and PSFC. Ignition delay and heat release rate are also well predicted. Also NO_x emissions are well predicted, whereas HC and CO emissions have been under-predicted which can be improved by increasing the number of particles in the discretized MDF.

2.1.3 Operator splitting and numerical solution

An operator splitting approach is employed [10] to solve the stochastic differential equation for the MDF at each time step. The differential operator is subdivided and the different physical and chemical processes are solved sequentially as shown in Figure 2. Each process is calculated at isobaric condition, which causes that the volume becomes different from the cylinder volume at the current time. The volume defect is corrected in the pressure correction procedure at the end of the operator splitting loop, using an adiabatic, isentropic compression.

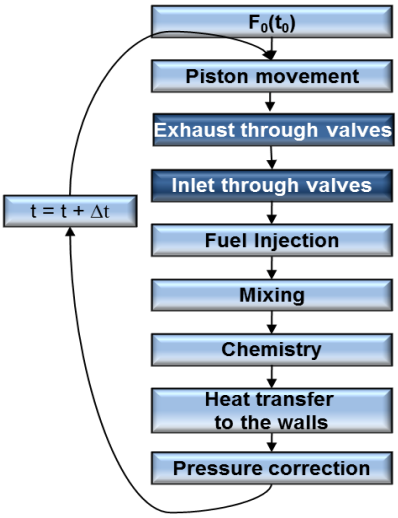

Figure 2: Operator splitting loop, including valve flow.

The initial conditions for the DICI-SRM calculation include global pressure, temperature, air/fuel ratio, EGR amount, residual gas composition, cylinder wall temperature, etc. . During model initialization, the mass within the cylinder is divided into an arbitrarily pre-set number of particles. Thus a discretized MDF is achieved. In the following the different terms in the MDF are briefly described.

During closed cycle the **piston movement** works against a closed cylinder, and gas compression of expansion occurs. During **gas exchange**, explained in more detail below, the pressure in the cylinder is almost constant. The gas exchange operators are grouped with the fuel-injection operator in order to perform all mass-exchange processes at the same time, see Figure 2. This avoids unrealistic pressure changes due to the separate treatment of exhaust and inlet fluxes. The pressure correction is performed after the treatment of all mass transfer terms in the MDF. The flow through the exhaust valve is treated before the flow through the inlet valve, avoiding an unrealistic selection of newly injected particles for the exhaust flow.

The **mixing** term results from the turbulent flow in the cylinder. The main effect of turbulence is spreading and dispersing inhomogeneities. Mixing / turbulence phenomena are themselves stochastic processes. A number of mixing models have been developed for PDF-methods in the past. The interaction by exchange with the mean (IEM) and the modified coalescence-dispersion C/D model are used in the current simulation code. For zone models such as the two-zone SI engine model, mixing occurs only within each zone.

Regarding the **chemistry** operator, for each particle a set of transient equations, equivalent to the set of equations describing a regular constant pressure reactor is solved. This step needs sub-cycling since the governing equations are highly nonlinear. A backward differential function method combined with a modified Newton algorithm is

used to solve this system of equations. The result is the new chemical composition for the particle at the next time step.

Heat transfer is a phenomenon directly responsible for temperature inhomogeneities within the engine cylinder gas. A particular strength of the SRM is its ability to model the inhomogeneities. Accordingly, the heat transfer model is of central importance to the SRM code. The implemented model uses the Woschni heat transfer model determining the total amount of heat transfer [11], but a stochastic approach [12] to decide the distribution of the heat transfer over the particles.

The **fuel injection** model employed can model multiple direct injections with arbitrarily shaped injection profiles. The vaporization rate of the fuel is given as input by the user.

2.1.4 The gas exchange model

A valve-flow model was added [13] to the existing SRM. The mass flow appears as a new term in the differential equation for the MDF. The valve-flow model needs pressure and temperature profiles of the pipes as user input, which can be provided by 1-D engine simulation tools. The equations for gas flow through valves follow entirely the description in [14].

The valve-flow model assumes a steady, adiabatic and reversible flow of an ideal fluid through a duct. The valve flow in an engine is not an ideal flow, and the discharge coefficient is introduced to account for real gas effects. The stochastic model for mass transfer through the exhaust valve is similar to the stochastic heat transfer model.

Regarding the inlet gas flow, the basic assumption is that the injected mass is not immediately mixed with the rest of the cylinder gas. The methodology resembles the one used for fuel injection. Stochastic particles from inlet pipes are preserved and directly inserted in the cylinder model, if pipes are connected to the cylinder within a reactor network.

2.2 The pipe sections model

The reactor network makes use of chains of stochastic perfectly stirred reactor models for pipe sections, giving the possibility to model inhomogeneities in the exhaust gas. Nusselt laws for pipes are used to calculate the heat transfer to the walls. The heat transfer is treated stochastically as in the DICI model.

2.3 The catalyst model

The transient 1D catalyst model [5] is capable of modelling catalytic reaction paths, surface site blocking and reactant interdependence, external heat and mass transfer, gas phase chemistry, reaction-diffusion in the washcoat and heat conduction through the substrate. The catalyst model consists of a number of representative channels. Gas and surface properties are calculated as functions of axial distance for each channel. Heat is transported between the representative channels by conduction in the substrate. Results from a single-channel model are presented in this article. The heat conduction model was deactivated, and will not be further discussed.

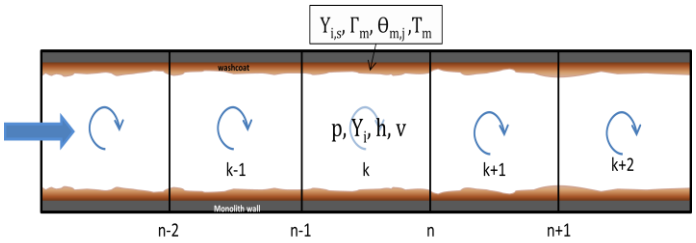

Figure 3: Illustration of the cell discretization in the catalytic channels.

The channel model is built by discretization of the pipe into a finite number of sections of length Δx (see Figure 3). The conservation equations for gas flow, chemistry and surface properties are solved using an operator splitting technique, decoupling the continuity and momentum equation from the species and energy conservation equations. The species and energy conservation equations for gas and surface sites are calculated for each section and the continuity and momentum equations are solved over all sections.

In each channel section the bulk gas is modelled as a 0D perfectly stirred reactor (PSR). To account for external diffusion the gas close to and inside the wall is modelled as a separate zone, called the *thin film layer*. Mass and heat transfer between the zones is accounted for through heat and mass transfer coefficients, calculated from the properties of the gas flow. To account for reaction-diffusion in the washcoat the effectiveness factor approach, used previously by e.g. Koop and Deutschmann [15], is invoked. The conservation equations for gas species mass fractions, gas enthalpy, surface temperature, thin film layer gas species mass fractions and surface site fractions are solved in each zone for each time step. The Navier-Stokes equations for pressure and flow velocity are solved over all sections in a separate step. The model is integrated into the DARS software package.

2.4 Diesel Particulate Filter model

The DPF is a transient 1D model [16] capable of modelling soot deposition in the wall, soot oxidation, gas kinetics and catalytic surface reactions throughout the channels together with heat conduction through the DPF. The DPF is modelled by a number of representative pairs of channels (Figure 4); each consisting of one inlet channel, a piece of substrate wall and one outlet channel. Gas properties and particulate mass accumulation and oxidation in the wall are calculated as functions of axial distance in each channel pair. Heat is transported between the representative channels by conduction in the substrate.

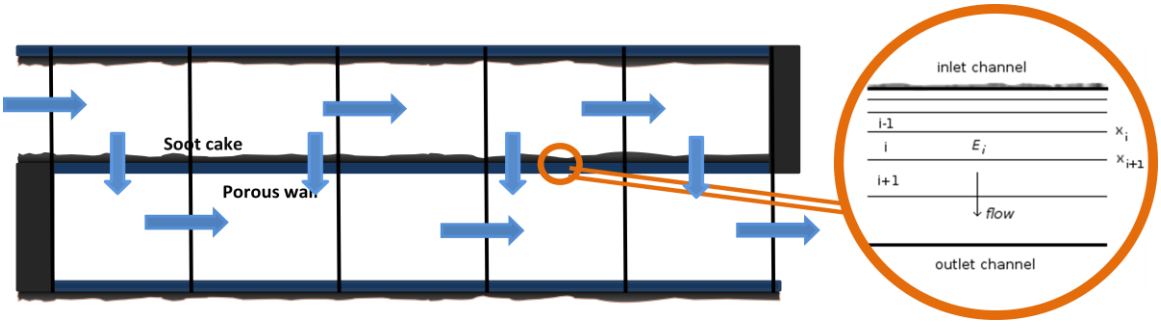

Figure 4: Illustration of the DPF model: representative channels and porous wall discretization

The Navier-Stokes equations for compressible flow, together with species and site conservation equations are the base for the channel model. The calculation of the flow in the inlet and outlet channels follows the lines in references [17] and [18]. An operator splitting method is applied to solve the governing equations. The pressure drop over the substrate wall is calculated by Darcy's law. Each channel section is modelled by a perfectly stirred reactor (PSR). The conservation equations for gas species mass fractions, gas specific enthalpy, and particulate matter deposit, oxidation and soot cake growth are solved at each time step at constant pressure. A number of parameters are required for a proper description of the DPF filter wall. Following the justification in reference [18], the micro-scale filter structure is approximated by spherical "unit" cells containing a collector which gradually fills, with particulate matter over time. Each filter cell is modelled as PSR, including soot deposition, soot oxidation, catalytic surface reactions and gas phase kinetics.

Soot cake forming above the filter wall is considered in the top filter cell. The top filter cell and the soot cake are treated through the two-layer model as described amongst others, in [18]. The particulate oxidation is assumed to follow a first-order heterogeneous process both in the presence or absence of catalytic materials (layer I and II respectively). Particulate oxidation by NO_2 is also accounted for. Carbon is oxidized through two reaction paths in layer I, considering the incomplete contact between particles and catalytic sites; a catalytic path over a certain fraction of the carbon specific area, β, and a non-catalytic thermal path over the remaining surface [19].

3. RESULTS AND DISCUSSION

In this section results from the individual models, described above are presented. The discussion of the interaction in between the models in a reactor sequence will be discussed in a following publication.

3.1 Results obtained with the DICI-SRM

DICI-SRM model results are presented for a VW direct injected engine. Figures 5 and 6 have been published before in reference [9]; they are shown here for demonstrating the model capabilities. Figure 7 shows further a joined PDF of NO mass fraction and temperature over the fuel air equivalence ratio. Emission concentrations at exhaust valve opening can be used for creating kinetic maps as functions of engine parameters. Figure 8 presents a typical emission map for CO as a function of EGR amount and IVC delay.

The engine calculation case in figures 5-8 had the following parameters: direct injection diesel engine, speed = 2000 rpm, bore = 81mm, stroke = 95.5 mm, compression ratio = 18, number of particles = 200, operator-split time-step size = 1 CAD, stochastic heat transfer coefficient = 15.

It was found that the DICI-SRM model calculates the NO_x emissions with an accuracy of 40% [21], 80% in [9], up to 88% in [20], while CO was strongly underpredicted in [9] (20%) and 60% [21]. Soot calculations were found indicative for general trends [20].

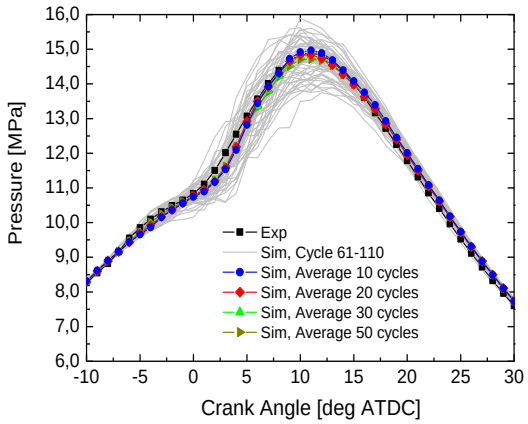

Figure 5: Pressure history variations, Average values from simulated cycles [9]

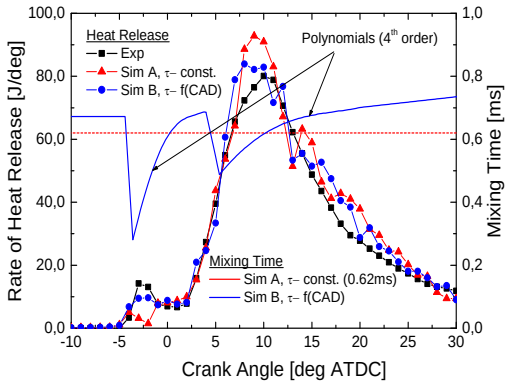

Figure 6: Simulated and experimental heat-release and in-cylinder pressure histories [9]

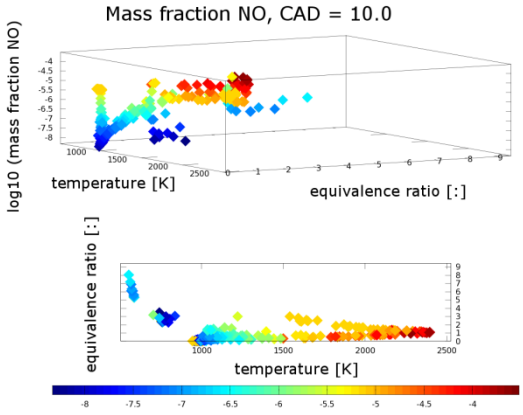

Figure 7: Nitric oxide mass fraction and temperature joined PDF map, as function of the fuel-air equivalence ratio

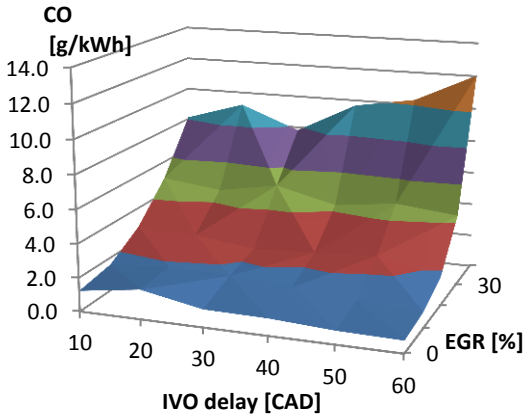

Figure 8: Engine emission map for CO as a function of EGR and IVO delay

Regarding the spark ignition engine model (SI-SRM), the tool is specifically designed to predict engine knock. It has been found that for this engine type the assumption of constant mixing time (in the interval 0.01...0.02s) provides fair results: knock can be predicted with accuracy within 1 CAD [20].

3.2 Results obtained with the catalyst model

The catalyst model is applied to experiments with a flat-bed reactor model catalyst published in references [15] and [22]. The catalyst is equipped with lateral outlets, giving the possibility to measure and study gas concentration profiles along the length of the catalyst. The experimental setup, measurements and catalyst used is thoroughly described in the references above. The model setup and further results are thoroughly described in reference [5].

The experiments are carried out under isothermal and steady state conditions in a flat-bed reactor manufactured by Delphi catalyst. A catalyst with a platinum γ-alumina wash coat carried by a monolithic honeycomb structure is used ([15], [22]). The space velocity of the gas is 40000 h^{-1}. A realistic model exhaust gas for Diesel engine emissions

under fuel lean and fuel rich conditions was used. The model gas includes CO, CO_2, O_2, H_2O, NO, NO_2, H_2 and C_3H_6. Propene is used as model species for reactive unburned hydrocarbons such as olefins or aromatics. An exemplary application of the model is shown in Figure 9 for fuel lean mixtures at 250 °C and 450 °C. The detailed kinetic scheme was taken from reference [15]. The concentration of C_3H_6 in the inlet gas was varied to study the inhibition effect of C_3H_6 on NO reduction. Intermediates from carbohydrate oxidation block the open surface sites for oxygen adsorption. Carbon monoxide is the most critical species in this respect. This was shown in reference [5] by comparing site fraction profiles. The inhibition effect is most pronounced at low temperatures, and vanishes at 450 °C. The agreement between DARS model calculations and experiments is very good (see Figure 9).

In Figure 10 the model response on transient hydrocarbon concentrations is reported. The initial condition for this calculation is a concentration of 90 ppm C_3H_6. At the time of 1 second all C_3H_6 is removed from the exhaust gas. The NO mole fraction in the gas as well as CO site fraction at the catalytic surface is presented in the figure. It is seen that NO oxidation follows CO site blocking, giving further proof that CO is the inhibiting intermediate from carbohydrate oxidation. The response time, defined as the time to move from 10% to 90% of conversion efficency in the case of no propene addition,of the catalyst is 5.5 sec(See Ref. [5] for more details.) This shows that site blocking is an important phenomenon. It is crucial to take it into account for accurate analysis of catalytic processes for complex gas compositions.

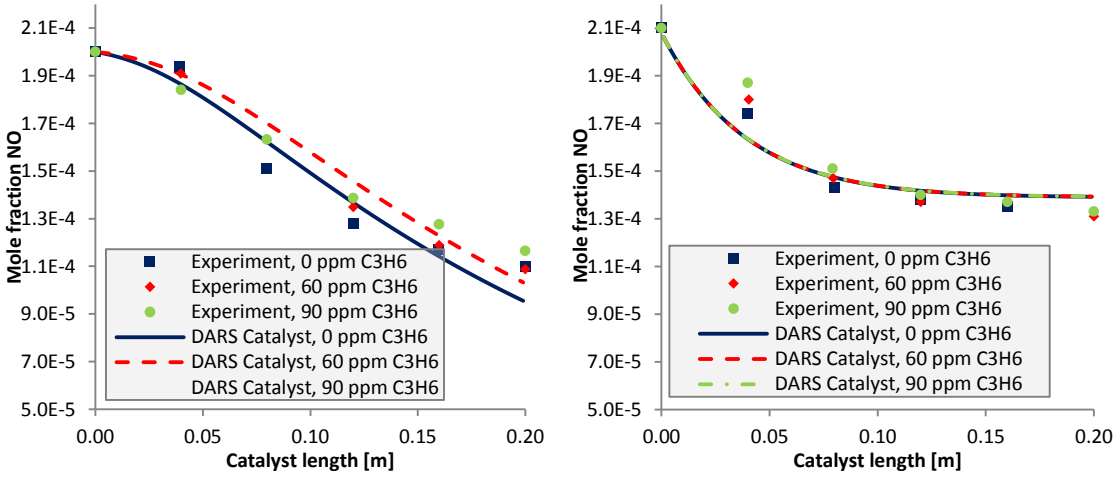

Figure 9: Application of the catalyst model in DARS BASIC 2.04: nitric oxide mole fraction in the burned gas mixture (250 ^{0}C and 450 ^{0}C) flowing along the catalyst pipe, as a function of distance – comparison to experiments (dots)

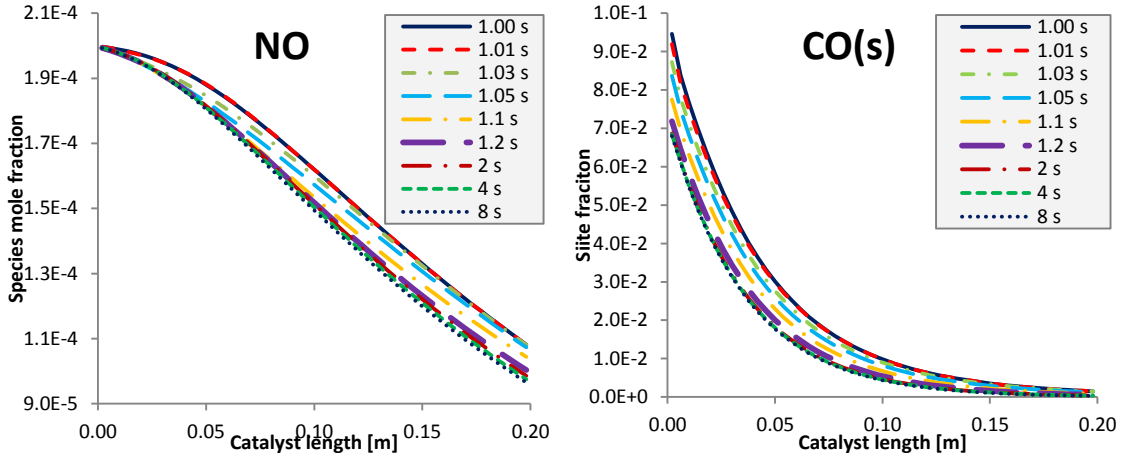

Figure 10: Application of the catalyst model in DARS BASIC 2.04: nitric oxide mole fraction and carbon monoxide site fraction (250 ^{0}C) along the catalyst channel, as a function of distance – time evolution for transition from 90 ppm C_3H_6 to 0 ppm C_3H_6

3.3 DPF model validation

The DPF model has been assembled and first plausibility tests are shown in this paper. For these tests experimental data have been taken from references [22], [24]. Figures 11 and 12 present DPF simulation results obtained for standard diesel engine exhaust gases. The main filter and exhaust gas parameters are the following: clean filter wall permeability = 5.3e-13 m^2, filter wall thickness = 0.43 mm, soot permeability = 1.8e-14, unit collector diameter = 10.5e-6 m, inlet gas temperature = 526 K, inlet soot mass fraction = 5.e-5, inlet pressure = 2 bar, outlet pressure =1 bar. Chemical kinetic data have been received from reference [25].

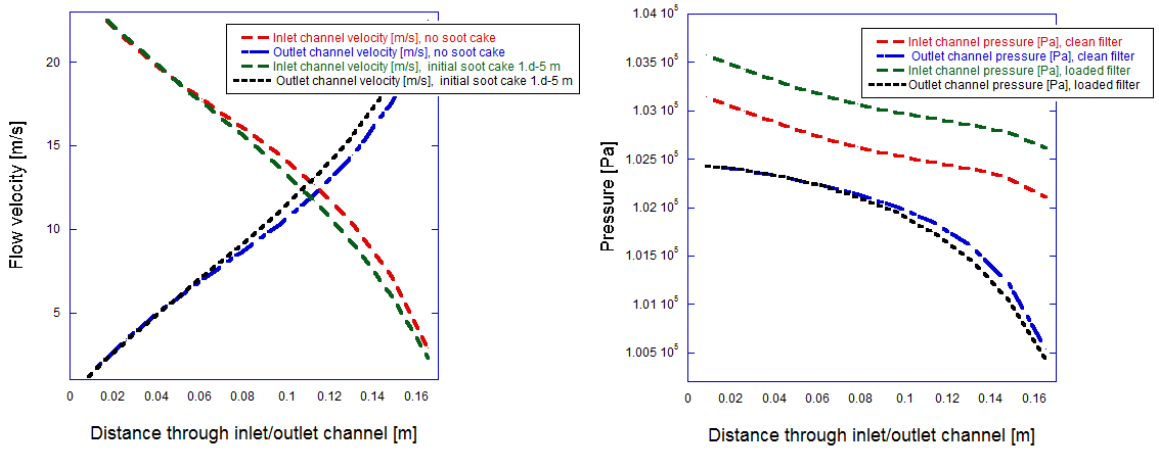

Figure 11: Simulation results obtained for the DPF model: flow velocities and pressure in the catalyst channel.

The calculated pressure drop over the filter wall and the calculated flow velocities (Fig. 11) agree with literature trends. A transient DPF calculation is shown in Figure 12. In an initial period soot is accumulated inside and on top of the filter. Thereafter the soot

load becomes stationary. This is evident from the filter wall permeability shown in Figure 12.

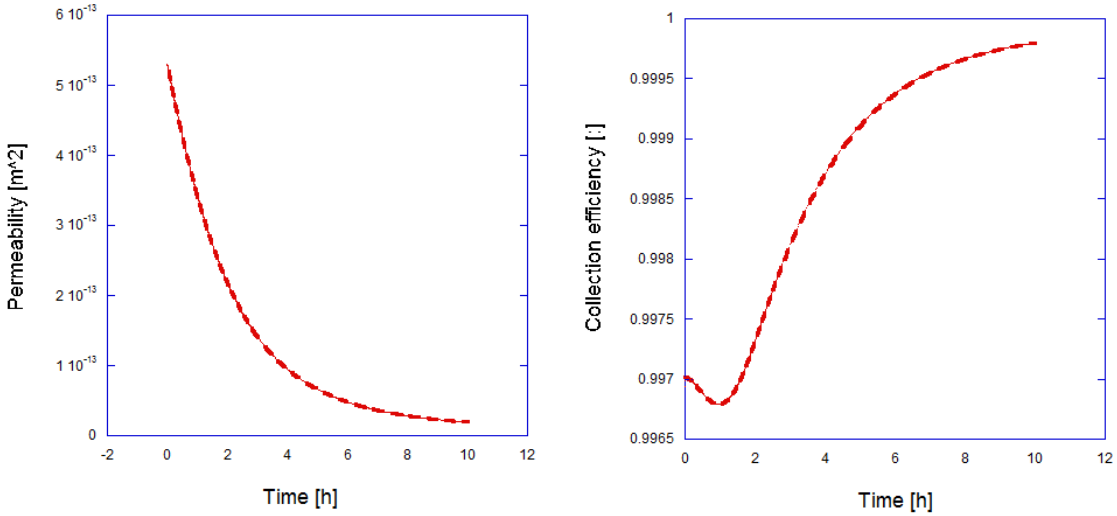

Figure 12: Simulation results obtained for the DPF model: filter wall permeability and collection efficiency

3.4 Discussion on model potential

The development has the potential to discuss kinetic effects in recirculated exhaust gases on the following engine cycle. For DISI engines it was demonstrated in reference [26], that the catalytic reformation of recirculated exhaust gases can limit engine knock, and thereby reduce fuel consumption.

The integrated DARS 1D reactor network tool is in the phase of further consolidation and testing. One important aspect of the usability of such a complex kinetic tool is the necessary CPU time for running each engine cycle.

The SRM-DICI model used in reference [27], coupled with Ricardo Wave needed 17 minutes for one engine cycle, if the PDF was resolved by 100 particles and a skeleton mechanism with 108 species and 2000 reactions was applied. It was found that this accuracy was acceptable for calculating pressure histories, or CO emissions. However other emissions, such as soot particles are in need of higher accuracy. The calculation time for 2000 particles was 5 hours and 40 minutes (340 minutes) [27]. Simulations were performed on one core of a 1.8 GHz dual core computer having 1 GB of RAM. Very recent calculations for the DICI-SRM dual fuel (one cycle in the range -120 to +120 CAD) with 1000 particles took 12 minutes on 32 cores AMD Opteron 4180 running at 2.6GHz with gigabit Ethernet interconnect and OpenMPI 1.4.3.

The transient catalyst cases, shown in Figure need 23 minutes for a transient calculation of 8 seconds using 40 cells. The time step size for the operator splitting was 0.3 msec. A reaction mechanism with 73 reactions and 22 surface sites and 11 gas phase species was applied on one core of an Intel Core 2 Duo CPU E8400 running at 3.00 GHz. In the future CPU time will be further reduced by an improved parallelization.

4. CONCLUSIONS

Stochastic models were developed for the investigation of spark ignition and direct injection diesel engines. The models predict combustion and emission trends in the engine. Stochastic models describe the interaction of turbulence and chemistry in detail. They are excellent tools for engine combustion and emission studies, with particular applicability for processes where detailed chemistry plays an important role (as knock or emission formation).

The catalyst model predicts conversion efficiencies of catalysts during steady state as well as transient conditions. The model has the potential to be applied in wide range operation studies, since it is based on a detailed kinetic model. The analysis of surface site concentration gives deep insight into important processes, such as site blocking of poisoning. The combination of the stochastic engine model with the transient catalyst model allows to understand transient lasting effects of inhibition by site blocking. In addition plausibility tests are shown for the detailed kinetic DPF model. All tools demonstrated in this paper can be connected in a one-dimensional reactor network. Besides full engine-aftertreatment system, other potential applications for DARS-1D include industrial catalysts, catalytic burners and Variable-Pressure Flow Reactors.

5. REFERENCES

1 Gamma Technologies Inc., GT-Power User's Manuals, version 7.0, 2009.
2 Ricardo Inc., WAVE User's Manual, WAVE 7.1 Help Suite, 2006.
3 http://www.loge.se/products-services.html
4 DigAnaRS LLC, DARS 2.0 Manual, Book 3 – Stochastic Reactor Models, 2010.
5 Fröjd, K., and Mauss, F., "A three-parameter Transient 1D Model for Catalyst Modeling", SAE-11PFL-0072, 2011.
6 Maigaard, P., Mauss, F., and Kraft, M., "Homogeneous Charge Compression Ignition Engines: A Simulation Study on the Effect of Inhomogeneities", ASME J. Engineering for Gas Turbines and Power 125 (2003) 466–471.
7 Challen, B., and Baranescu, R., "Diesel Engine Reference Book", Second edition, SAE International, 1999.
8 Samuelsson, K., Gogan, A., Netzell, K., Lehtiniemi, H., Sunden, B., and Mauss, F., "Modeling Diesel Engine Combustion and Pollutant Formation Using a Stochastic Reactor Model Approach", Intl. Conf. Clean Diesel Combustion, Lund, 2005.
9 Pasternak, M., Mauss, F. and Bensler, H., "Diesel Engine Cycle Simulation with Reduced Set of Modeling Parameter Based on Detailed Kinetics", SAE 2009-01-0676.
10 Yang, B., and Pope, S. B., "An investigation of the accuracy of manifold methods and splitting schemes in the computational implementation of combustion chemistry", Combust. Flame 112 (1998) 16 –32.
11 Woschni, G., "A Universally Applicable Equation for the Instantaneous Heat Transfer Coefficient in the Internal Combustion Engine", SAE 670931.

12 Bhave, A., Balthasar, M., Kraft, M., and Mauss, F., "Analysis of a natural gas fuelled homogeneous charge compression ignition engine with exhaust gas recirculation using a stochastic reactor model", Int. J. Engine Res. 5(1) (2004) 93–103.
13 Fröjd, K., "Diesel engine cylinder model including gas exchange", Internal Report LOGE AB, 2009.
14 Heywood, J. B., "Internal Combustion Engine Fundamentals", McGraw Hill, New York, 1988.
15 Koop, J., and Deutschmann, O., Applied Catalysis B: Environmental 91 (2009) 47–58.
16 Perlman, C., "Diesel particulate filter model", Internal Report LOGE AB, 2010.
17 Bissett, E.J., "Mathematical Model of the Thermal Regeneration of a Wall-flow Monolith Diesel Particulate Filter", Chemical Engineering Science 39 (1984) 1233–1244.
18 Konstandopoulos, A.G., Kostoglou, M., Skaperdas, E., Papaioannou, E., Zarvalis, D., and Kladopoulou, E., "Fundamental Studies of Diesel Particulate Filters: Transient Loading, Regeneration and Aging", SAE Technical Paper Series 2000-01-1016
19 Konstandopoulos, A.G., and Kostoglou, M., "Reciprocating Flow Regeneration of Soot Filters", Combust. Flame 121 (2000) 488–500.
20 Gogan, A., PhD Thesis, "Full Cycle Engine Simulations with Detailed Chemistry", Lund Institute of Technology, 2006, ISBN 978-91-628-6765-2.
21 Pasternak, M., Mauss, F., and Bensler, H., "Stochastic Reactor Model Based Diesel Engine Cycle Simulation", Fourth European Combustion Meeting, Vienna, Austria, April 14–17, 2009.
22 Schmeisser, V., Perez, J.D., Tuttlies, U., and Eigenberger, G., "Experimental Results Concerning the Role of Pt, Rh, Ba, Ce and Al_2O_3 on NO_x-Storage Catalyst Behaviour", *Topics in Catalysis* 42–43 (2007) 15–19.
23 A.G. Konstandopoulos, and J.H. Johnson, "Wall-Flow Diesel Particulate Filters – Their Pressure Drop and Collection Efficiency", SAE Trans. 98 sec. 3 (J. Engines) Paper No. 890405.
24 C.T. Huynh, J.H. Johnson, S.L. Yang, S.T. Bagley, and J.R. Warner, "A One-Dimensional Computational Model for Studying the Filtration and Regeneration Characteristics of a Catalyzed Wall Flow Diesel Particulate Filter", SAE Technical Paper Series 2003-01-0841.
25 Piscaglia, A., and Ferrari, G., "A Novel 1D Approach for the Simulation of Unsteady Reacting Flows in Diesel Exhaust After-Treatment Systems", Energy 34 (2009) 2051–2062.
26 Hoffmeyer, H., Montefrancesco, E., Beck, L., Willand, J., Ziebert, F., and Mauss, F., "CARE – Catalytic Reformated Exhaust Gases in Turbocharged DISI-Engines", SAE Int. J. Fuels Lubr. 2 (1) (2009) 139–148.
27 Tunér, M., Pasternak, M., Bensler, H., and Mauss, F., "A PDF-Based Model for Full Cycle Simulation of Direct Injected Engines", SAE 2008-01-1606.

NOMENCLATURE

Abbreviations

CAD Crank Angle Degree

CFD	Computational Fluid Dynamics
DI	Direct Injection
EGR	Exhaust Gas Recycling
HCCI	Homogeneous Charge Compression Ignition
IVO	Inlet valve Opening
MDF	Mass Density Function
PDF	Probability Density Function
SRM	Stochastic Reactor Model