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Characterisation and Model Based Optimization of a Complete Diesel Engine/SCR System

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ABSTRACT

In order to make efficient use of a Diesel engine equipped with an SCR system, it's important to have a complete system approach when it comes to calibration of the engine and the aftertreatment system.

This paper presents a complete model of a heavy duty diesel engine equipped with a vanadia based SCR system. The diesel engine uses common rail fuel injection, a variable geometry turbocharger (VGT) and cooled EGR.

The engine model consists of a quasi steady gas exchange model combined with a two-zone zero dimensional combustion model. The combustion model is a predictive heat release model. Using the calculated zone temperatures, the corresponding NO_x concentration is given by the original Zeldovich mechanism. The SCR catalyst model is of the state space type. The basic model structure is a series of continuously stirred tank reactors and the catalyst walls are discretized to describe mass transport inside the porous structure. Implicit methods are used to solve the ODEs which allow long time steps and high computational efficiency.

The combined engine-SCR model is a useful tool to characterize the system. A number of critical operating sequences are studied; step response from steady state low load conditions to high load and vice versa and also cold start experiments. Model based optimization is used aiming at achieving Euro VI emission levels while minimizing the brake specific fuel consumption (including Urea cost) by simultaneously optimizing the engine and SCR control parameters.

INTRODUCTION

Urea SCR is currently the industry standard for NO_x aftertreatment on heavy vehicles and is rapidly gaining popularity on larger diesel passenger cars as well [1]. Although the technology is maturing, implementation and control of an SCR system is not a straightforward task. The first generation SCR engines were more or less retrofitted with an SCR catalyst and a Urea dosing system. Little or no modifications were performed to the engine itself and simple look up table based control systems were applied.

In order to reach future emission standards, Euro VI and beyond, substantially higher conversion rates (>90%) over the catalyst should preferably be realized. Also, moving from the European Transient Test Cycle (ETC) to World Harmonized Transient Test Cycle (WHTC) will result in lower exhaust temperatures, which will further complicate the conditions for the SCR system. One of the key factors to achieve these goals is to have a complete system approach; i.e. to optimize the engine and SCR system as one unit. A novel approach to solve these problems is to use model based control and optimization.

Computationally efficient models of the diesel engine and SCR system have been presented in previous publications by the authors [2,3]. This is the third paper in our study and describes the combined model. Improvements, mainly in the combustion model, are also presented. The complete model is a useful tool for a variety of purposes. In this paper, model based optimization is performed on step response experiments which are identified to be important to the performance of the complete system.

MODELS

In this section the complete model of the engine / SCR system is described. All models are implemented in Matlab Simulink.

THE ENGINE MODEL

The engine model is an improved version of the model presented by Ericson et al. [2]. The gas exchange model is not modified from its original form however. The combustion model is improved to fit a wider range of operating conditions. The basic assumptions and structure (as schematically described in Figure 1) supporting the original combustion model remain unchanged.

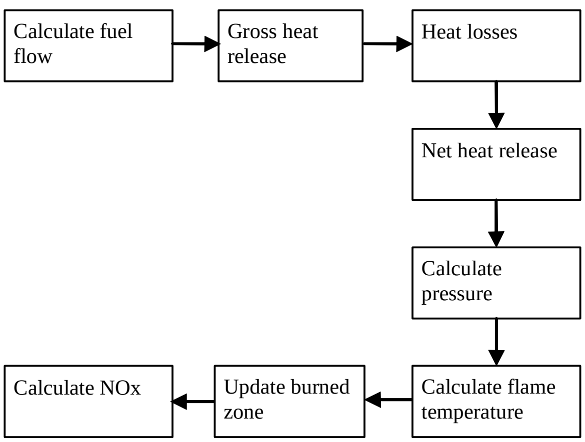

Figure 1 Flowchart of the combustion model

Modifications to some of the submodels have been implemented and will be presented below.

Fuel flow and heat release calculations

The ignition delay is modeled using the following expression:

$$\alpha_{SOC}-\alpha_{SOI}= \\ = f_1\left(N_{eng}\right)\cdot f_2\left(\delta_{pilot}\right)\cdot c_{O_2}{}^{k_1}\cdot p_{rail}{}^{k_2}\cdot \mathrm{e}^{k_3\left(\frac{1}{R\cdot T_{SOI}}-\frac{1}{k_4}\right)} \qquad (1)$$

where k_x are constant parameters tuned to fit measured ignition delay. The correlation is basically the inverse of a second order reaction rate. The concentration of vaporized fuel inside the cylinder is not easily calculated however; instead fuel injection pressure is used as a measure of available fuel. f_1 and f_2 are polynomial functions compensating for deviations at low engine speeds and pilot injections respectively. The (inlet) oxygen concentration is given by:

$$c_{O_2}=\frac{p_{SOI}}{T_{SOI}\cdot R}\cdot 0.21\cdot\left(1-\frac{x_{EGR}}{\lambda}\right) \qquad (2)$$

The premixed combustion is calculated according to:

$$\frac{dQ_{g,premix}}{d\theta}=f_{pre1}\left(Q_{premix,tot}\right)\cdot\left(\theta-f_{pre2}\left(Q_{premix,tot}\right)\right)^2 \\ +f_{pre3}\left(Q_{premix,tot}\right) \qquad (3)$$

In other words, the premixed heat release rate is a second order function. The duration of the combustion is empirically determined to be a fixed value. The parameters f_{prex} are calculated to fit the integrated area under the curve to the total energy to be released ($Q_{premix,tot}$). The energy is given by:

$$Q_{premix,tot}=\frac{dQ_{fuel,inj}}{d\theta}\cdot \\ \cdot\min\left(\alpha_{EOI}-\alpha_{SOI},\alpha_{SOC}-\alpha_{SOI}-\alpha_{mix}\left(N_{eng}\right)\right) \qquad (4)$$

where α_{mix} is a fuel mixing parameter. The addition of a mixing time is required to get an accurate balance between premixed and diffusion combustion at high load operating conditions with long ignition delays.

Diffusion combustion heat release rate is calculated using the difference between injected and released fuel energy:

$$\frac{dQ_{g,diff}}{dt}=C_{diff}\left(Q_{fuel,inj}-Q_{g,diff}\right) \qquad (5)$$

In previous publications [2,4], C_{diff} is considered a constant. This will not describe the combustion accurately at highly varying EGR rates and fuel injection pressures. Instead, a modified version of the Chmela model for diffusion combustion [6] presented by Andersson et al. [5] is used. Lumping the constant parameters together, the following expression is achieved:

$$C_{diff}=c_{O_2}{}^{1/3}\sqrt{k_{spray}\cdot p_{rail}\cdot x_{O_2}\cdot e^{-k_{fade}\cdot\tau_{AEOI}}+k_{swirl}\cdot N_{eng}^2} \qquad (6)$$

Note that the cylinder pressure, compared to the fuel injection pressure, is neglected. The constant parameters k_{spray}, k_{fade} *and* k_{swirl} are tuned to fit measured heat release rates.

Combustion

The burned zone calculations are performed in a similar manner to the previous models [2] except for two details:

1. In order to improve computational efficiency, the adiabatic flame temperature is calculated using simplified enthalpy calculations. The temperature range in the burned zone is quite limited; therefore the enthalpy can be approximated as a linear function of

temperature. The result is that no iterations are needed.

2. The radiative heat loss factor has empirically been determined to be a linear function of oxygen fraction. This is a reasonable; decreased oxygen content typically results in higher soot production and in return higher radiative heat losses.

Pre and Post Processing

In order to save computational time, the heat release loop is executed from SOI until 30 degrees ATDC only. The pressure at SOI is calculated according to:

$$p_{SOI} = p_{IVC} \cdot \left(\frac{V_{IVC}}{V_{SOI}}\right)^{\gamma_{IVC-SOI}} \quad (7)$$

The polytropic exponent is given by a black box expression:

$$\gamma_{IVC-SOI} = \gamma_{IVC-SOI}\left(N_{eng}, \alpha_{SOI}, \delta_{main}, \delta_{pilot}\right) \quad (8)$$

The temperature dependency and operating condition dependent heat losses will be compensated for by equation 8. The pressure at IVC is given by:

$$p_{IVC} = p_{BDC} \cdot \left(\frac{V_{IVC}}{V_{BDC}}\right)^{\gamma_{BDC-IVC}} \quad (9)$$

where the polytropic exponent has a constant value.

The pressure and temperature at EVO is calculated using polytropic expansion using the exponent calculated at 30 degrees ATDC. The exhaust manifold temperature T_{em} is correspondingly given by:

$$T_{em} = T_{EVO} \cdot \left(\frac{p_{em}}{p_{EVO}}\right)^{\frac{\gamma_{em}-1}{\gamma_{em}}} \quad (10)$$

where γ_{em} is a constant.

Indicated mean effective pressure (*IMEP*) can be calculated in two steps:

1. Numerical integration of the pressure trace given by the heat release loop from SOI to 30 deg. ATDC.

2. Analytical integration of the pressure from BDC to SOI and 30 deg. ATDC to BDC (using the polytropic constants given in equations 8 and 9).

Brake mean effective pressure is given by:

$$BMEP = IMEP\text{-}PMEP\text{-}FMEP \quad (11)$$

PMEP is estimated using inlet and exhaust manifold pressures. *FMEP* can essentially be divided into two parts:

$$FMEP = FMEP_{fric} + FMEP_{hpp} \quad (12)$$

The first term describes the friction related to the moving parts of the engine and also auxiliary units such as the engine coolant pump and fan. $FMEP_{fric}$ typically has a second order relation to engine speed:

$$FMEP_{fric} = k_{F,1} + k_{F,2} \cdot N_{eng} + k_{F,3} \cdot N_{eng}^{\ 2} \quad (13)$$

$k_{F,x}$ are empirically determined constant parameters. The second part of *FMEP* describes losses in the high pressure fuel pump:

$$FMEP_{hpp} = k_{F,4} \cdot p_{rail}^{\ k_{F,5}} \cdot \delta_{main}^{\ k_{F,6}} \cdot \left(1 + k_{F,7} \cdot N_{eng}^{\ k_{F,8}}\right) \quad (14)$$

Using the calculated value of BMEP, other quantities such as torque and BSFC are easily calculated.

THE EXHAUST SYSTEM MODEL

The temperature after the turbine is given by:

$$T_{atrb} = T_{em} \cdot \left(\frac{p_{amb}}{p_{em}}\right)^{\frac{\gamma_{em}-1}{\gamma_{em}}} f_{atrb}\left(W_{trb}, x_{EGR}, \delta_{main}, \alpha_{SOI}\right) \quad (15)$$

where f_{atrb} is a black box compensation factor. The black box correction factor will correct the values for heat transfer to and from the engine block, exhaust manifold and turbocharger. The exhaust temperature will be further reduced and smoothed before the exhaust gas reaches the catalyst. This is related to heat transfer to and from the exhaust system. A dynamic mean value exhaust system model is presented by Eriksson [8]. This model is used in a simplified form; the heat conduction between engine and exhaust system is neglected. The exhaust system energy balance is given by:

$$\begin{aligned} \frac{dT_w}{dt} m_{exh.sys} c_{p,exh.sys} = {} & A_{exh.sys}\Big(h_{gi}\left(T_{atrb} - T_w\right) \\ & - h_{cve}\left(T_w - T_{amb}\right) - F_v \varepsilon \sigma \left(T_w^4 - T_{amb}^4\right)\Big) \end{aligned} \quad (16)$$

T_w is the exhaust system wall temperature. The external convection heat transfer coefficient, h_{cve} and the gray body view factor, F_v as well as the emissivity, ε are assumed to be constant. σ is the Stefan-Boltzmann constant. The generalized internal heat transfer coefficient is given by [8]:

$$h_{gi} = \frac{1 - e^{-\frac{h_{cvi} A_{exh.sys}}{W_{eng,in} c_{p,exh}}}}{\frac{h_{cvi} A_{exh.sys}}{W_{trb} c_{p,exh}}} h_{cvi} \tag{17}$$

The internal convective heat transfer coefficient is highly flow dependent, and is estimated using the Nusselt number:

$$h_{cvi} = \frac{Nu \lambda_{exh}}{d_{exh.sys}} \tag{18}$$

where the Nusselt number is estimated using the following relation [8]:

$$Nu = 0.48 Re^{0.5} \tag{19}$$

Finally, the pre-silencer / catalyst temperature is given by:

$$T_{precat} = T_w + \left(T_{atrb} - T_w\right) e^{\frac{h_{cvi} A_{exh.sys}}{W_{trb} c_{p,exh}}} \tag{20}$$

THE SCR CATALYST MODEL

The SCR catalyst model is based on a state space concept. The catalyst is discretized into six continually stirred tanks in the axial direction, and two wall layers are used to model the mass transfer in the catalyst wall (Figure 2).

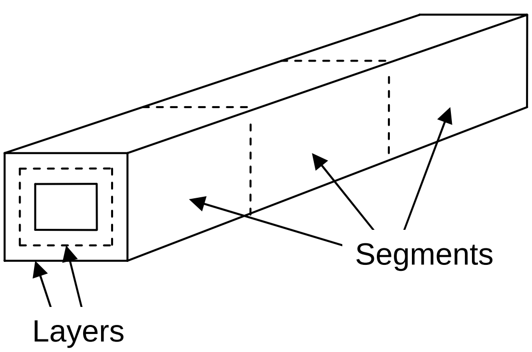

Figure 2 Illustration of the catalyst discretization principle

Uniform radial flow and concentration distribution over the catalyst cross section is assumed; therefore it is sufficient to model one channel only. Eley-Rideal kinetics is applied to calculate the reaction rates on the catalyst surface. The model is described in more detail in previous publications [3,7].

THE COMPLETE MODEL

The engine, SCR and exhaust system models are combined and implemented in a common Simulink model. The flow of inputs, outputs and signals between the submodels is shown in Figure 3.

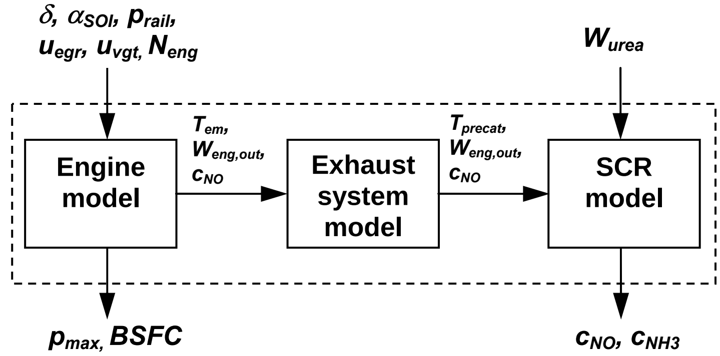

Figure 3 The complete model

A simplified engine control system is added, calculating injected fuel, VGT and EGR actuator signals depending on desired versus actual torque, desired EGR rate and injection timing, illustrated in Figure 4.

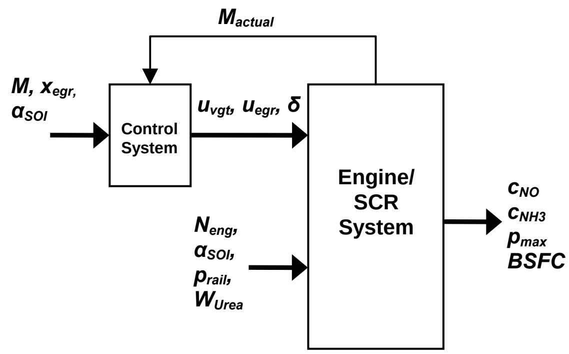

Figure 4 Schematic view of the complete system

The differential equations of the gas exchange model are solved using the Euler method with a step of 10 ms to ensure stability. The SCR catalyst can use substantially longer step lengths (0.5 s) using customized ODE solvers [3,7]. The combustion model is executed with a 0.1 s interval which is sufficient for the intended application. Due to the slow dynamics of the SCR catalyst, a shorter interval for the combustion model does not offer improved accuracy of the complete model. The simulation performance of the combined model is faster than 10 X real time (using the uncompiled Simulink code on a 2.67 GHz CPU).

CALIBRATION

The combustion model is tuned to fit a large set of steady state measurements. The set consists of ~ 800 operating conditions where all relevant degrees of freedom are varied (engine speed, torque, injection timing, injection pressure, EGR, pilot injections). The gas exchange model parameters are tuned using transient test cycles (ETC) measured in the engine test bed as well as real world driving (on road) measurements.

Step response experiments from the engine test bed are used to tune the SCR catalyst model. In order to differentiate the transient response of the catalyst from the engine, and also to minimize uncertainties in the initial conditions of the catalyst, the engine is run at a constant load and steps are performed in the Urea dosing.

VALIDATION

The complete model was validated using transient test cycle experiments (ETC) measured in the engine test bed. The experimental engine is a 12.8 litre, 6 cylinder in-line engine equipped with common rail fuel injection, two stage cooled EGR and a variable geometry turbocharger (VGT). The SCR system consists of a vanadia based SCR catalyst and an air assisted Urea injection system. The NOx flow engine out is predicted with excellent accuracy, Figure 5 shows a sequence of the ETC. Specific NOx for the test cycle is predicted with less than 1% relative error.

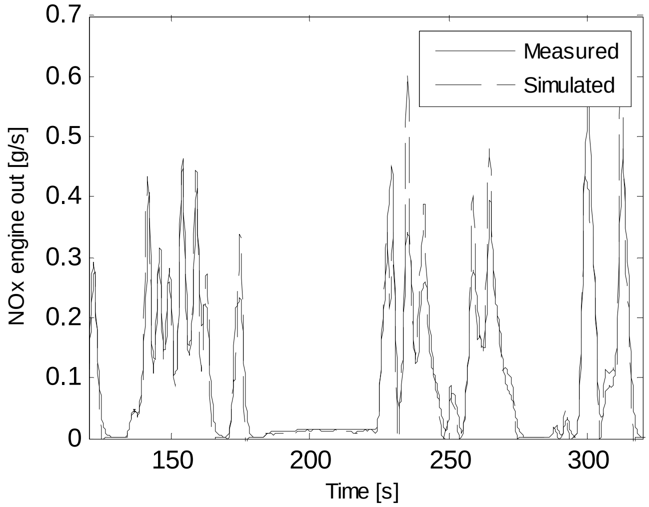

Figure 5 Measured and simulated NOx flow engine out

The SCR catalyst model also performs adequately (Figure 6). Despite the sparse discretization of the catalyst wall, the transient mass transport phenomena are captured. Specific tailpipe NOx for the ETC is slightly over predicted (21.2% relative error).

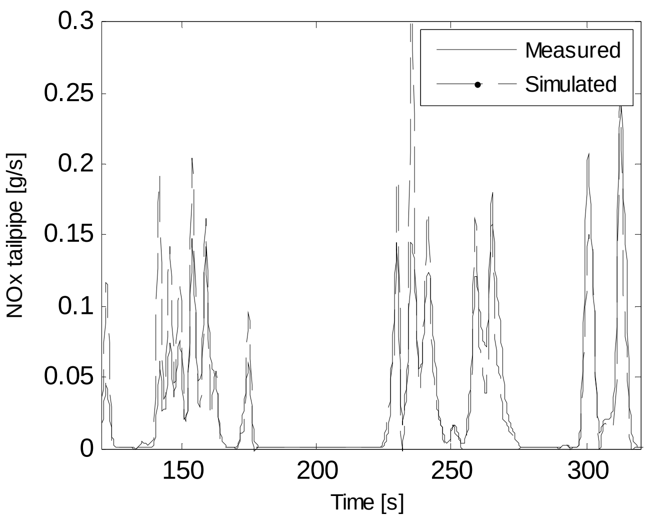

Figure 6 Measured and simulated NOx tailpipe

Ammonia slip is consistently under-predicted by the SCR catalyst model, Figure 7. The mean simulated ammonia slip is 10.5 ppm compared with the measured value of 16.3 ppm. The deviation is likely related to errors in the inputs to the model. The Urea decomposition model (which describes the thermolysis reaction in gas phase between the Urea injector and catalyst substrate) is a known weak link.

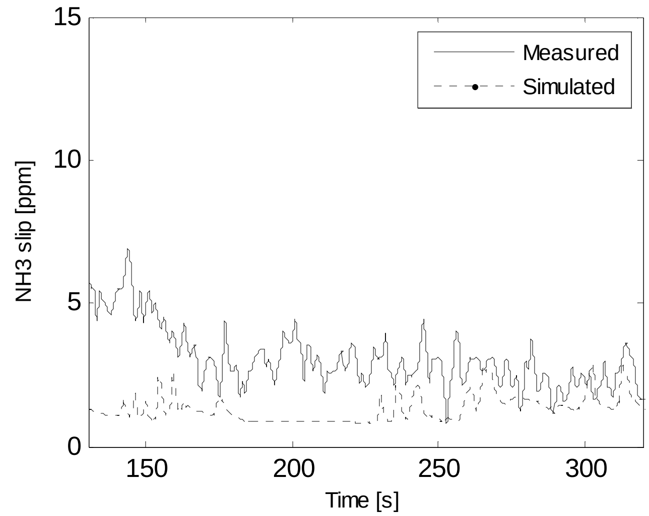

Figure 7 Measured and simulated NH3 slip

Torque simulated by the engine model shows excellent agreement with measured values (Figure 8).

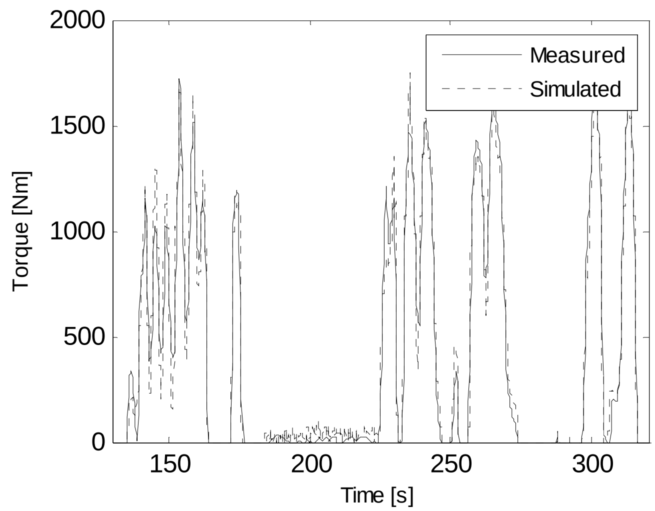

Figure 8 Measured and simulated Torque

Simulated EGR rate shows a reasonably small deviation from the measured rate. The deviations during rapid transients are likely related to the dynamics (low pass filtering) of the measurement system. One indication of this is that the engine out NOx level, which is closely related to the EGR rate, shows good agreement with measurements (Figure 5).

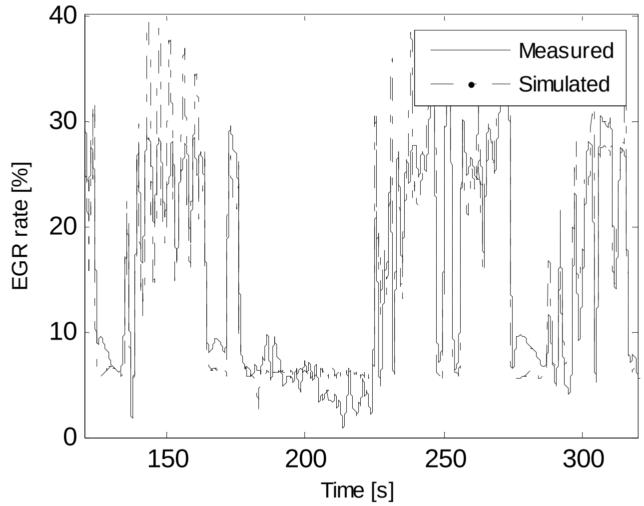

Figure 9 Measured and simulated EGR rate

OPTIMIZATION

One of the most interesting applications of the described model is model based optimization. By varying both the engine and SCR inputs, an optimized complete system can be achieved.

CRITICAL OPERATING SEQUENCES

There are a number of critical operating sequences which will be important to the overall performance of the system:

The first case is a positive load transient; as the temperature of the catalyst increases with increasing engine load, the equilibrium ammonia coverage decreases and stored ammonia will be released from the surface. In order to avoid ammonia slip, the Urea dosing and possibly engine out NOx must be controlled. Also, the rapidly increasing NOx flow due to the higher load must be handled either at the source (EGR / retarded injection timing) or in the catalyst.

The second case is a negative load transient, i.e. moving from a high load to low load. The decreasing exhaust temperature (and catalyst temperature) will decrease the NOx reduction capacity of the SCR catalyst. In order to improve reaction rates at the lower temperature, more ammonia must be stored in the catalyst. At the same time, the urea dosing can not be overly excessive; this will result in ammonia slip.

The third case is a special case of case one; cold start, i.e. a positive load transient starting from ambient catalyst (and exhaust system) temperature. Apart from the lower initial temperature, the main difference between case one and three is that urea dosing will not be possible right from the start; at temperatures below ~180^{o}C the urea will not be sufficiently evaporated in the exhaust stream.

THE OPTIMIZATION PROBLEM

The optimization problem studied is targeted at minimizing fuel consumption (including Urea cost) while achieving Euro 6 emission levels (NO_x and NH_3 slip) and not exceeding the construction limits of the engine. For a simple case, the goal function can be brake specific fuel consumption and is given by:

$$f\left(\delta,\alpha,x_{egr},W_{Urea},p_{rail}\right)= \frac{m_{fuel}\left(\delta,\alpha,x_{egr},p_{rail}\right)+m_{Urea}\left(W_{Urea}\right)}{\int_0^{t_{sim}} P\cdot dt} \qquad (21)$$

where P is engine power and t_{sim} is the simulation (test cycle) time. m_{fuel} is calculated by the engine model, taking injection timing and EGR rate into account. The specific fuel consumption is the accumulated value for the whole test cycle (i.e. $f\in R^1$). The equivalent urea consumption is given by:

$$m_{Urea}\left(W_{Urea}\right)=EQ_{Urea}\int_0^{t_{sim}} W_{Urea}dt \qquad (22)$$

where t_{sim} is the duration of the test cycle. EQ_{Urea} is the relative cost of Urea to diesel fuel (in Europe 2008 typically 0.25).

The parameters all have physical limitations; injected fuel mass is limited by the injectors, injection timing can not be varied excessively without avoiding misfire and cylinder liner wetting. EGR rate is limited by the gas exchange system (in order to maintain a high enough air-fuel equivalence ratio) and the Urea dosing is limited by the injection system. This can be formulated mathematically according to:

$$\delta\in\Omega_{\delta} \quad \in R^m \qquad (23)$$

$$\alpha\in\Omega_{\alpha} \quad \in R^m \qquad (24)$$

$$x_{egr}\in\Omega_{egr} \quad \in R^m \qquad (25)$$

$$W_{Urea}\in\Omega_{Urea} \in R^m \qquad (26)$$

$$p_{rail}\in\Omega_{prail} \in R^m \qquad (27)$$

Where m is the number of time steps in the simulation/cycle. There are also a number of non linear inequality constraints:

$$c_{NOx}\left(\delta,\alpha,x_{egr},W_{Urea},p_{rail}\right)\le LD_{NOx} \qquad (28)$$

$$c_{NOx,NTE}\left(\delta,\alpha,x_{egr},W_{Urea},p_{rail}\right)\le NTE_{NOx} \qquad (29)$$

$$c_{NH3}\left(\delta,\alpha,x_{egr},W_{Urea},p_{rail}\right)\le LD_{NH3} \qquad (30)$$

$$c_{NH3,NTE}\left(\delta,\alpha,x_{egr},W_{Urea},p_{rail}\right)\le NTE_{NH3} \quad (31)$$

$$c_{P\max}\left(\delta,\alpha,x_{egr},W_{Urea},p_{rail}\right)\le p_{\max} \quad (32)$$

Equations 28-31 describe the legal limits and not to exceed (NTE) limits for NO_x and NH_3 respectively. Equation 32 limits the maximum cylinder pressure in order not to exceed the construction limit of the engine. The legal limit constraints are calculated as accumulated values for the entire test cycle (scalar), whereas the NTE and cylinder pressure constraints are vector valued i.e:

$$c_{NOx},c_{NH3}\in R^1 \quad (33)$$

$$c_{NOx,NTE},c_{NH3,NTE},c_{P\max}\in R^m \quad (34)$$

The NTE constraints for a time step *n* will depend on the parameters leading up to time *n* (*1-n*) because of the accumulative properties of the SCR catalyst. For a constraint *c* and a parameter *x*, this can be formulated in terms of a triangular constraint Jacobian:

$$J_c=\begin{pmatrix}\frac{\partial c_1}{\partial x_1} & \cdots & 0\\ \vdots & \ddots & \vdots\\ \frac{\partial c_m}{\partial x_1} & \cdots & \frac{\partial c_m}{\partial x_m}\end{pmatrix} \quad (35)$$

Defining the sparsity structure of the Jacobians to the optimizer will greatly improve optimization time.

A suitable optimization routine should fulfil the following criteria:

- Nonlinear optimizer.
- Capable of nonlinear constraints.
- Efficient for large scale problems with expensive goal and constraint functions.
- Possibility to define a sparsity structure of the constraint jacobian.

The chosen routine is SNOPT [9,10] which is based on a Sequential Quadratic Programming (SQP) algorithm. The Tomlab SOL Matlab toolbox [11] includes a version of SNOPT which has been used in the optimization work.

STEADY STATE OPTIMIZATION

Steady state optimization for various operating conditions has been performed in order to get suitable initial values for the transient optimization experiments. The optimization problem can be formulated according to:

$$\min_{\alpha\in\Omega_\alpha,x_{egr}\in\Omega_{egr},W_{Urea}\in\Omega_{Urea}} f\left(\alpha,x_{egr},W_{Urea}\right)$$

$$s.t.$$

$$c_{NOx}\left(\alpha,x_{egr},W_{Urea},p_{rail}\right)\le LD_{NOx}$$

$$c_{NH3}\left(\alpha,x_{egr},W_{Urea},p_{rail}\right)\le LD_{NH3}$$

Fuel rail pressure is not an optimization parameter; instead it is calculated as a linearly increasing function of EGR rate. Since no model for engine out PM emissions is included in the complete model, rail pressure is chosen to ensure reasonable PM levels based on measurement data. Injected fuel mass is calculated backwards from brake efficiency as a function of EGR and injection timing.

The target and constraint values are calculated by running the complete model with constant inputs (parameters) for a sufficiently long time to reach steady state, typically < 600 s. The constraint limits are set to:

$LD_{NOX}=0.5$ *g/kWh*

$LD_{NH3}=10$ *ppm*

The non-smooth target function will result in different local optima depending on the initial values. Figure 10 shows an example of simulated steady state brake efficiency where the non-smooth property is obvious.

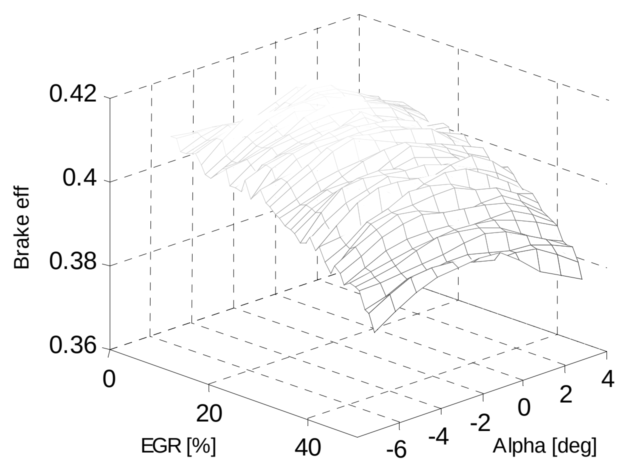

Figure 10 Brake efficiency, 1250RPM / 600Nm load

One way of solving the problem is to fit a second order surface to the steady state simulation results, and replace the actual combustion / NO_x model with surface approximations for brake efficiency, NO_x, exhaust temperature and maximum cylinder pressure. This will guarantee a smooth target function. Using the second order simplifications, results according to Table 1 are achieved for typical operating conditions.

Torque [Nm]	Injection timing [deg]	EGR [%]	Urea flow [kg/h]	NOx Reduction [%]
400	0.00	31.00	0.31	86
600	0.00	18.99	0.94	92
1800	-1.57	26.82	1.08	84

Table 1 Steady state optimization results, 1250 RPM

STEP RESPONSE OPTIMIZATION

In order to study the three critical operating cases mentioned earlier, optimization of step response sequences is performed. All step responses are defined in the following way:

- Initial values for all temperature, pressure and coverage states in the model are set to the steady state solution corresponding to the initial operating condition.
- The step is performed at time *t=0*. In other words, the optimizer has no look-ahead information.

Step response optimization is not just of theoretical interest; if simplified methods to solve the optimization problems are developed, it could be applied in a model predictive control (MPC) application.

The second order surface approximations are also used in the step response optimizations. The actual engine model is used during the initial transient part of the step response although (typically before the engine reaches within 5% of the desired torque level), and the second order simplifications are used thereafter. Another benefit from using the second order simplifications is simulation performance; the complete model is typically a factor 5-10 faster when the combustion/ NOx formation model is disabled.

The optimization problem is formulated in a similar way as the steady state optimization:

$$\min_{\alpha \in \Omega_\alpha, x_{egr} \in \Omega_{egr}, W_{Urea} \in \Omega_{Urea}} f\left(\alpha, x_{egr}, W_{Urea}\right)$$

$$s.t.$$

$$c_{NOx}\left(\alpha, x_{egr}, W_{Urea}, p_{rail}\right) \leq LD_{NOx}$$

$$c_{NOx,NTE}\left(\delta, \alpha, x_{egr}, W_{Urea}, p_{rail}\right) \leq NTE_{NOx}$$

$$c_{NH3}\left(\alpha, x_{egr}, W_{Urea}, p_{rail}\right) \leq LD_{NH3}$$

$$c_{NH3,NTE}\left(\delta, \alpha, x_{egr}, W_{Urea}, p_{rail}\right) \leq NTE_{NH3}$$

Note that the NO_x and NH_3 constraints are calculated as accumulated values for the whole step response. Also, NTE conditions are added in order to allow temporarily higher emissions. In all cases, the constraint limits are set to:

LD_{NOX}*=0.5 g/kWh*

NTE_{NOX}*=1.0 g/kWh*

LD_{NH3}*=10 ppm*

NTE_{NH3}*=25 ppm*

<u>Additional constraints</u>

The initial step response optimization attempts resulted in disappointing results; the optimum solution was highly oscillative, indicating a poorly conditioned problem. The conclusion was that some type of constraint must be added which defines how the catalyst is to be emptied or filled (with NH_3), depending on step response case. Two different options were successfully used:

a. Positive/negative sign of the coverage gradient, i.e. the catalyst must be filled or emptied monotonously. This will decrease the degrees of freedom and prevent oscillating solutions.

b. Positive/negative sign of the NO_x conversion gradient, i.e. the NO_x conversion must increase/decrease monotonously. This constraint is suitable in cases where the temperature is increasing while the initial coverage (and therefore NO_x conversion) is low.

The gradient constraints are typically applied to tank 1. This will offer the shortest time constant between Urea dosing and the constraint. Also, most of the NOx reduction does occur in the very beginning of the catalyst.

Another problem encountered is that the optimum solution typically results in low NH_3 coverage at the end of the simulation, i.e. most of the NH_3 which is stored initially is consumed. This is solved in two steps:

1. Add consumption of stored ammonia to the target function, i.e. consuming ammonia from the surface costs equally much as injecting the corresponding amount of Urea.
2. Add end value equality constraints; at the end of the simulation the coverage profile should equal the steady state profile corresponding to the target load. Typically, it is sufficient to use equality constraints for the first three tanks; most NO_x reduction does occur in the first half of the catalyst. Also, the slow dynamics will result in great difficulty to achieve steady state coverage in the entire catalyst at the end of the simulation (when the temperature has just recently reached steady state).

Case 1 Positive Load Transient

The positive load transient studied is a step response from 400Nm to 1800Nm at constant engine speed, 1250 RPM. This will result in a catalyst temperature increase of approximately 250 degrees. The simulation time is set to 240 seconds, the time it takes for the entire catalyst to deviate less than 1% from the corresponding steady state temperature. A parameter step length of 10 s is chosen to get a reasonable number of parameters and optimization time. The initial values of the optimization parameters in all time steps are set to the steady state optimum according to Table 1. Constraint a is the most appropriate in Case 1; the rapid increase in temperature calls for a decreasing coverage.

Optimization parameters	**NO_x [g/kWh]**	**Peak NO_x [g/kWh]**	**NH_3 slip [ppm]**	**Peak NH_3 slip [ppm]**	**Norm. BSFC [%]**
Initial values	0.23	0.70	93.63	406.50	100.0 (ref)
Urea	0.50	1.00	25.07	127.17	99.7
Urea+EGR	0.50	1.00	10.00	25.00	99.9

Table 2 Optimization results, Case 1

The initial parameter values results in low NOx emissions, but at the expense of severe NH_3 slip, as shown in Figure 12. This is expected; the rapid temperature increase will result in lower equilibrium coverage which results in NH_3 slip. The fluctuations in EGR rate in the beginning of the step is related to the transient response of the engine (and its simplified control system).

Optimizing the Urea dosing only (with the EGR rate fixed at the steady state optimum) does improve the NH_3 slip problem, but a peak value of more than 120 ppm is still higher than the target NTE value (Table 2). In fact, even if the Urea dosing is turned off during the whole step response, the NH_3 slip constraints still can not be fulfilled. By simultaneously optimizing Urea dosing and EGR rate, all constraints can be met. Meanwhile the combined BSFC is slightly reduced compared to the initial values.

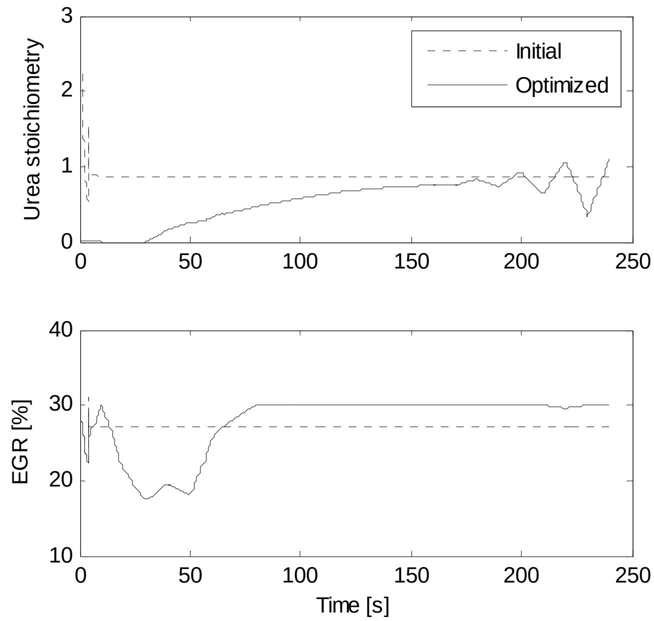

Figure 11 Optimized EGR and Urea parameters, Case 1

The optimum solution (Figure 11) is to reduce the EGR rate during the first ~50 s in order to get higher engine out NOx which consumes NH3 from the catalyst surface. The consumption of stored NH3 is further enhanced by zero Urea dosing for the first 30 seconds. Thereafter the Urea dosing is slowly ramped up to close to stoichiometric conditions. The EGR rate is increased to a higher level than the steady state optimum. This is required in order to meet the average NH_3 slip constraint.

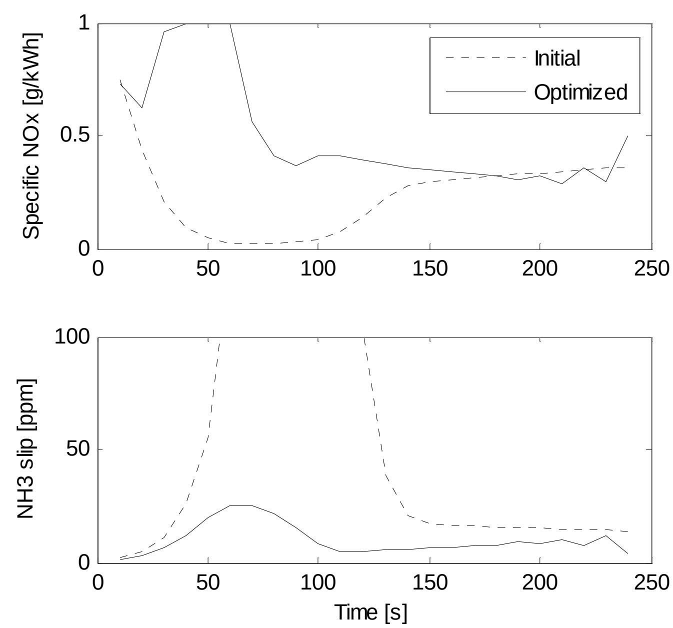

Figure 12 Optimization results, Case 1

The end value coverage profile constraints are met by the optimum solution as shown in Figure 13.

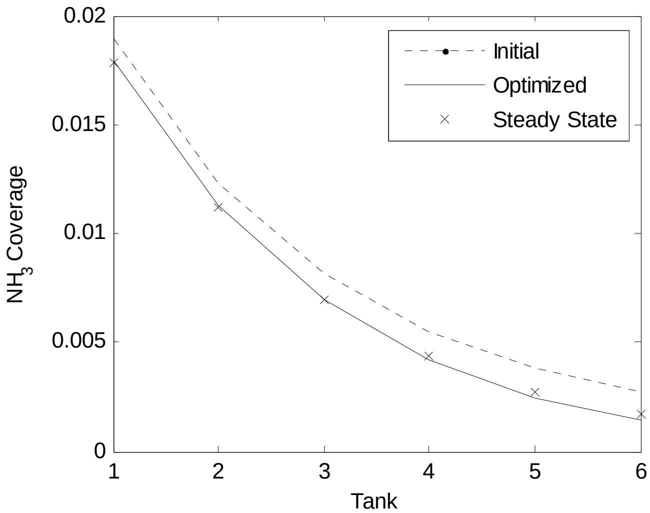

Figure 13 NH_3 Coverage Profile at t=240s, Case 1

Case 2 Negative load transient

The negative load transient is the inverse of case 1; i.e. a step from 1800Nm to 400Nm. A simulation time of 420 seconds is required to reach temperature equilibrium and the parameter step is 20 s. The optimization parameter initial values are set to the steady state optimums. Constraint a is suitable; the decreasing catalyst temperature requires an increased NH_3 coverage to maintain NO_x conversion.

Optimization parameters	**NO_x [g/kWh]**	**Peak NO_x [g/kWh]**	**NH_3 slip [ppm]**	**Peak NH_3 slip [ppm]**	**Norm. BSFC [%]**
Initial values	1.49	1.74	0.24	2.23	100.0
Urea	0.43	1.00	1.85	6.11	100.6

Table 3 Optimization results, Case 2

Using Urea dosing only as optimization parameter, all constraints can be met (Table 3). Very slight gains (<0.02%) can be achieved by using both EGR and Urea dosing as parameters. The optimum solution is quite intuitive; after the temperature has started to decrease, Urea is dosed over-stoichiometric in order to increase the NH3 coverage, followed by a slow decrease down to the steady state optimum (Figure 14).

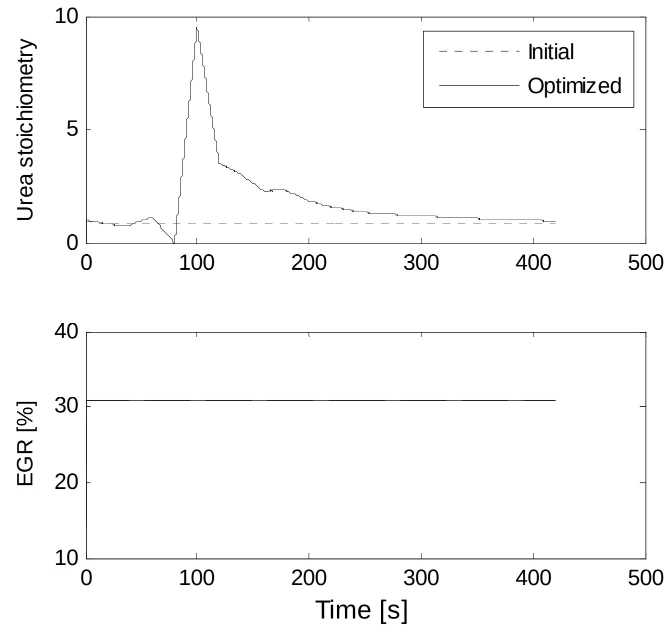

Figure 14 Optimized EGR and Urea parametes, Case 2

The NOx and NH3 constraints are all achieved (Figure 15). The end value coverage profile constraints are also met (the first three tanks in Figure 16). The optimum solution does however deviate from the steady state solution further down the catalyst (tank 4-6).

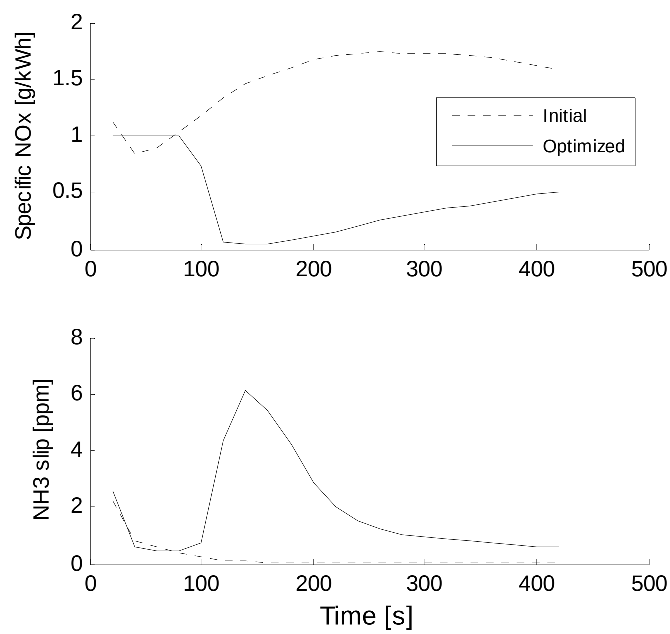

Figure 15 Optimization results, Case 2

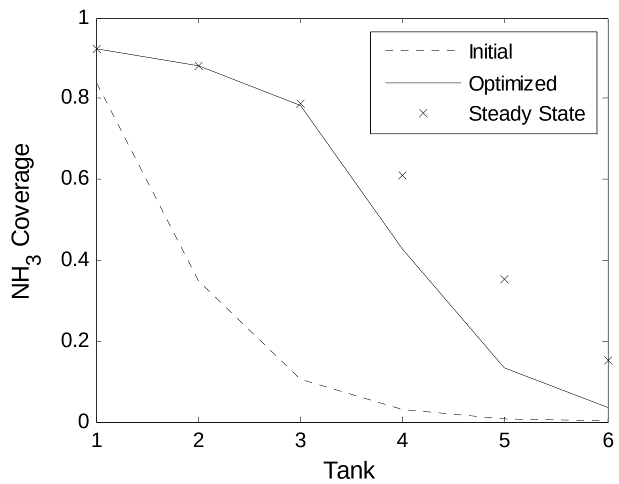

Figure 16 NH_3 Coverage profile at t=420s, Case 2

Case 3 Cold Start

The cold start optimization is defined as a step from idle to 600Nm at 1250 RPM. Initially, the catalyst is at ambient temperature and has zero NH3 coverage, i.e. the catalyst is empty. The engine is warm started; no capability to simulate the influence of coolant and oil temperatures is included in the engine model. Simulation time is fixed at 720 s, and a parameter step of 30 s is used. Urea dosing is deactivated in the model if the pre-catalyst exhaust temperature is below 450 K.

The catalyst temperature will slowly increase from ambient up to ~550K. Because of the low initial coverage, the catalyst should be filled rapidly. Since the temperature is increasing, the equilibrium coverage will decrease (opposite to Case 2); therefore it is desirable to allow overshoots in the NH3 coverage, which obviously excludes constraint a. Instead constraint b is chosen; the NO_x conversion will increase from zero up to the goal of 92% monotonously, even though the NH_3 coverage is higher than the steady state optimum at certain points.

Optimization parameters	NO_x [g/kWh]	Peak NO_x [g/kWh]	NH_3 slip [ppm]	Peak NH_3 slip [ppm]	Norm. BSFC [%]
Initial values	2.10	6.41	0.99	2.36	100.00
Urea	1.56	6.41	15.09	25.16	100.71
Urea+EGR	0.60	4.33	1.26	2.70	102.53
Modified initial values	0.42	0.68	2.98	7.62	101.40
Urea+EGR	0.54	0.99	1.06	2.30	101.40

Table 4 Optimization results, Case 3

The optimization result, as shown in Table 4, states that using only Urea dosing as optimization parameters, all constraints can not be met. Because the initial coverage is zero and the temperature is too low to allow Urea dosing during the first ~100 seconds (Figure 17), no NO_x conversion is possible and the NTE constraints can not be met. The combined fuel consumption is increased; this is expected since more NO_x is reduced. Using both EGR rate and Urea dosing as optimization parameters, the result is disappointing (Table 4). The number of iterations is high, and the optimizer terminates with a solution with high BSFC and none of the constraints fulfilled.

The optimizer would likely benefit from a more intelligent guess of initial values. A set of modified initial values is given by calculating the required engine out NO_x (and the corresponding EGR rate) to achieve 0.5 g/kWh throughout the whole simulation based on the NO_x conversion obtained with the initial value Urea dosing. As can be seen in Figure 17, the result is higher EGR rate in the beginning (in order to compensate for the poor NO_x conversion) ramping down to the steady state optimum towards the end of the simulation. Using the modified initial values, a new optimization is performed with improved results (Table 4, Figure 18). All constraints are fulfilled, except for the LD NO_x constraint which is slightly exceeded. The obvious response would be to increase the Urea dosing. This is not possible however in order to meet the end of simulation NH_3 coverage constraints (Figure 19). Possibly a longer simulation time is needed to fulfill all constraints.

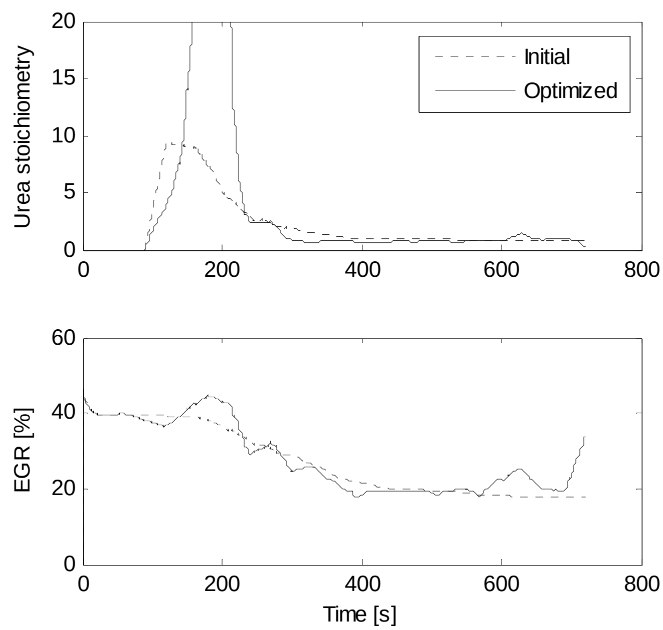

Figure 17 Optimized EGR and Urea parameters, Case 3

The EGR rate is at a higher level than the steady state optimum during the first ~400s of the step response (Figure 17) in order to achieve the NTE constraints. Meanwhile, the Urea dosing is over stoichiometric to increase the NH_3 coverage rapidly. From 400-550s the EGR rate is close to the steady state optimum and the Urea dosing is roughly around stoichiometric conditions. The fluctuations in EGR rate and Urea dosing from 600-

720s is related to altering the NH_3 coverage profile in order to achieve the end value constraints (Figure 19).

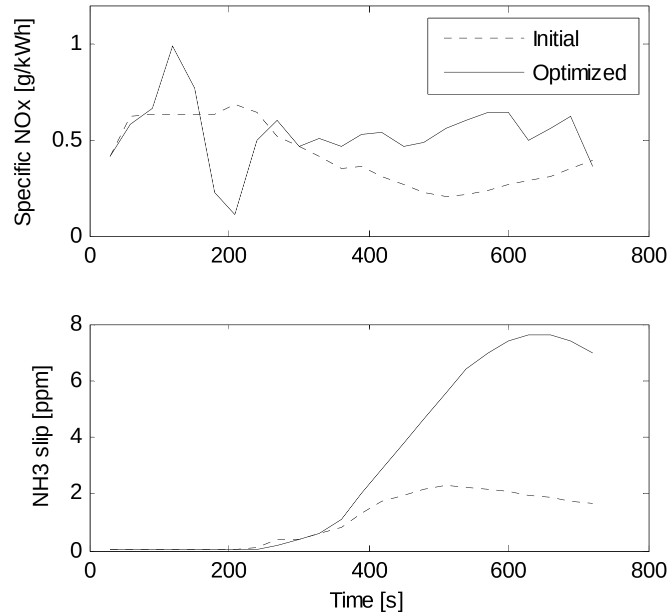

Figure 18 Optimization results, Case 3

Note that the modified initial values results in a higher NH_3 coverage than the steady state optimum in tank 3-6. This will result in NH_3 slip problems if the exhaust temperature is increased. The optimum solution is closer to the desired coverage profile (Figure 19), but still outside the constraint tolerance; another indication that a longer simulation time is needed in order to meet all constraints.

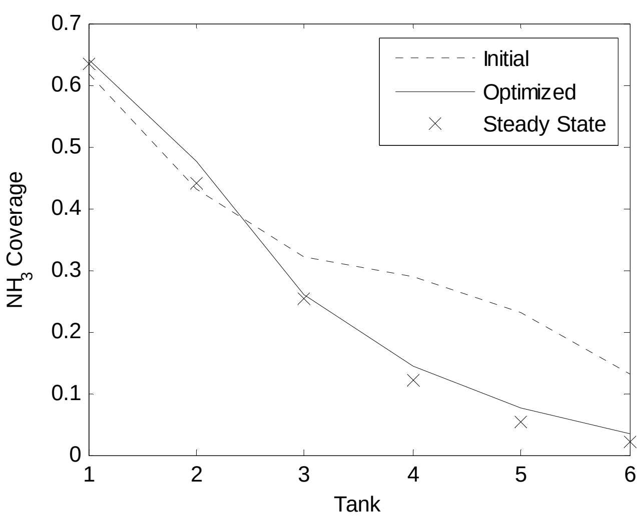

Figure 19 NH3 Coverage profile at t=720s, Case 3

CONCLUSIONS

A complete model of a heavy duty diesel engine plus SCR system is presented. The model includes a quasi steady gas exchange model, a zero dimensional combustion and NOx formation model, a mean value exhaust system model and a state space model of the SCR catalyst. The model shows excellent agreement with measurements and the computational performance is faster than 10 X real time using uncompiled Simulink code on a standard PC. Using second order simplifications for the combustion model in steady state, the computational performance is even faster.

Three operating sequences which are critical for the performance of the SCR system are identified. Using the complete model, a model based optimization problem is formulated. Considering the structure of the problem, the choice of optimization routine is discussed. Other important aspects of the problem are also identified, such as the importance of using constraints to define the end value states and the filling/ emptying process of the catalyst.

Optimization of typical examples of the three critical operating sequences is performed. The results show that by using a complete system approach, i.e. optimizing the balance between engine out emissions and NO_x reduction in the catalyst, Euro VI level NO_x emissions can be achieved while maintaining good fuel economy.

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DEFINITIONS, ACRONYMS, ABBREVIATIONS

ATDC	After Top Dead Center
BDC	Bottom Dead Center
BMEP	Brake Mean Effective Pressure
BSFC	Brake Specific Fuel Consumption
EGR	Exhaust Gas Recirculation
ETC	European Transient Cycle
EVO	Exhaust Valve Opening
FMEP	Friction Mean Effective Pressure
IMEP	Indicated Mean Effective Pressure
IVC	Inlet Valve Closing
LD	Legal Demand
NTE	Not To Exceed
ODE	Ordinary Differential Equation
PMEP	Pumping Mean Effective Pressure
SCR	Selective catalytic reduction
SOC	Start Of Combustion
SOI	Start Of Injection
SQP	Sequential Quadratic Programming
VGT	Variable Geometry Turbocharger
WHTC	World Harmonized Transient Cycle

$\alpha_{IO\Sigma}$ / α_{IOE}	[deg]	Start / end of injection
$\alpha_{\xi\iota\mu}$	[deg]	Fuel mixing parameter
$\alpha_{XO\Sigma}$	[deg]	Start of combustion
$\gamma_{X\varsigma I-X\Delta B}$	[1]	Polytropic exponent, compression from BDC to IVC
$\gamma_{\mu\varepsilon}$	[1]	Polytropic exponent, exhaust manifold
$\gamma_{IO\Sigma-X\varsigma I}$	[1]	Polytropic exponent, compression from IVC to SOI
θ	[deg]	Crank angle degree
δ_{main}/ δ_{pilot}	[mg/stroke]	Main / pilot injected fuel mass
ε	[1]	Emissivity
λ	[1]	Air fuel equivalence ratio
λ_{exh}	[W/mK]	Thermal conductivity of exhaust
σ	[W/m^{2}K^4]	Stefan-Boltzmann constant
τ_{AEOI}	[s]	Time after end of injection
Ω_X	[1]	Feasible set of parameter x

$A_{exh.sys}$	[m^2]	Exhaust system surface area
C_{diff}	[1/s]	Diffusion combustion rate
$c_{p,x}$	[J/kgK]	Specific heat value of x
c_{O2}	[mole/m3]	Oxygen concentration
c_x	[-]	Constraint x
$c_{x,NTE}$	[-]	NTE constraint x
d_{exh}	[m]	Exhaust system inner diameter
EQ_{Urea}	[1]	Relative cost of Urea
F_v	[1]	Gray body view factor
f_x	[1]	Black box function x
h_{cve} / h_{cvi}	[J/s m^{2}K]	External / internal convective heat transfer coefficient
h_{gi}	[J/s m^{2}K]	Internal generalized heat transfer coefficient
J_c	[-]	Jacobian of constraint c
k_x	[1]	Constant parameter x
$m_{exh.sys}$	[kg]	Exhaust system mass
m_x	[kg]	Mass of component x
N_{eng}	[rpm]	Engine speed
Nu	[1]	Nusselt number
p_{amb}	[bar]	Ambient pressure
P	[kW]	Engine power
p_{em}	[bar]	Exhaust manifold pressure
p_{max}	[bar]	Maximum cylinder pressure
p_{rail}	[bar]	Fuel rail pressure
p_{SOI}/p_{IVC}/p_{BDC}/ p_{EVO}	[bar]	Pressure at SOI/ IVC/ BDC/ EVO
$Q_{fuel,inj}$	[J]	Injected fuel energy
$Q_{g,diff}$	[J]	Gross heat release, diffusion combustion
$Q_{g,premix}$	[J]	Gross heat release, premixed combustion
$Q_{premix,tot}$	[J]	Totalt heat release, premixed combustion
R	[J/kgK]	General gas constant
Re	[1]	Reynolds number
t	[s]	Time
T_{amb}	[K]	Ambient temperature
T_{atrb}	[K]	Temperature after turbine
T_{em}	[K]	Exhaust manifold temperature
T_{precat}	[K]	Temperature pre catalyst
T_{SOI}/T_{EVO}	[K]	Temperature at SOI / EVO
T_w	[K]	Exhaust system wall temperature
V_{SOI} /V_{IVC} /V_{BDC}	[m3]	Cylinder volume at SOI/ IVC / BDC
W_{trb}	[kg/s]	Exhaust mass flow through turbine
W_{Urea}	[kg/s]	Urea mass flow
x_{EGR}	[1]	EGR fraction
x_{O2}	[1]	Oxygen molar fraction