

Three-Way Catalyst Light-off During the NEDC Test Cycle: Fully Coupled 0D/1D Simulation of Gasoline Combustion, Pollutant Formation and Aftertreatment Systems

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ABSTRACT

The introduction of more stringent standards for engine emissions requires a steady development of engine control strategies in combination with efforts to optimize in-cylinder combustion and exhaust gas aftertreatment.

With the goal of optimizing the overall emission performance this study presents the comprehensive simulation approach of a *virtual vehicle* model. A well established 1D gas dynamics and engine simulation model is extended by four key features. These are models for combustion and pollutant production in the cylinder, a model for the conversion of pollutants in a catalyst and a model for the effect of manifold wall wetting and fuel evaporation. The general species transport feature is linking these model together as it allows to transport an arbitrary number of chemical species in the entire system. Finally this highly detailed engine model is integrated into a vehicle model.

The presented model is used to investigate the effect of retarded spark timing on the engine out emissions and the tailpipe emissions during the first 60 seconds of the NEDC emission test cycle. Based on the presented results one can conclude that this simulation approach has the potential to reduce the number of experiments on a roller dynamometer in future.

1 Introduction

Current and future legislative restrictions on vehicle emissions draw attention to the design of exhaust gas aftertreatment systems in combination with optimized engine performance. Nowadays, three-way catalysts reach conversion efficiencies of up to 95% for the three main pollutants (carbon monoxide, to-

tal hydrocarbons and nitric oxides) when the converter is fully warmed up. It can take up to two minutes after the engine cold-start until the catalyst is heated by the hot exhaust gas stream. However, in order to meet today's very stringent emission requirements, the light-off of the close coupled catalyst must be achieved within the first 30 seconds of the test cycle.

A great number of modeling studies on a reduction and optimization of the cold start phase, supported by experimental data, are presented in literature. Brinkmeyer et al. [1] apply a 1D model that explicitly focus on the transient heat-up of the catalyst. Missy et al. [2] present a 3D model approach where they simulate the exhaust manifold and the converter heat-up. Using a simplified set of boundary conditions (taken from 1D engine cycle simulations) they consider the influence of flow pulsation as typically given by engine exhausts. The work from Onorati et al. [3, 4] considers the entire exhaust piping within a 1D fluid dynamic model and additionally uses 0D cylinder combustion models for predicting the exhaust gas composition.

For the simulation of the cold start phase this paper presents the following comprehensive model approach:

1. Build a steady-state engine model for the engine under consideration.
2. Validate the emission model parameters using experimental data (see i.e. Bozza and Gimelli [5]).
3. Extend the steady-state engine model by a transient model for the port fuel injectors.
4. Build a model for the close coupled three-way catalyst (TWC).

5. Validate the TWC model using experimental data (see i.e. Brinkmeyer et al. [1], Peters et al. [6]).
6. Link the TWC model to the engine model by using the general species transport feature.
7. Link the engine model (with catalyst) to a vehicle model as sketched in Fig. 1.
8. Run the vehicle+engine+catalyst model for the emission test cycle under consideration.

The major focus of this study is to numerically investigate the effect of spark timings aggressively retarded from maximum brake torque (MBT) timings on the engine out emissions (CO, HC and NOx) as well as on the heat-up and on the time required for light-off of the close coupled TWC.

2 Vehicle Model

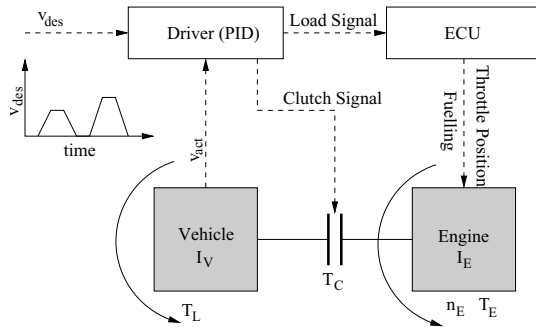


Figure 1: Sketch of the two-body system engine/vehicle and of the control signal flow.

The simulation of emission test cycles such as the NEDC or the FTP cycle requires the consideration of the dynamic behaviour of the two-body system vehicle and engine which can be decoupled by an open or slipping clutch as shown in Fig. 1. For the case that the actual clutch torque is lower than the maximum clutch torque (clutch does not slip: $T_C < T_{C,max}$) the engine speed (and the corresponding vehicle speed) is calculated according to:

$$(I_E + I_V) \cdot \frac{d\omega_{sys}}{dt} = T_E + T_L \quad (1)$$

For the case of a slipping clutch the transferred torque is equal to the maximum clutch torque. Then

the engine and the (reduced) vehicle speed can be described by:

$$I_E \cdot \frac{d\omega_E}{dt} = T_E + T_{C,max} \quad (2)$$

$$I_V \cdot \frac{d\omega_V}{dt} = T_L + T_{C,max} \quad (3)$$

wherein $T_{C,max}$ is a function of clutch pedal position. The process of gear shifting is modeled by defining a specific time profile for load signal and clutch pedal position as described in AVL BOOST AVL List GmbH [7].

The rotational inertia of the engine is defined as a constant value, for the vehicle it is defined by the sum of the drivetrain inertia and the rotational inertia of the vehicle:

$$I_V = I_{DT} + m_V \cdot r_T^2 \quad (4)$$

The load moment is calculated as follows:

$$M_L = r_T \cdot F \quad (5)$$

where the vehicle load F is calculated as $F = a + b \cdot v_V + c \cdot v_V^2$.

The driver model tries to follow a specified vehicle speed course by calculating the load signal depending of the deviation of the actual vehicle speed from the desired one. Here the driver is represented by a simple PID controller:

$$LS = G_P \cdot (n_{des} - n) + G_I \cdot \int_0^t (n_{des} - n) + G_D \cdot \frac{d}{dt} (n_{des} - n) \quad (6)$$

Finally the ECU uses the load signal in order to set the throttle position and the fueling for the engine model as sketched in Fig. 1.

3 Engine Model

The 1D engine simulation and gas exchange model AVL BOOST (AVL List GmbH [7]) comprises a list of individual components that can be combined in a variable way. Elements such as cylinders, pipes, plena, junctions, injectors, turbo chargers, catalytic converters, air coolers and filters can be assembled

to an engine model comprising a complete description of all cylinders and the intake and exhaust systems. Typically, the aim of gas exchange simulation is to predict and optimize air delivery ratio, power, torque, fuel consumption or tail-pipe noise. With the goal of modeling the efficiency of aftertreatment systems this classic approach needs to be extended by four key-features:

1. Transient formation of a fuel puddle in the intake port and evaporation of fuel from it.
2. Predictive in-cylinder combustion and emissions modeling in order to calculate engine-out conditions during a transient operation of the engine.
3. Transport of all chemical species (arbitrary number and type) through all elements of the model.
4. Consideration of the heterogeneous chemical reactions and the related release of heat in the catalytic converter.

In the following subsections these four models are described in more detail.

3.1 Species Transport Model

A minimum list of species, which is arbitrary in general, is defined by the reaction chemistry of the main pollutants under legislative control. The species are CO, C₃H₆, C₃H₈, CO₂, H₂, NO, NO₂, O₂, OH, H₂O, O, H and N₂. Starting with air and fuel in the cylinder these species need to be produced, transported through the ducts and finally converted in the catalyst. Please refer to Wurzenberger et al. [8] for details on this model.

3.2 Transient Fuel Injector Model

Under the practical driving conditions represented by an emission test cycle, PFI gasoline engines are operated under highly transient conditions, which cause significant air-fuel ratio excursions. As most of the engine out unburned hydrocarbon (UHC) and CO emissions are produced during cold start and under transient conditions, it is of particular importance to take into account the formation and the evaporation of a liquid fuel film on the intake port wall and the intake valve surface. The liquid fuel film acts as a source or sink of fuel under cold start and transient conditions.

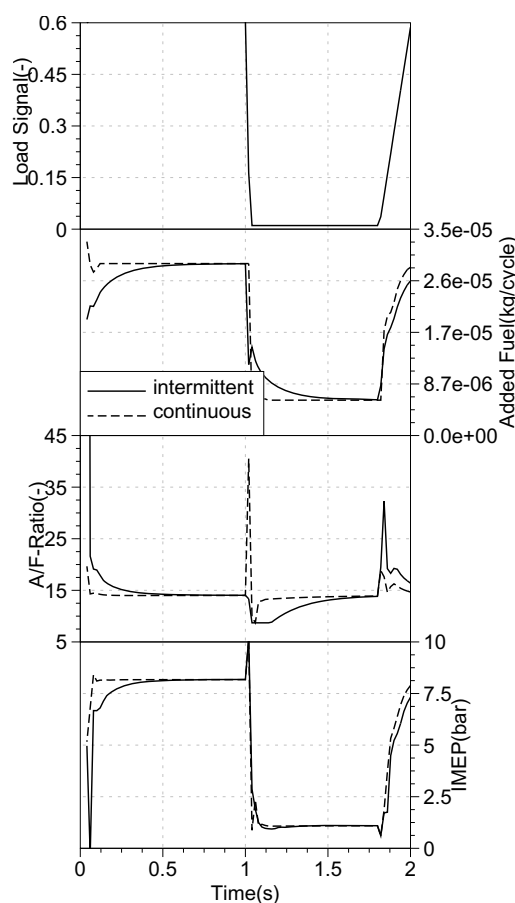


Figure 2: Transient injector modelling: Effect of fuel puddle on air/fuel ratio and engine performance.

On this phenomenon one can find a variety of models of different complexities in the literature. Starting from full 2D or 3D simulations (AVL FIRE AVL List GmbH [9], Cho et al. [10]) several simplified approaches have been developed to model this effect in a more system-oriented way. Aquino [11] proposed a simple time-constant based model, together with a fraction X describing the amount of fuel that gets deposited on the port surface. The time constant and the value of X must be determined experimentally. Although this model is simple to use, especially for control applications, its disadvantage is that it is non-predictive. It does not allow extrapolation of the parameters for different fuel types or different wall temperatures. As the focus of this paper is to model the entire engine including also the in-cylinder combustion and the aftertreatment system it is neither feasible to model all details of these

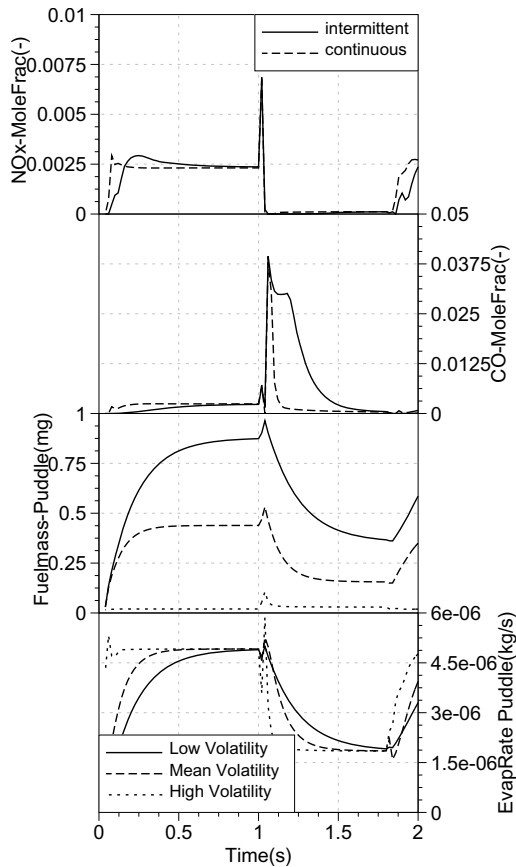


Figure 3: Transient injector modelling: Effect of fuel puddle on engine out emissions.

complex and multi-dimensional processes nor to rely on a very simple control oriented approach. Based on the work that was previously done in this area we here present a model that considers the effects of fuel injection, fuel deposition, fuel evaporation and fuel transport. The objective is to account for the effect of fuel puddling on engine performance, combustion fuel-air ratio, engine-out emissions and performance (light-off) of the close coupled three-way catalyst.

The fuel injection process is described as a pulse with given start timing, pulse duration and injection rate. The model is neglecting any transients caused by the spray but adds the injected mass of fuel according to a user-prescribed fraction X directly into the gas phase or into the fuel puddle along the port walls.

The evaporation characteristics of gasoline fuel is typically described by a distillation curve (please refer to www.chevron.com [12]). Components with

higher volatility evaporate at lower temperatures (approx. 50 degC), components with lower volatility evaporate at higher temperatures (approx. 170 degC). In order to take this effect into account the actual amount of injected fuel $\dot{m}_F$ is split into Q different packages where each fuel package has different evaporation properties depending on the user-specified distillation curve.

$$\dot{m}_F = \sum_{q=1}^Q \dot{m}_q \quad (7)$$

For each package q the actual mass in the fuel puddle is calculated from a simple balance equation:

$$\frac{dm_{P,q}}{dt} = (1 - X) \cdot \dot{m}_q - \dot{m}_{evap,q} - C_P \cdot m_{P,q} \quad (8)$$

The rate of evaporation of fuel package q is given by

$$\dot{m}_{evap,q} = C_{evap} \cdot k_q \cdot A_P \cdot \rho_{g,i} \cdot \left(\frac{y_{q,sat} - y_i}{1 - y_{q,sat}} \right) \quad (9)$$

wherein A_P is the actual port area that is covered by the fuel puddle. It is calculated using the actual mass of fuel in the puddle, a reference diameter and a user-prescribed thickness of the fuel film. The saturation mole fraction for fuel q is calculated using Raoult's law ($y_{q,sat} = p_{q,sat}/p$), the saturation vapour pressure for each boiling range can be derived from the distillation curve for the given fuel. k_q is the convective mass transfer coefficient and is calculated using the following relation for the Sherwood number:

$$Sh_q = \frac{k_q \cdot d_{ref}}{D_q} = 0.023 \cdot Re^{0.8} \cdot Sc^{0.22} \quad (10)$$

For a very simple test case (prediction of throttle transients for a fixed engine speed) the impact of the fuel puddling on engine performance and engine out emissions is shown in Figs. 2 and 3. At time $t = 0$ the calculation is started with the throttle wide open. Without the fuel puddle model (=continuous injection) the target combustion air/fuel ratio is immediately reached, with the fuel puddle model it takes approximately 0.5s. During this period more fuel is added to the puddle than is evaporat-

ing from it. Therefore less fuel is added to the gas phase, the engine is running lean and the IMEP is below its target value. After coming to a steady state the throttle is closed at around 1 sec. Again, without the puddle model the target air/fuel ratio is immediately reached. With the fuel puddle model the engine is running rich (fuel is evaporating from the puddle) for the next 0.5s. This has no significant influence on the IMEP. However, the CO emissions are significantly higher during this period. On the other hand the NOx emissions are lower. Figure 3 also shows, that the actual mass of a certain package q that can be stored in the puddle depends on its volatility: higher volatility result in higher evaporation rates and a lower amount of liquid fuel in the puddle.

3.3 Cylinder Model

The thermodynamic state within a cylinder is represented by its mass, temperature, species composition, and pressure (see Fig. 4). In order to describe the state during an engine cycle, conservation and state equations need to be solved. Two different sets of 0D equations are used in the present model approach. A *single zone* model is used for the gas exchange phase and a *two zone* model is applied during the high pressure phase. Please refer to Wurzenberger et al. [8] for details on the conservation equations during the different phases and for a detailed description of the 'Fractal Combustion Model'.

3.3.1 Burned Zone Stratification Model

As shown in Fig. 4, the model divides the combustion chamber into two different zones. The *unburned zone* comprises the state of the unburned air/fuel mixture in front of the ignition front. The *burned zone* describes the state behind the front, where combustion products are part of the gas mixture. The mass and the enthalpy of the unburned zone are transferred to the burned gases as the combustion proceeds. Chemical kinetic models can be applied to both the burned zone (pollutant formation) and the unburned zone (i.e. knock and HCCI simulation).

It is well known in fact that mixture which burns early in the combustion process is further compressed after combustion as the remainder charge is burned (D'Errico et al. [13]). On the contrary, mixture which burns late is compressed prior to combustion and therefore ends up at a different final state. Typically temperature differences of about 100-200 K

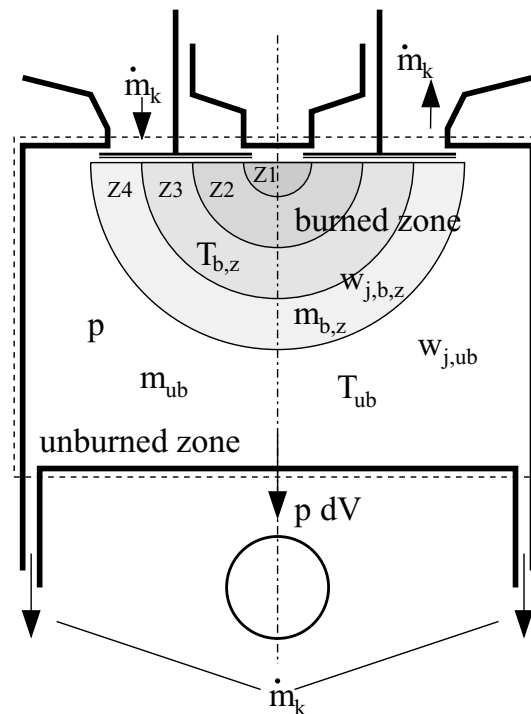


Figure 4: Schematic of the main state variables and fluxes in a two zone cylinder model. Burned zone stratification model: The mass in the zones 1, 2 and 3 is constant, zone 4 is burning.

have been reported between the first and last burned regions. Neglecting this effect by using a standard two zone model would typically result in a significant underprediction of the CO and NOx emissions.

The burned zone stratification model splits the 'average' burned zone into a total number of Z stratified zones. It assumes that each zone, except the last zone (the currently burning zone), has the same constant amount of mass. The mass of the last zone results from:

$$m_b = \sum_{z=1}^Z m_z \quad (11)$$

The model furthermore assumes that there is no mass exchange between the zones, each zone is spherical with its center located on the spark plug position, each zone exchanges heat with the cylinder walls according to the respective wetted area.

For all burned zones except the last the temperature is calculated from: