A Novel 1D Co-Simulation Framework for the Prediction of Tailpipe Emissions under Different IC Engine Operating Conditions

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Abstract

The accurate prediction of pollutant emissions generated by IC engines is a key aspect to guarantee the respect of the emission regulation legislation. This paper describes the approach followed by the authors to achieve a strict numerical coupling of two different 1D modeling tools in a co-simulation environment, aiming at a reliable calculation of engine-out and tailpipe emissions. The main idea is to allow an accurate 1D simulation of the unsteady flows and wave motion inside the intake and exhaust systems, without resorting to an over-simplified geometrical discretization, and to rely on advanced thermodynamic combustion models and kinetic sub-models for the calculation of cylinder-out emissions. A specific fluid dynamic approach is then used to track the chemical composition along the exhaust duct-system, in order to evaluate the conversion efficiency of after-treatment devices, such as TWC, GPF, DPF, DOC, SCR and so on. This co-simulation environment is validated against a real engine configuration which was instrumented and tested at EMPA labs. A 4-cylinder SI, turbocharged, CNG engine is investigated at different loads and revolution speeds, to allow a wide validation with experimental data and verify the predictiveness of engine performances and pollutant emissions.

Introduction

The current European legislation concerning pollutant emissions from IC engine vehicles is very stringent and demanding. In addition, the CO2 fleet emission must obey to a significant reduction path during the next decade, to cope with the prescribed targets recently agreed.

In general, the prediction of pollutant emissions from IC engines has been a challenge since the introduction of the emission regulation legislation. During the last decade, along with the more tightening limits and increased public concern about air quality, the capability of simulating different operating conditions and driving cycles with an acceptable computational effort has become a key feature for modern simulation codes.

Nowadays advanced simulation tools give the opportunity to investigate how to achieve high engine efficiency, low fuel consumption and emissions while keeping good performances, on the basis of the typical operating conditions requested by the WLTP cycle and the new Real Driving Emission (RDE) homologation procedure.

The role of 1D thermo-fluid dynamic simulation models is extremely important to achieve this task, in order to investigate the performances of the next generation of IC engines working over a wide range of operating conditions, under steady-state and transient conditions.

Many 1D simulation tools are available on the market, offering real time models capable of achieving the simulation of any driving cycle in limited time frames. These approaches are generally based on the extreme simplification of the engine geometry or on the adoption of engine maps, which, for any engine operating condition, give the engine output in terms of power, torque, and exhaust gas composition. Specific fluid dynamic models can be used to track the composition along the exhaust system and, with the aid of ad-hoc modules, to evaluate the conversion efficiency of after-treatment devices, such as TWC, GPF, DPF, DOC, SCR and so on.

This work is based on the idea of integrating two different 1D simulation tools in a co-simulation environment, realizing a strict numerical coupling between the two codes. The main goal is to allow an accurate 1D simulation of the unsteady flows and the wave action along the intake and exhaust systems, without resorting to over-simplified geometrical discretization, and to rely on advanced thermodynamic combustion models for the calculation of cylinder-out emissions.
emissions. The simulation of the after-treatment systems is then performed resorting to a steady state model with a detailed chemistry approach. In this scenario, the choice of the coupling strategy is a key issue, since an unsteady model must be coupled to a steady one. In particular, this last element may flatten the unsteady pattern of the flow, imposing unreal boundary conditions at the engine exhaust manifold and increasing the risk of misleading results. For this reason, the chemical and the fluid-dynamic behavior have been decoupled, allowing the 1D unsteady solver to propagate pressure waves along the complete system, preserving all the characteristic lengths (acoustic and fluid dynamic). For every after-treatment device a specific steady-state 1D model is used to predict the chemical conversion phenomena and the heat transfer involved. The boundary conditions for the steady state solver are provided by the 1D unsteady solver, suitably averaged over the time. The steady-state solution is then sent back to the 1D unsteady solver and suitably over-imposed: temperature of the substrate, friction coefficient and gas composition. This co-simulation environment is validated against a real engine configuration which was tested at the experimental labs of EMPA research center. An SI, 4-cylinder, turbo-charged, CNG engine has been simulated at different loads and speeds and results are compared with the experimental measurements, to verify the prediction of engine performance and pollutant emissions.

**Methodology**

**Governing Equations**

The code used in this work is *gasdyn*, a 1D thermo-fluid dynamic model that is being continuously developed and enhanced by the researchers of Politecnico di Milano and Exothermia. The main features of the numerical code have been described in previous works [1, 2, 3, 4]. The model has been developed for the simulation of internal combustion engines coupled to their complete intake and exhaust systems. This allows for a detailed analysis of the fluid dynamic, thermal and chemical behaviour of the whole engine system. The partial differential equations describing the mass, momentum and energy conservation for each computational mesh are written in matrix form as follows [1, 2]:

\[
\frac{\partial W(x,t)}{\partial t} + \frac{\partial F(W)}{\partial x} + B(W) + C(W) = 0
\]

\[
W = \begin{bmatrix}
\rho F \\
\rho UF \\
\rho e UF \\
0 \\
0
\end{bmatrix}, \quad F(W) = \begin{bmatrix}
\rho UF \\
\rho UF U^2 + p \\
\rho UF h_F \\
0 \\
0
\end{bmatrix},
\]

\[
B(W) = \begin{bmatrix}
0 \\
-\frac{p}{\rho} \frac{\partial F}{\partial x} \\
0
\end{bmatrix}, \quad C(W) = \begin{bmatrix}
0 \\
\frac{2}{D} \rho U [k] f_s F \\
-\rho (q + q_{t, F}) F
\end{bmatrix}
\]

The source term \( q_{i, F} \) in the energy equation represents the heat released by the chemical reactions occurring in the gas phase (per unit mass per unit time) and \( q \) is the sum of the convective and radiative heat transferred from the gas to the pipe walls. The information concerning the tracking of chemical composition along the duct systems is accounted for by solving the mass conservation equation for each chemical specie considered:

\[
\frac{\partial \rho Y_i F}{\partial t} + \frac{\partial (\rho Y_i UF)}{\partial x} = Y_i
\]

where \( Y_i = m_i/m \) is the mass fraction in the control volume for the \( i \)-th specie and \( Y_i \) is the rate of variation of mass fraction due to chemical reactions involving the \( i \)-th specie. The system of conservation equations represents a quasi-linear hyperbolic problem which can be solved by means of shock-capturing numerical methods. The *gasdyn* code makes use of a set of different numerical solvers, among which symmetric, TVD finite difference techniques with 2nd order accuracy described in [2]. Boundary conditions and intra-pipe connections for the representation of devices such as turbochargers, multi-pipe junctions, abrupt area changes, inlet and outlet and similar, are developed following a characteristic-based approach for the calculation of Riemann variables [6].

For the purpose of this work the *gasdyn* 1D model has been coupled to the *axisuite* code, developed by Exothermia, which is able to deal with any reaction scheme and rate expressions (“elementary” and “global” reactions) [7, 8, 9]. The *axisuite* code allows 1D, 2D or 3D discretization at the device level and 0D, 1D and quasi-2D in the wall direction, used when washcoat diffusion limitations need to be accounted for.

**Balance Equations**

The simplified 1D + 0D version of the *axisuite* model adopted in this work exploits the assumption of simplified single channel. In this context the calculation of the temperature and species concentrations in the channel is based on the solution of the quasi-steady equations for the gas phase heat and mass transfer:

\[
\rho C_p \frac{\partial T}{\partial z} = -h \cdot \left( \frac{S_g}{\varepsilon} \right) \cdot (T_e - T_s)
\]

where \( \rho \) is the density, \( C_p \) the specific heat capacity, \( v \) the gas velocity, \( T \) the temperature, \( h \) the heat transfer coefficient, \( S_g \) the monolith specific surface area and \( \varepsilon \) the substrate void fraction. Subscripts \( g \) and \( s \) denote the exhaust gas and the solid substrate respectively.

Similarly, a “film” approach is also used to account for the gas phase mass transfer resistance:

\[
\frac{\partial (y_j y_{s, i})}{\partial z} = -k_i \cdot \left( \frac{S_g}{\varepsilon} \right) \cdot (y_{s, j} - y_{j, i})
\]

where \( y_j \) is the molar fraction of species \( j \) and \( k_i \) the mass transfer coefficient of species \( j \). In these equations the heat and
mass transfer coefficients are calculated based on the following definitions:

\[ h = \frac{Nu \cdot \lambda_{sk}}{d_h}, \quad k_j = \frac{Sh \cdot D_{mol,j}}{d_h} \]

where \( \lambda_s \) is the thermal conductivity, \( D_{mol,j} \) the molecular diffusion and \( d_h \) the hydraulic diameter. Provided that the influence of internal diffusion is considered negligible, there is no concentration gradient in the washcoat and therefore only one surface species concentration is defined. Therefore, the total reaction rate on the surface for each species (including storage reactions) is equal to the local external species mass transfer \( \text{to/from the exhaust gas:} \)

\[ \rho \frac{M_j}{M_g} k_j \left( \frac{S}{E} \right) (y_{s,j} - y_{s,i}) = R_j \]

where \( M_j \) is the gas molecular weight. The surface reaction rates for each species \( R_j \) are calculated based on the specific reaction scheme and are functions of local surface concentrations, coverages and temperature.

The thermal balance of solid phase is taken into account by solving the energy conservation equation also accounting for the transient behaviour:

\[ \rho_s C_{ps} \frac{\partial T_s}{\partial t} = \lambda_s \frac{\partial^2 T_s}{\partial z^2} + \frac{S}{1-E} (T_g - T_s) + \frac{1}{1-E} \sum_{k=1}^{n} \Delta H_k R_k \]

which considers, in the right hand side, the contribution of convective heat transfer of the gas flow in channels and of the heat released or adsorbed by chemical and adsorption reactions.

In many catalyst applications, the thickness and effective diffusivity of the active layer may not allow the simplifying assumption of negligible internal diffusion resistance. In these cases, a more detailed approach which models mass transfer both in the gas phase and in the washcoat active volume pores may be used.

**Coupling Strategy**

To carry out a detailed simulation of the after-treatment system, the \textit{gasdyn} code has been coupled to \textit{axisuite}. Since the numerical approaches of the two codes are different, the authors have developed a hybrid coupling to allow an unsteady approach and a steady-state one coexist in the same simulation framework. The main target of the developed strategy is to preserve the unsteady nature of the flow, with the transport of pressure pulsations, while exploiting the detailed calculation of the chemical reactions provided by the steady-state solver. To achieve this goal the coupling approach is based on the duplication of the catalyst element, by generating two overlapping elements that are solved in parallel and suitably merged in the final solution.

The wave motion and the flow pulsations are predicted by \textit{gasdyn}. Then, the passage of values from \textit{gasdyn} to \textit{axisuite} relies on the averaging of mass flow, gas temperature and chemical composition along a single (or a fraction of) thermodynamic cycle. These averaged pipe quantities, as shown in Figure 1, are assigned as inlet boundary conditions to \textit{axisuite}. In this framework, the time step used for the integration of the steady state problem is larger than the time step used in \textit{gasdyn}, which is subject to the CFL stability condition. Therefore, during the \textit{axisuite} time step, quantities are integrated at the inlet and then used to perform the steady state calculation, when the cumulative time step of \textit{gasdyn} has reached the \textit{axisuite} one. Once \textit{axisuite} has performed its time step, the solution is then mapped back to \textit{gasdyn}, transferring the quantities referred to the chemical activity and to the fluid dynamic processes occurring inside the catalyst: the wall temperature calculated node by node, the gas-wall heat flux at every node, the friction factor and the outlet species concentrations. The heat flux and the friction factor are then considered in \textit{gasdyn} as source terms in the governing equations \((f_w \text{ and } q)\) and they are fully integrated in the stencil of the numerical method. The outlet concentration of chemical species is overwritten to the concentration tracked by \textit{gasdyn}. This can be realized only with the option of constant thermophysical properties implemented in the \textit{gasdyn} solver: the \( c_p \) and molecular mass of the gas are considered constant regardless of the changes in the gas composition. The outlet concentration of \textit{axisuite} is assigned to the last and second last node of the \textit{gasdyn} domain and then passed as a zero-gradient trend to the characteristic-based approach. This allows to advect the desired concentration along the path lines and track it downstream of the catalyst, following the pulsations of the gas flow.

**Combustion and Pollutant Emissions Models**

With regard to SI combustion model, a primary requirement is an accurate prediction of the flame front velocity, which is influenced by a large number of factors, such as thermodynamic and chemical properties, turbulence intensity, chamber design and heat fluxes through the boundaries. In order to predict the in-cylinder pressure development, a multi-zone, quasi-dimensional combustion model has been used for the
simulation of the SI turbocharged engine, to evaluate the thermodynamic and chemical gas properties inside the combustion chamber [4] where the fully developed turbulent flame speed has been computed applying the Zimont model [10]. Therefore, even accepting all limitations due to a quasi-dimensional approach, it is fundamental to account for the turbulence generation and dissipation within the combustion chamber and to rely on appropriate laminar flame speed correlations. For the former aspects, the turbulent intensity \( u' \) has been evaluated by the two-equation model \( K-k' \) from the knowledge of the turbulent kinetic energy, \( k \), and the mean flow kinetic energy, \( K \) [4]. The convective heat transfer rate to the combustion chamber walls is calculated as indicated in [4], whereas the heat transfer coefficient has been calculated by applying the Woschni correlation [11].

The \textit{gasdyn} code is able to predict the concentration of the main chemical species such as NO, CO, CO\(_2\), HC, O\(_2\), etc., during the combustion process and their concentration in the exhaust gases discharged by cylinders at EVO. In particular, the combustion model adopts an equilibrium approach to evaluate the concentrations of the major species (H\(_2\)O, H, H\(_2\), CO, CO\(_2\), O, O\(_2\), OH, N\(_2\), NO), considering the following six reactions [12]:

\[
\begin{align*}
CO + H_2O & \rightleftharpoons CO_2 + H_2 \\
2CO_2 & \rightleftharpoons 2CO + O_2 \\
H_2 + O_2 & \rightleftharpoons 2OH \\
H_2 & \rightleftharpoons 2H \\
O_2 & \rightleftharpoons 2O \\
O_2 + N_2 & \rightleftharpoons 2NO
\end{align*}
\]

The resulting equilibrium composition is calculated resorting to a fast computation method, described in [12]. Some species are satisfactorily calculated on the basis of the equilibrium assumption, such as H\(_2\)O, H\(_2\), CO\(_2\), O\(_2\), N\(_2\), whereas some other species, essentially CO, NO and HC, must be properly evaluated resorting to kinetic sub-models, since the equilibrium assumption is not acceptable. With regard to NO, the extended 6 reaction Zeldovich [13] model has been used to predict the kinetically controlled NO formation process:

\[
\begin{align*}
O + N_2 & \rightleftharpoons NO + N \\
N + O_2 & \rightleftharpoons NO + O \\
N + OH & \rightleftharpoons NO + H \\
N_2O + O & \rightleftharpoons 2NO \\
N_2O + O & \rightleftharpoons N_2 + O_2 \\
N_2O + H & \rightleftharpoons N_2 + OH
\end{align*}
\]

from which the NO production rate \( (d[NO]/dt) \) can be derived [11].

To improve the reliability of the predictions, this approach is coupled to a multi-zone thermal model for the calculation of temperature gradients in different regions of the burned gas [4,11], which significantly influence the global NO concentration.

Many experimental evidences proved that the CO concentration in SI engine exhaust gas has to be considered kinetically controlled, because it is lower than the maximum value measured into the combustion chamber, but higher than the corresponding equilibrium value. Hence, the classical kinetic sub-model described in [11] has been included in \textit{gasdyn} to evaluate the production/destruction rate of this specie, on the basis of the following reactions:

\[\begin{align*}
CO + OH & \rightleftharpoons CO_2 + H \\
CO_2 + O & \rightleftharpoons CO + O_2
\end{align*}\]

The resulting CO reaction rate can be expressed as follows [11]:

\[
d\left[\frac{[CO]}{t}\right] = (R_1 + R_2) \left(1 - \frac{[CO]_e}{[CO]_c}\right)
\]

where \([CO]_c\) is the predicted equilibrium concentration of CO, and the rates \( R_1, R_2 \) are given by:

\[
R_1 = k_1 \cdot [CO]_c \cdot [OH]_c \\
R_2 = k_2 \cdot [CO]_c \cdot [O_2]_c
\]

In this work, as an alternative the CO concentration, related to the actual equilibrium value \( CO_{eq} \), has been computed by applying the Baruah semi-empirical method on the basis of the maximum equilibrium values, \( CO_{max} \), achieved in the combustion chamber [14]. The simple following equation has been proposed:

\[
[CO] = [CO]_{eq} + f_{CO} \cdot \left([CO]_{max} - [CO]_{eq}\right)
\]

where \( f_{CO} \) is a calibration factor (\( f_{CO} = 0 \div 1 \)). However, such a method is not fully predictive, since it must be calibrated at least for one operating point.

The sub-model for unburned HC is based on the approach described in [15, 16, 17, 18, 19, 20], taking account of the hydrocarbons released by the top land crevice and by the oil film. Once the cylinder pressure is known from the multi-zone combustion model, the mass of fresh charge in the crevice can be determined by means of the ideal gas equation.

Hence, the storage and release of unburned hydrocarbons from the top land crevice during the thermodynamic cycle can be evaluated, depending on the variation of cylinder pressure.

Moreover, the absorption and desorption of HC from the lubricating oil layer can be modeled. The oil film thickness is an input data (typical values are in the range 0.4-1 \( \mu \text{m} \) [17]); the oil film is considered at the same cylinder wall temperature, which is a function of engine speed, load and location on the cylinder liner, as suggested in [17,20].

The absorption/desorption process of hydrocarbons by the oil layer is modelled as function of different complex
factors, such as the fuel solubility into the oil, the air/fuel ratio, the cylinder wall temperature, the oil film thickness and the engine speed. An analytical solution of the fuel profile distribution inside the oil film is obtained by solving the following diffusion equation [19]:

$$\frac{\partial Y}{\partial t} - D \frac{\partial^2 Y}{\partial x^2} = 0$$

where \( Y \) is the fuel mass fraction in the oil and \( D \) is the corresponding diffusion coefficient. The above equation can be solved numerically by a first order finite difference scheme, assuming a zero gradient concentration at the oil layer-wall interface, and assigning variable conditions at the other boundary depending on the flame front and piston position [19]. The result, in terms of hydrocarbons release per cycle, is clearly affected by the oil film thickness and wall temperature.

The HC released by the crevice and the oil layer in the burnt gas after the arrival of the flame front, are subject to a post-flame oxidation and can produce unburned hydrocarbons in the exhaust products. A significant part of the total mass of unburned HC released in the cylinder during the post-flame stage generally is rapidly oxidized in the hot bulk gas (then it does not contribute to final HC emissions), whereas the remaining part is entrained in the colder thermal boundary layer adjoining cylinder walls. Hence, it is slowly oxidized and finally released as unburned hydrocarbons at the exhaust valve opening. An empirical constant must be fixed to assign this subdivision of the unburned HC mass. An Arrhenius type, global reaction rate equation has been adopted to model the slow post-oxidation of HC in the thermal boundary layer, as suggested in [15]:

$$\frac{d[H C]}{dt} = R_{HC} = -c_{HC}A_{HC}e^{-E_{HC}/RT_{wall}}[H C][O_2]^b$$

where \( R_{HC} \) is the rate of HC post-flame oxidation, \( A_{HC} \) and \( E_{HC} \) are constants equal to 7.7x10^9 (m^3/mole)arbs^-1/s and to 156222 (1/mole), respectively, \( R \) is the universal gas constant equal to 8314 (J/mole/K), \( T_{w} \) is the average gas temperature in the thermal boundary layer, assumed equal to \( (T_{w} + T_{cyl,wall})/2 \), with \( T_{w} \) equal to cylinder bulk gas temperature (calculated by the multi-zone combustion model) and \( T_{cyl,wall} \) equal to cylinder wall temperature at that location. \([H C]\) and \([O_2]\) are the concentrations of HC and \( O_2 \) (mole/m^3) in the gas, \( a \) and \( b \) are exponents generally equal to 1.0 and \( c_{HC} \) is a calibration constant used to adjust the reaction rate to a specific case. In fact, the unburned HC sub-model requires a minimum of initial calibration to provide satisfactory results.

### Engine Modelling

The first step of this research activity required a complete 1D modelling of the engine, on the basis of the known geometrical layout, including complex devices such as the NG injectors, the intercooler and the three-way catalysts. In Figure 2 the schematic of a SI, turbocharged, natural gas engine, realized by means the gasdynpre graphical interface, has been depicted: all the geometrical characteristics of the intake and exhaust systems, including the turbocharger group with wastegate and the air cooler have been introduced. Figure 2 shows also the three catalytic converters placed along the exhaust line, which have been coupled to the axisuite code, with the schematic of the representation of a single channel.

The focus of this work was to investigate the behaviour of the after-treatment components, therefore only the first part of the exhaust system (without the silencers) was considered. The 1D model was applied in order to run a first level analysis, able to characterize the overall performance of the engine. As a second step, detailed simulations were carried out to confirm the validity of the gasdyn-axisuite coupling, in order to investigate the behaviour of the catalysts by a chemical point of view. The accurate 1D modelling of the turbocharger represents a challenging task. The most common approach is based on the use of performance steady-flow maps [15], which are determined experimentally by the manufacturer and stored by the simulation model into dedicated look-up tables.

### Engine Type

In this study a light duty 3.0L SI, NG, turbocharged engine was considered. The engine is fuelled by natural gas (NG), which is injected inside the primary ducts by a port fuel injection (PFI) system, adopting a sequential and phased strategy. The engine is supercharged by means of a turbocharging group with a single stage fixed geometry turbine (FGT) and a wastegate (WG). In the induction system an intercooler is adopted, in order to increase the volumetric efficiency and to reduce the knocking propensity. Three catalytic converters are located downstream of the turbine: one pre-cat, based on a metallic support, one ceramic main catalyst and a third monolith, not loaded with precious metals.

This engine has been instrumented and investigated experimentally on the test bench at EMPA labs, to study and optimize the combustion process and reduce the pollutant emission formation. It has to be pointed out that the engine is not equipped with its serial-production engine control unit (ECU) but with a rapid-prototyping ECU with in-house coded functionalities. The main specifications of the engine investigated are reported in Table 1.
Experimental Activity

Methodology

The experiments were concerned with a series of operating points from the entire engine map consisting of:

- predefined maximum load (determined by boost pressure and limited by the cylinder head temperature),
- medium load - 0.6 MPa of BMEP,
- low load - 0.25 MPa of BMEP.

The natural gas used as fuel contained on the average 94.5% Mol-% of methane with only a small variation among different batches. The second frequent component, in respect to molar shares, is ethane with 3.5%. The molar shares of these two components reach 98% in total. The share of all the other combustible components, higher hydrocarbons and hydrogen, is 0.7%. The remaining 1.3% consisted of the inert gases carbon dioxide and nitrogen.

Experimental Setup

Engine tests have been performed on a Schenck Dynas bench with a Horiba STARS automation system. Figure 3 features a view of the test bench. Figure 4 shows the major measurement devices and their placement. Natural gas mass flow was measured with a Rheonik RHM 015 GNT Coriolis-type flow-meter. The associated measurement uncertainty was at 0.2%.

The combustion air provided to the engine is conditioned in terms of temperature and humidity. All tests are performed with combustion air at 24 °C and 60% of relative humidity. The intake air mass flow is measured by a hot-film anemometer ABB Sensyflow FMT700-P which guarantees a measurement uncertainty of 1%.

Measurement data are collected on two different systems:

- Crank-angle based indication using a Kistler Kibox triggered by a Kistler 2614A1 crank angle sensor. Additionally, cylinder 1 is equipped with a piezoresistive Kistler 4007B sensor in the intake and a water cooled piezoresistive Kistler 4049B10 sensor in the exhaust manifold. The Kibox derives near-real-time data from those signals which is transferred to the ECU and is used to control the spark timing, namely the centre of combustion and a cylinder-pressure derived knock index.

- Time-based data is recorded by the test bench automation system (pressures, temperatures, mass flows, feedback signals from actuators and data from exhaust gas analyzers, scalar data from the Kistler Kibox). Each analogic channel is equipped with an anti-aliasing filter; 60 seconds of measuring time are recorded with a frequency of 1Hz.

Figure 5 shows all pressure, temperature and wide-band lambda sensors mounted on the engine.

Discussion of Results

The initial step has been an extended validation of the 1D simulation on the basis of experimental measurements. These simulations have been carried out for some operating points at full load, from minimum up to maximum engine speed, as well as at part load at 2000 rpm.
With regard to the simulations at full load, the comparisons between measured data and predicted results are useful to evaluate the correct behaviour of the turbocharger group and to analyse the values of the main fluid-dynamic parameters (air mass flow, gas pressure and temperature along the duct systems, etc.).

Figures 6 and 7 show the comparison between experiments and prediction of air mass flow rate delivered by the compressor, as well as the boost pressure achieved, the latter being targeted by a PID controller. The good agreement between the measured and computed data is also due to the well captured interaction between the gaseous fuel injected into the primary ducts and the mass flow towards the cylinders. As expected, the natural gas injection points out a significant influence on the air mass flow rate, due to its high specific volume, which limits the air mass in-to the cylinder during the induction phase.

In Figures 8 it is reported the comparison between the computed and the measured air temperature after the compressor. Downstream of the compressor, the intercooler performs the cooling of the fresh charge reaching the delivery gas temperature, thanks to a PID controller set on the gas temperature. Overall, the map-based model of the turbocharger is acceptably reliable for the prediction of the fluid dynamic processes occurring in the turbine and the compressor.

About the turbocharger group, Figure 9, for the sake of completeness, shows the compression ratio as a function of the mass flow parameter, reported on the compressor map, which reports also the iso-efficiency zones. The compressor works closed to its the maximum efficiency only at high engine revolution speed, whereas at medium-low engine speed (lower mass flow parameter) the efficiency is very low. Figure 10 highlights the corresponding fluid dynamic behaviour of the turbine (the expansion ratio is reported as a function of the mass flow parameter).
In the model, the fuel mass is injected according to the experimental injection strategy fixed by ECU (in terms of mass injected per cycle and timing). In this way the corresponding in-cylinder air-fuel ratio is determined only by the local thermo-fluid dynamic conditions into the ducts and by the possible differences among the volumetric efficiency for each cylinder.

To predict realistic values of in-cylinder pressure traces, a multi-zone, quasi-dimensional combustion model [4] has been applied for the simulation of the engine, to evaluate the thermodynamic and chemical gas properties into the combustion chamber. The correct flame front velocity propagation depends on the turbulence intensity in the cylinder and on the air-fuel ratio, which define the laminar flame speed, the turbulent flame speed and, as a consequence, the correct heat release ratio. In particular, the model uses the actual spark timing (data extracted from the ECU). In Figure 11 the calculated in-cylinder peak pressure is compared with the corresponding measured value.

In Figures 12.a and 12.b the pressure trace as a function of in-cylinder volume has been reported. The diagrams related to 800 rpm and 1200 rpm at full load, show a rather good behaviour of the combustion model and also a rather good prediction of the in-cylinder pressure during the open valve period.

Once the global parameters have resulted in rather good agreement with the experimental data, the 1D model can be used to transport the chemical species along the exhaust ducts and then evaluate the conversion process through the catalysts.

Figure 13 shows the normalized NOx, CO, HC and O2 concentrations discharged by the cylinders at EVO. It is possible to notice that the trend is in rather good agreement with the measured data. In particular, the NOx trend changes, as a function of engine speed, according to the A/F ratio and the in-cylinder peak pressure. With regard to CO and HC concentrations (the latter expressed as carbon equivalent), the emission sub-models have been tuned at 1200 rpm, full load, and the same tuning values have been used for all the operating conditions. The tuning of HC has also an influence on the computed O2 concentration mainly because of its presence in the mixture stored and released by the crevices. The reason for this evident mismatch between experimental and computed HC emissions could be partly related to the fact...
that the experimental data are referred to the inlet of the ATS, whereas the computed data are referred to the composition of the gas discharged by the cylinder, just downstream the exhaust valves. Probably, in the path between the exhaust valves and the inlet of the ATS, some post-oxidation reactions could occur which, in these simulation campaign, have not been considered. Moreover, in order to justify this possible explanation, new experimental measurements have been planned. Concerning the simulations at variable load and constant regime, the comparison between computed and measured data is related to six different loads, identified as percentage of the maximum BMEP at 2000 rpm. In particular, the load percentages are the following: 25%, 35%, 45%, 55%, 65% and 75%.

In Figure 14 some typical global parameters have been reported. In particular, the computed turbocharger speed, the air mass flow rate, the BMEP and the in-cylinder peak pressure have been compared to the measured data. As can be noted, Figure 14 shows a rather good agreement between the two sets of data, pointing out the reliable prediction of the model also at partial loads.

For the same operating points at part load reported in Figure 14, the corresponding cylinder-out emissions have been computed and compared to the experimental data. Figure 15 shows the normalized CO, CO₂, NOₓ, HC and O₂ concentrations discharged by the cylinders at EVO.

The cylinder-out gas composition calculated by gasdyn is then tracked downstream of the cylinder head, along the exhaust system, thanks to the possibility of advecting the chemical species in the calculation nodes. Along the exhaust line the gas then flows through the catalytic converter where, by means of the coupling with axisuite, the heterogeneous reactions occurring on the washcoat surface are modeled.

Figure 16 shows the comparison between the measured and calculated species conversion of CH₄, CO, NOₓ and O₂ at full load, across the whole after-treatment system (ATS), considering the pre-catalyst and the main catalyst in cascade. From the analysis of the combustion process in the previous section, it appears that the exhaust gas contains both oxygen and unburned hydrocarbons due to the particularly slow kinetics of CH₄ into the cylinder. This results in a gas
composition typical of lean burn conditions where O₂ is present, even if the engine feeding condition was slightly rich.

The catalytic converters adopted in this exhaust system are typical TWC for SI engines. Despite the geometrical parameters of the three catalysts where fully known, the chemical composition of their washcoats was guessed on the basis of typical catalyst properties, since the manufacturer has not provided complete information about them. Therefore, these devices have been modelled exploiting the pre-defined chemical libraries of *axisuite* for the simulation of three-way catalysts. In particular, the set of reaction that have been considered are the following ones:

1. CO + 0.5 O₂ → CO₂
2. H₂ + 0.5 O₂ → H₂O
3. CH₄ + 2 O₂ → CO₂ + 2 H₂O
4. CO + NO → CO₂ + 0.5 N₂
5. H₂ + NO → H₂O + 0.5 N₂
6. CH₄ + H₂O → CO + 3 H₂
7. CO + H₂O ↔ CO₂ + H₂

Additionally, the submodel of oxygen storage has been considered to account for eventual fluctuation of the cylinder feeding conditions. As can be seen in Figure 16, the oxygen contained in the gas stream is completely consumed at every operating condition. This is due to the presence of CO, ceria oxides (in the washcoat) and to the presence of CH₄, which are competing towards the oxygen. These oxidation reactions appear to be important in the first part of the ATS along with the reduction of NOₓ consuming CO.

The comparison with the measured data shows that the calculations can predict the conversion efficiency of CH₄ and NOₓ, whereas the conversion of CO from suffers the uncertainty about the washcoat composition, which should condition the balance between water gas shift reaction, methane steam reforming and the oxidations. The steam reforming seems to prevail at high temperature, explaining why the efficiency of the CO abatement decreases with the engine speed. With this reaction further CO is produced and not oxidized due to the absence of oxygen.

To better understand the impact of every single reaction, in Figures 17 and 18 the concentration of CO, NO and CH₄ (normalized with respect their values at the inlet) along the axial coordinate of the precat and maincat are plotted for the case at 2400 rpm full load. It is possible to see that in the precat (Figure 17) the oxygen is captured by the ceria oxides which are creating the reducing environment to promote the reaction between CO and NO.

The methane is then oxidized by the small amount of oxygen which is contained in the gas stream. Conversely, in the main catalyst the methane appears follow the steam reforming path which generates CO and H₂[16,17]. This can be seen by the increase of the carbon monoxide, which explain the low abatement efficiency of CO along the ATS (see Figure 18). Figure 19 shows the comparison between the calculated and measured fluid dynamic quantities. In particular, the gas temperature at the inlet of the ATS is reported, showing that the model can correctly predict the heat transfer in the pre-turbine exhaust manifold and the expansion of the gas through the turbine. A correct prediction of the gas temperature is important to
evaluate the volumetric flow at the inlet of the ATS and therefore the pressure loss caused by the resistance of the substrate. Moreover, the comparison between the measured and calculated gas temperature shows that there is an overestimation of the temperature level. Since this temperature reflects the chemical activity of the catalysts, it can be explained by the overestimation of the CO oxidation reaction.

Conclusions

In this paper the application of an integrated approach based onto a strict numerical coupling between the gasdyn and axisuite codes has been proposed, with the main goal of allowing the detailed simulation of engine performance based on 1D unsteady models with a detailed simulation of chemical reactions in the after-treatment devices. To this purpose the authors have developed an original strategy to couple a code based on the unsteady formulation of the conservation equations (gasdyn), necessary to capture the wave action in the ducts and to estimate the engine performance, to a steady state approach for the simulation of after-treatment systems (axisuite). The strategy makes possible the continuous transfer of information between the models at synced time steps, due to the difference of the time marching procedure of the codes. The numerical approach has been tested on an industrial case: a 4-cylinder, spark ignition, CNG fuelled heavy duty engine. Several operating conditions at partial and full load, for different engine revolution speeds, have been simulated, showing that the global engine performance parameters can be predicted with fairly good accuracy as well as cylinder-out emissions. The coupling strategy has proved to be successful, allowing the flow unsteadiness to propagate along the system, while advecting the chemical species from the engine head to the tailpipe outlet, through the catalytic converters. The calculated results have shown that, by this coupling, it is possible to predict the abatement of chemical species such as CH₄, NO and CO inside catalytic converters placed in cascade configuration. The agreement with the measured abatement efficiency has shown that the matching is fairly good overall, with the exception of the CO caused by the lack of information about the formulation of the washcoats.

References


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