Diesel efficiency improvement with Particulates and emission Reduction

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Project partners:
1 - AVL - AVL List GmbH - AT
2 - REN - Renault SAS - FR
3 – IFP – Energies nouvelles – IFPEN – FR
4 - CMT - Universitat Politecnica de Valencia – ES
5 - JM - Johnson Matthey Plc - UK
6 – CONTI – Continental Automotive France SAS – FR
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Publishable Executive summary

The objective of the task 4.5 is to complete the research and development of the rest of partners in order to model the engine emissions in transient operation. With this purpose, a platform for engine simulation available at CMT Motores Térmicos (Virtual Engine Model -VEMOD-) has been completely refined and adapted to perform an assessment of different strategies at cold and low pressure ambient conditions as the main objective of this task.

Task 4.5 includes three main subtask (not explicitly named in the proposal):

- 4.5.1: Submodels refinement, integration and tuning for fast simulation of engine transients.
- 4.5.2: Calibration of engine model for the engine demonstrator.
- 4.5.3: Projection of vehicle emissions to high altitude and low temperature operation conditions.

As scheduled, this report covers the two first subtask that have been performed by CMT, with the collaboration of Renault for the engine calibration.

In the framework of subtask 4.5.1 and 4.5.2, the integrated Virtual Engine Model (VEMOD) has been rebuilt as a standalone tool to simulate new standard testing cycles. The VEMOD is based on a wave-action model that carries out the thermo-and fluid dynamics calculation of the gas in each part of the engine. In the model, the engine is represented by means of 1D ducts, while the volumes, such as cylinders and reservoirs, are considered as 0D elements. VEMOD includes different sub-models that have been refined and/or adapted to retain the main physics of the most relevant phenomena whilst providing fast response for accurate simulation of engine fast transients (boosting and EGR behaviour) and low transient (engine warm-up) cycles. The improvements carried out deals with the following:

- **1D/0D thermo-and-fluid dynamic**: it is the core or the simulation and most of the calculation time is due to this subsystem, thus the numerical method for solving the physical equations has been modified from finite differences to finite volumes. This numerical technique is extremely conservative so big mesh size can be used to reduce computation time from the original 50 times slower than real time to the current 10 times slower than real time. Also the model has been improved through the identification and quantification of water condensation at different engine elements, key issue during cold starting. Finally, the blow-by model, used to evaluate the gas leakage and to set the boundary condition for the friction calculation in the piston, has been reviewed to consider the effect of ambient conditions.

- **Virtual injector**: the main input for the combustion model is the injection rate, thus a new simple injection model to reproduce the actual injection rate has been included in VEMOD. The model simulates the instantaneous fuel injection based on straight part that takes into account the initial and final transient periods and the steady state part in long injections.

- **Combustion and emissions** formation models: **combustion** process is calculated based on the Apparent Combustion Time (ACT) 1D model [1], responsible for the prediction of the rate of heat release and NOx formation. ACT is a mixing controlled combustion model that has been improved with a CFD-based correction of the transient processes at SOI and EOI. Thus, during quasi-steady conditions, a physical approach based on turbulent gas jet theory is used to calculate the air entrainment in each fuel parcel injected. During the transient process at the start/end of injection a parameterized correction based on CFD calculations is applied. The ignition delay model, which is based in the Shell model, tracks the Livengood & Wu [2] integral accounting for the instantaneous thermodynamic conditions and the local composition. It has been upgraded to make it more suitable for low T conditions. Finally, the premixed combustion is reproduced by means of an empirical model based on the propagation velocity of a premixed flame. Regarding the **emissions**, in the case of NOx a physical (chemical) approach is applied, considering all the relevant mechanisms for NOx formation (thermal or Zeldovich, prompt and via N_2O) and reduction (reburning mechanism, relevant at high EGR rates and F/A ratios). In order to reduce the computation time, the model is implemented in a computational efficient way by means of tabulated chemistry. For the rest of pollutants (soot, CO and UHC emissions), which fundamentals are unclear and/or affected by many local phenomena, an Artificial Neural Network (ANN) approach has been used to determine them.

- In order to predict tailpipe pollutant emissions to the ambient, different **aftertreatment** systems models have been upgraded (DOC, DPF) or completely developed (SCR y LNT) to reproduce the behavior of the devices in the exhaust system. Thus, the DPF model have been improved to consider PSD variation due to filtration, DOC model considers UHC accumulation and SCR and LNT have been included in VEMOD. Main physical/chemical processes taking place in each EATS element are approached to be solved based on a lumped model approach.

- **Heat transfer** (HT) model in VEMOD is based on lumped conductance models (engine block, ducts and turbo) to take into account the heat transferred between the different fluids of the engine (gas and liquids –coolant and oil-). Thus, the lumped conductance model allows linking in-cylinder, port and turbocompressor processes with hydraulic circuits through the heat rejection calculation: 0D in-cylinder model, 1D ports model and 0D turbo and compressor models provides boundary conditions of gas temperature and heat transfer coefficient to calculate heat flux, while the nodal model provides detailed wall temperature and heat transfer repartition to coolant and oil circuit. The model has been improved to include the oil-coolant heat exchange through the block, the thermal inertia of liquids (coolant and oil) and the metal heating, all of them key issues during transient operation starting from cold conditions. Finally, the model has been adapted to evaluate different thermal management strategies with split cooling system (independent coolant circuit in the cylinder-head and block).

  Being the heat transfer in the chamber the main source of heat rejection, it is a critical issue during the operation in cold conditions such as that in the WLTC after the engine start at -7ºC. With the aim of assessing the validity of the VEMOD HT model, a critical review of convective HT models has been carried out. The main conclusion found is that the influence of room temperature on the heat transfer fitting coefficient is smaller than engine speed influence, and hence there is no evidence that the Woschni-based HT model of VEMOD is not valid for both hot and cold environment conditions.

- The VEMOD includes **coolant and lubricant circuits** linked, on the one hand, with the engine block and the turbocharger through heat transfer lumped models; and on the other hand with the engine heat exchangers. The hydraulic models have been upgraded to include all the required heat exchangers (gas-liquid, liquid-liquid…) and the effect of the vehicle velocity on the radiator. Also hydraulic circuit model has been modified in order to consider split cooling in combination with the lumped conductance model.

- An existent dedicated **friction and auxiliaries** model [7] has been included in VEMOD to obtain the brake power starting from indicated power. Friction losses (piston pack, bearings and valve train) are calculated taking into account the instantaneously lubrication regime, kinematics and dynamics of the mechanisms. Specific upgrade to consider rolling cam follower in the valve train and oil viscosity at low temperatures (up to -35ºC) have been carried out. Auxiliaries system has been considered in a simple way, taking into account the power to drive fuel, coolant and oil pumps.

- A **control system** emulating the ECU along with a vehicle and driver models allow completing the engine simulation tool. On the one hand the control system has been upgraded to include all the necessary sensors (torque, mass flow, p and T in pipes…) and actuators (EGR, swirl valves, turbine position, engine speed, injection settings…) in order to simulate both stationary and transient tests (WLTP…) by considering different engine settings and operations modes. Thus, the VEMOD is now able to reproduce experimental conditions by imposing measured settings and engine speed (no vehicle is considered) or a fully predictive evolution where the vehicle is considered and the setting are taken from the calibration tables in the virtual ECU in order to follow a track.

After the VEMOD upgrading, sub-model geometry was adapted to the characteristics of the specific engine and the properties of different elements (turbocharger maps, pump curves, thermostat settings, heat exchangers efficiencies, virtual ECU calibration…) were set according to the information provided by Renault or specific tests performed at CMT. The calibration of the model was performed in steady state operating condition using experimental results at different operating points and ambient temperature conditions (from -7ºC to 25ºC). When possible, the sub-models were calibrated independently of the rest:

- The injector model was calibrated with a complete experimental matrix in an injector test rig.
- Aftertreatment models were calibrated (and validated) in stand-alone executions in against experimental data.
- The friction model calibration, aimed at obtaining an accurate prediction of the brake efficiency, was performed with stationary operating points in the complete engine map both at cold and hot ambient conditions.
- Heat tranfer model calibration was performed by means of a methodology developed at CMT in which a combination of experimental and simulated in-cylinder cycles in motoring and combustion tests allows obtaining the heat transfer model constants.

In the case of the combustion model (and hence emissions sub-models that are directly dependent on it) a dedicated calibration was performed after the heat transfer model calibration, which affects the experimental heat release (main input for the combustion model).

After the calibration of the different models, the complete VEMOD has been validated with experimental tests using steady and WLTC tests. The result showed that key variables were well predicted during WLTC such as engine torque (ε=2 %), turbine outlet temperature (ε=6 %), CO_2 emissions (total cumulated $\varepsilon < 1$), and NOx with a good performance during the WLTC cycle except at the last part (high load and speed) having a mean error of 14 %.

Dissemination of the project results:

1. Martin, J., Arnau, F., Piqueras, P., and Auñon, A., "Development of an Integrated Virtual Engine Model to Simulate New Standard Testing Cycles," SAE Technical Paper 2018-01-1413, 2018, doi:10.4271/2018-01-1413.
2. Broatch, A., Olmeda, P., Martin, J., and Salvador-Iborra, J., "Development and Validation of a Submodel for Thermal Exchanges in the Hydraulic Circuits of a Global Engine Model," SAE Technical Paper 2018-01-0160, 2018, doi:10.4271/2018-01-0160.
3. Payri, F., Arnau, F.J., Piqueras, P., and Ruiz, M.J., "Lumped Approach for Flow-Through and Wall-Flow Monolithic Reactors Modelling for Real-Time Automotive Applications," SAE Technical Paper 2018-01-0954, 2018, doi:10.4271/2018-01-0954.

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