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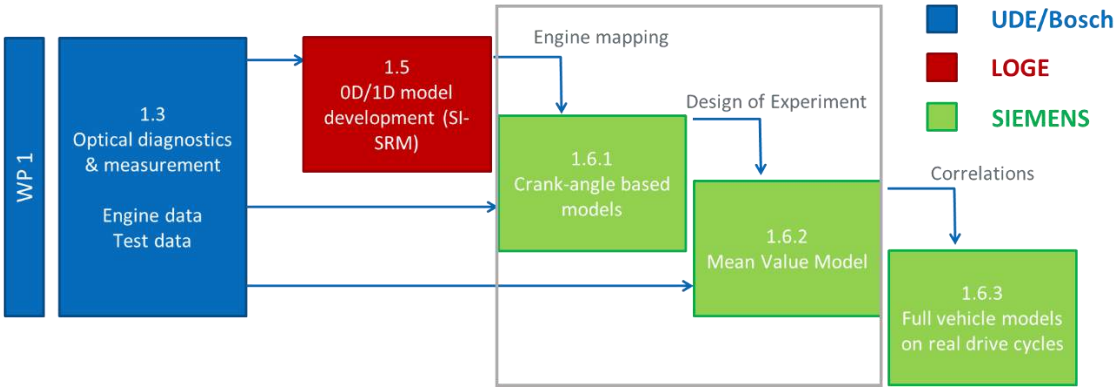
Summary

In the framework of the PaREGEn project, Siemens aims to investigate and develop modelling capabilities and associated methodologies in order to leverage the findings and results obtained by partners in Work Package 1 (WP1, Advanced Combustion Technologies) lead by BOSCH. Indeed, most of the WP1 activities are related to comprehensive research, testing and modelling activities toward the measurement and understanding of the root cause of soot formation plus the development of a locally complex modelling approach. In this context, Siemens wants to offer a way to extend the range of the investigation, from a local perspective (at the level of the cylinder) to a system perspective (at the vehicle level). The final goal of the PaREGEn project is to demonstrate the value of the developments in demonstrator cars from JLR and DAIMLER, evaluated on real driving cycles. Hence, it makes sense to apply the same kind of approach by simulation, meaning that the modelling approaches developed during the project can be implemented in full vehicle models to give an evaluation of the emissions and soot within virtual environments.

The report D1.4 presents the Siemens activities in Tasks 1.6.1, entitled "Phenomenological high frequency to mean value models", and an introduction to the Task 1.6.2, "Correlated mean value models". The connection of these tasks with the rest of the works in WP1 is illustrated in the figure below.



From this, the present report is focused on the modelling activities by Siemens extending the scope of the analysis from the combustion itself, to a single-cylinder approach and then onto the reduction of the phenomenological models into a Mean Value Engine Model (MVEM). This later approach is the most convenient option for a further integration of the engine model including its air path system, in a full powertrain and vehicle model, mainly due to the reduced simulation times. The actual work on the multi-cylinder engine modelling and integration in a vehicle context is the purpose of the Task 1.6.3 to be completed by Siemens during the second half of the project.

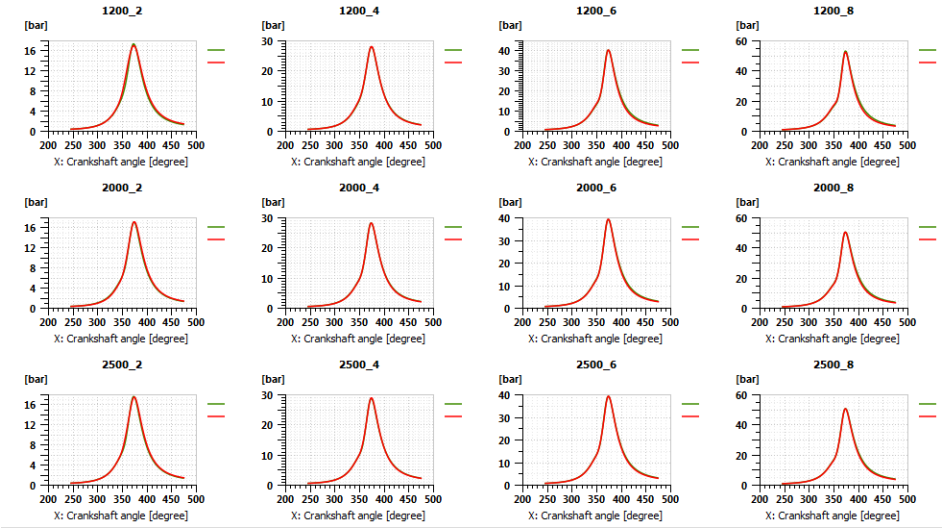
The workflow proposed, developed and illustrated by Siemens in the D1.4 report is the following:

- Develop phenomenological crank-angle based models and methods to address the simulation of the combustion heat release
- Develop phenomenological crank-angle based models and methods to address the simulation of a single-cylinder engine in combination with a prediction of engine-out emissions thanks to an interface with LOGE's Spark-Ignited Stochastic Reactor Model (SI-SRM)
- Develop a methodology to reduce the phenomenological crank-angle based model to a Mean Value Engine Model

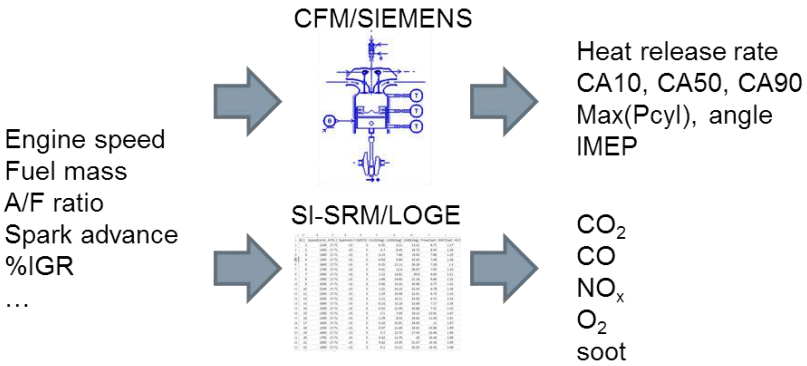
The research and modelling activities conducted by Siemens in collaboration with LOGE are structured around a common application case. This corresponds to a single-cylinder research engine set-up by BOSCH. The engine and component characteristics, including geometry as well as its control, are well known. This corresponds to a direct injection, spark ignited and homogeneous combustion application. In practice, a test

data set composed of 12 operating points, covering various engine speeds from 1200 to 2500 rpm and loads between 2 and 8 bar IMEP, is used for the modelling and validation tasks.

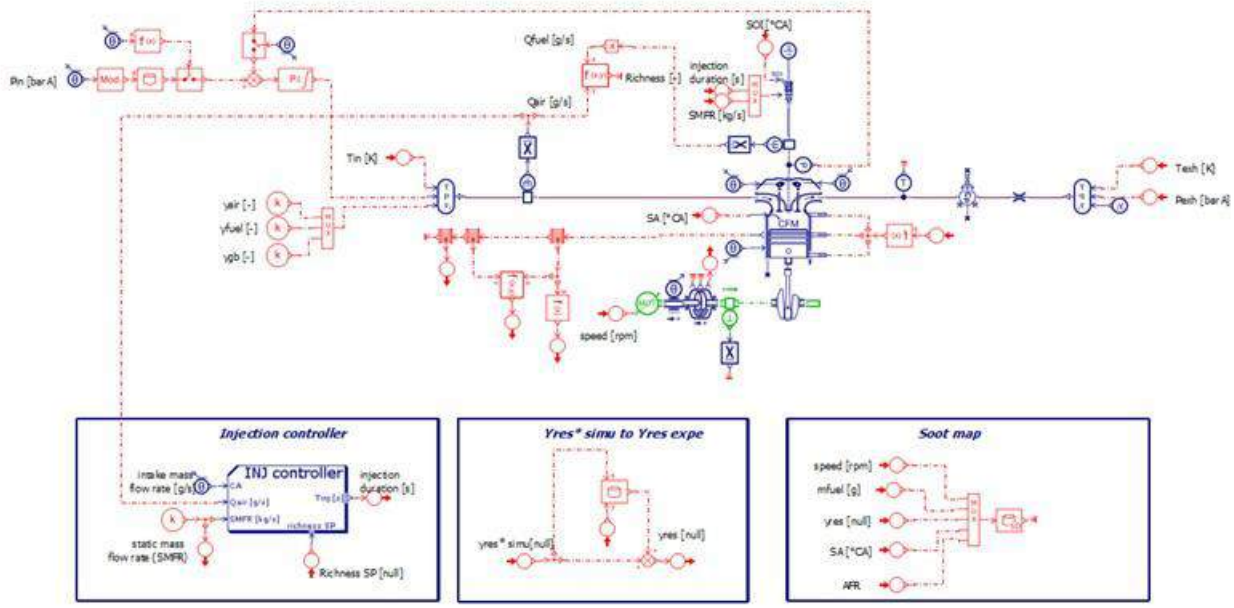
The first activity of Siemens is related to the set-up of a phenomenological combustion model based on the CFM (Coherent Flame Model) in order to predict accurately the combustion heat release for various boundary and initial conditions. A validation is performed on the 12 reference operating points and illustrated in the plots below, comparing simulated (red) and measured (green) pressure traces for various engine speed and loads.



Then, a coupling strategy with the engine-out and soot models is developed based on the principle given in the figure below. A parallel approach is retained after an evaluation of the possible options. The differences in the approaches by LOGE and Siemens in terms of the modelling and calibration strategy raises some technical difficulties for interfacing the two models. Some solutions are investigated and implemented by Siemens in order to ensure consistency of the data shared at the interface.

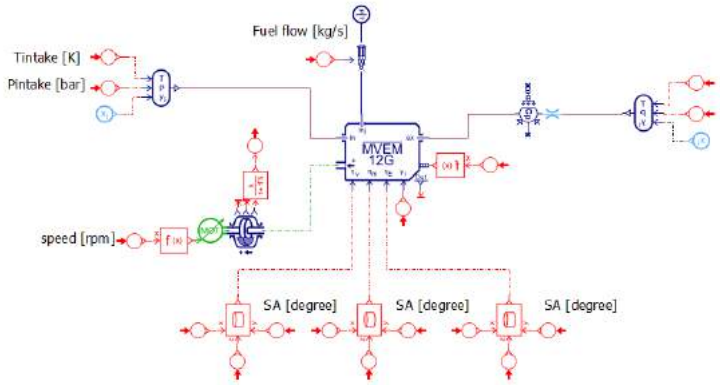


A representation of the reference single-cylinder engine model resulting from the Siemens activities is presented below. It includes the phenomenological combustion model (CFM) and the map-based model for the emissions by LOGE.



Once again, the 12 reference operating points are used to validate the retained options and the developed model. The single-cylinder engine model is fully capable of predicting the heat release and pollutant emissions for varying engine speeds, manifold conditions, equivalence ratios and spark timings.

The last step is dedicated to the reduction methodology. Starting from the reference phenomenological model, the purpose is to generate the right data to feed an equivalent Mean Value Engine Model, which would enable faster simulation (a factor 1000 is observed at this stage) toward the method's final implementation in larger vehicle models. The resulting model uses the same boundary conditions and controls as the reference model, as shown below. The same interface is set-up with the map-based pollutant model, for a prediction of the NO_x and soot in particular for various operating conditions.



The validation is again done based on the 12 reference operating points, completed by parameter sweeping in order to assess the quality of the model outputs in terms of NO_x and soot emissions.

These activities, conducted by Siemens during the first part of the project, will be extended towards the implementation of an air path system model, and the integration of the engine in a full vehicle model which includes a driver model. The final goal is to develop a demonstrator for a vehicle model including the soot model developed in WP1, evaluated over realistic driving cycles.

Contents

1 Introduction 8
1.1 Contribution in PaREGEn 8
1.2 Methodology 8
1.3 Data used for the modelling and validation tasks 9
2 Methods and results 10
2.1 In-cylinder process simulation 10
2.1.1 Heat release modelling 10
2.1.2 Simulation using SI-SRM and investigation of possible interfaces 17
2.2 Single-cylinder simulation 24
2.2.1 Modelling approach, definition of the boundary conditions and injection 24
2.2.2 Physical consistency using imposed mean manifold conditions 25
2.2.3 Iterative calibration process for the CFM 27
2.2.4 Results of the single-cylinder model 28
2.2.5 Direct interface with LOGE data using map based model 31
2.3 Reduced Mean Value Engine Model 33
2.3.1 Introduction to the MVEM 33
2.3.2 Introduction to the migration workflow 35
2.3.3 Application of the methodology for the PaREGEn project 36
3 Discussion and Conclusions 39
3.1 Discussion and future works 39
3.2 Conclusion 39
4 Deviations and Risks 40
4.1 Deviations 40
4.1.1 Description of work related to deliverable in GA Annex 1 – Part A 40
4.1.2 Time deviations from original planning in GA Annex 1 – Part A 40
4.1.3 Content deviations from original plan in GA Annex 1 – Part A 40
4.2 Risk Register 40
5 References 41
Appendix A – Acknowledgement 42
Appendix B – Quality Assurance 43
Abbreviations and Nomenclature 44

Figures

Figure 1-1 Interface of the Siemens activities in WP 1. 8
Figure 1-2 Level of model addressed by Siemens in PaREGEn and illustrated in the report. 9
Figure 1-3 Research engine mapping on the dyno (12 operating points). 9
Figure 2-1 The Coherent Flame approach. 10
Figure 2-2 Definition of the mean flame surface. 11
Figure 2-3 Mean flame surface evolution, assuming a pancake geometry for the combustion chamber. 11

Figure 2-4 Calibration process applied for the CFM model set-up. 12
Figure 2-5 Results of the CFM model for the 12 operating points (red = simulation, green = measure). 14
Figure 2-6 Details for the point 1200 rpm, 2 bar (red = simulation, green = measure). 14
Figure 2-7 Initiation of the combustion, point 1200 rpm, 4 bar (red = simulation, green = measure). 15
Figure 2-8 Tumble and cut-off maps from the CFM calibration (3 curves for engine speed 1200, 2000 and 25000rpm) 15
Figure 2-9: Concept of modelling the mean representative mixing time for the SI-SRM simulations of spark-ignited engines with port injection. 19
Figure 2-10: Visualization of the flame surface described using a set of nodes at regular angular intervals. 20
Figure 2-11 Methodology for engine mapping with the SI-SRM. 21
Figure 2-12 Interface using a parallel modelling approach for heat release & emissions. 22
Figure 2-13 Interface using a two steps modelling approach for heat release & emissions. 22
Figure 2-14 Comparison between measurement (yellow) and SI-SRM results (blue) for the CA50. 22
Figure 2-15 Emission table for CO_2 (humid basis) generated by Siemens. 24
Figure 2-16 Single-cylinder engine model in Simcenter Amesim. 24
Figure 2-17 Measured pressures imposed at the valves vs at the boundaries of a CFD1D model (red = CFD1D model) 26
Figure 2-18 Impact of the modelling of the boundary conditions on the in-cylinder process simulation (red = reference model). 27
Figure 2-19 Updated calibration process applied for the single-cylinder model set-up. 28
Figure 2-20 Results of the single-cylinder model for the 12 operating points (red = simulation, green = measure). 28
Figure 2-21 Impact of the residual gas content on the combustion heat release (Yres = 0.1, 0.15, 0.2). 29
Figure 2-22 Results for the exhaust temperature by the SI-SRM model. 31
Figure 2-23 Simple conversion function from simulated *Yres** to the values used as input of the SI-SRM model *Yres*. 31
Figure 2-24 Final single-cylinder model including estimation of combustion heat release and emissions (blue circle). 32
Figure 2-25 Validation of the NO_x emissions by comparing the test data vs SI-SRM (left) and single-cylinder engine model (right). 32
Figure 2-26 Soot emissions for various equivalent ratios at 2000 rpm, 6 bar IMEP. 33
Figure 2-27 Soot emissions in rich conditions (equivalent ratio = 1.2) as a function of IMEP, 2000 rpm. 33
Figure 2-28 Cylinder energy balance in the MVEM. 34
Figure 2-29 Migration from a crank-angle resolved model to a Mean Value Engine Model. 35
Figure 2-30 Migration workflow by the MVEM tool. 36
Figure 2-31 Control of the single-cylinder engine model. 36
Figure 2-32 Control of the MVEM equivalent model. 37

Tables

Table 1-1 Signals measured on the research engine. 10
Table 2-1 Comparison of the estimations of the residual gas content (Siemens vs engine dyno). 13
Table 2-2 Validation of the CFM for the prediction of the pressure peak (engine dyno vs simulation). 16
Table 2-3 Validation of the CFM for the prediction of the peak pressure angle (engine test vs simulation). 16
Table 2-4 Validation of the CFM for the prediction of indicated mean effective pressure (engine test vs simulation). 16
Table 2-5 Validation of the CFM for the prediction of the timing for 50 % fuel burned “CA50” (engine test vs simulation). 17
Table 2-6 Inputs and outputs of the SI-SRM model for engine mapping. 21
Table 2-7 Comparison of the estimations of the residual gas content (Siemens vs engine dyno). 29
Table 2-8 Results for the single-cylinder engine model. 29
Table 2-9 Results for the intake mass flow rate. 30

Table 2-10 Results for the exhaust temperature. 30
Table 2-11 Outputs of the single-cylinder engine model for data processing. 36
Table 2-12 Comparison between the MVEM and reference model for the IMEP production. 37
Table 2-13 Comparison between the MVEM and reference model for the air mass flow rate. 37
Table 2-14 Comparison between the MVEM and reference model for the exhaust temperature. 38

1 Introduction

1.1 Contribution in PaREGEn

The report D1.4 reflects the activities conducted by Siemens in collaboration with LOGE and other partners in Work Package 1 (Advanced Combustion Technologies) of the PaREGEn project, towards the development of modelling capabilities for a multi-level approach to emissions simulation with a special focus on particulate matters. Indeed, starting from the work, findings and data generated through Tasks 1.1 to 1.5, related to the development of innovative soot measurement tools and comprehensive 3D simulation approaches, Siemens is in charge of the research and development of modelling strategies to extend the scope of the analysis, from a local perspective to a system approach. The main goal of Siemens in the PaREGEn project is to develop modelling approaches and methodologies in order to be able to support investigations, not only at the level of the cylinder but also at the engine level and finally at the vehicle level. The final target is to support the evaluation of soot emissions in vehicles running on real driving cycles. Thus at the end, the resulting modelling approach would be put in perspective of the testing activities conducted for the evaluation of the demonstration cars at the end of the project.

The present report covers the Task 1.6.1, entitled “Phenomenological high frequency to mean value models” and gives an introduction to the Task 1.6.2, “Correlated mean value models”. The connection of these tasks with the rest of the work in WP 1 is illustrated in Figure 1-1.

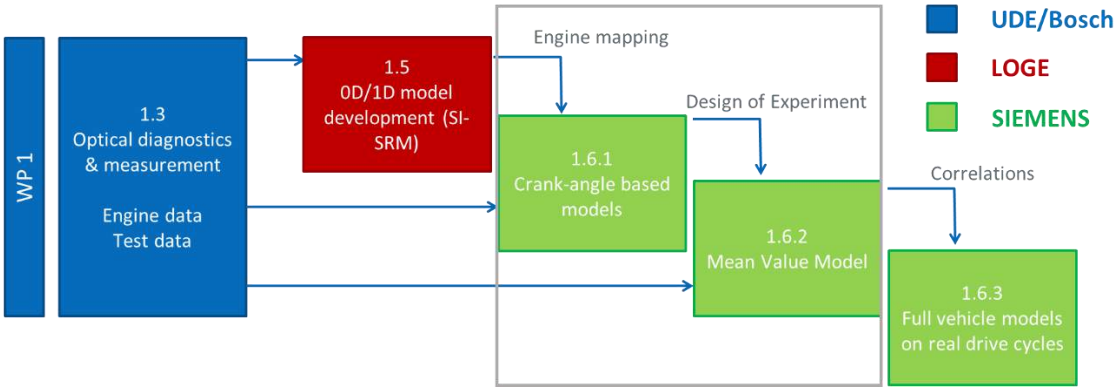


Figure 1-1 Interface of the Siemens activities in WP 1.

1.2 Methodology

The methodology applied by Siemens for the PaREGEn project, see Figure 1-2, relies on a general workflow, supported by its commercial software Simcenter Amesim™ [1] [2] completed with new methodologies and with the set-up of an interface with the LOGEengine software from LOGE for the evaluation of emissions including soot. This interface ensures consistency of the Siemens model capabilities for soot emissions with the developed data and models by BOSCH, EDU, ETH and LOGE.

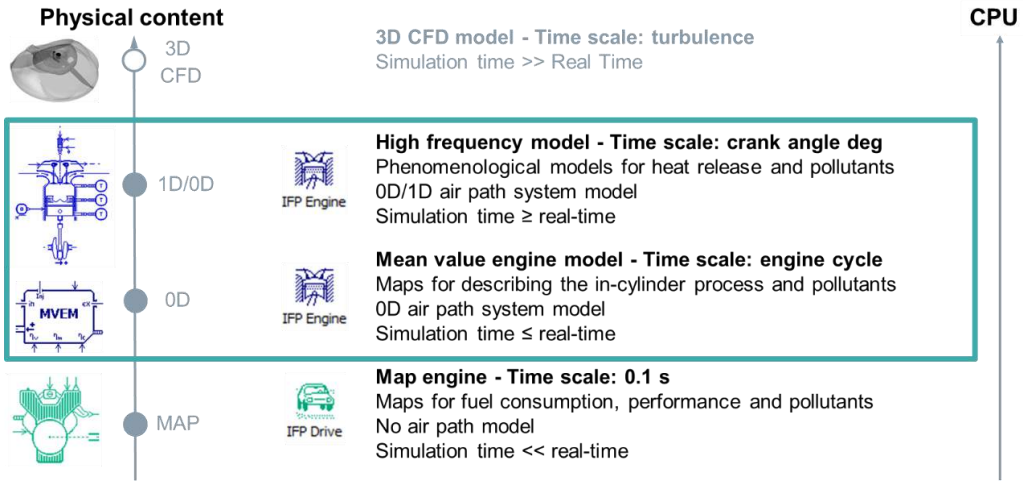


Figure 1-2 Level of model addressed by Siemens in PaREGEn and illustrated in the report.

The workflow proposed by Siemens is the following:

- Develop phenomenological crank-angle based models and methods to address the simulation of the combustion heat release in the context of the activities conducted by partners in WP1
- Develop phenomenological crank-angle based models and methods to address the simulation of a single-cylinder engine in combination with a prediction of engine-out emissions thanks to an interface with SI-SRM
- Develop a methodology to reduce the phenomenological crank-angle based model to a Mean Value Engine Model

This workflow is reflected in the structure of the present document which details each step in the following chapters. This workflow mentioned above will be completed within the PaREGEn project by the following extensions through the Tasks 1.6.2 and 1.6.3 for “Driving emission prediction capabilities”:

- Coupling of the MVEM with an air path system model,
- Integration of the full engine model in a vehicle model evaluated on a RDE compliant driving cycle.

1.3 Data used for the modelling and validation tasks

The research and modelling activities conducted by Siemens and LOGE are structured around a common application case. This corresponds to a single-cylinder research engine set-up by BOSCH. The engine and component characteristics including geometry as well as its control, are well known. This corresponds to a direct injection, spark ignited and homogeneous combustion application. In practice, a test data set composed of 12 operating points, covering various engine speeds from 1200 to 2500 rpm and loads between 2 and 8 bar IMEP, is used for the modelling and validation tasks, see Figure 1-3.

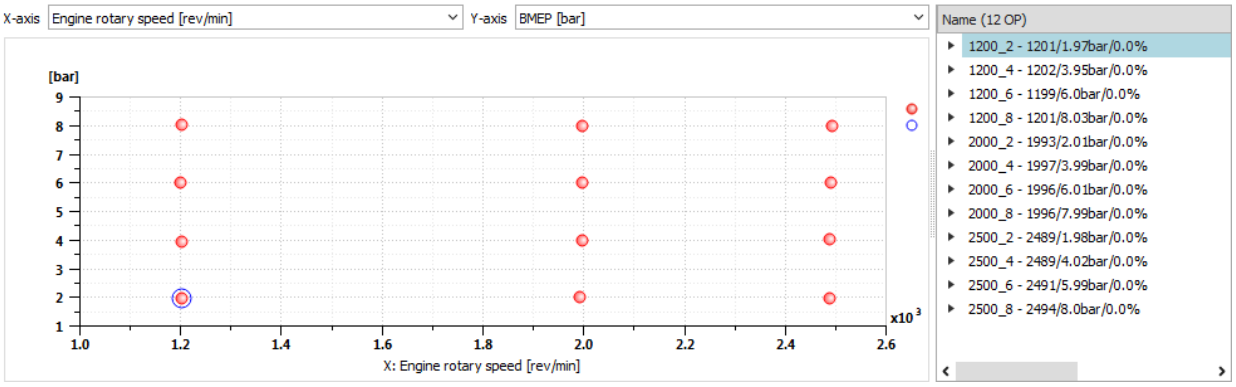


Figure 1-3 Research engine mapping on the dyno (12 operating points).

The signals available from the engine dynamometer and used for the modelling and validation activities are listed in Table 1-1.

Table 1-1 Signals measured on the research engine.

Signal	Unit	Comment
T_intake	°C	Mean value
T_exhaust	°C	Mean value
p_intake	mbar	Mean value and crank-angle resolved
p_exhaust	mbar	Mean value and crank-angle resolved
P_cylinder	bar	Crank-angle resolved
engine speed	rpm	Mean value
lambda	-	Mean value
m_air	kg/h	Mean value
m_fuel	mg/stroke	Mean value
start of injection	°CA (crank-angle)	Control
duration of injection	ms	Control
ignition angle	°CA	Control
internal EGR rate	%	Estimation
IMEP	Bar	Mean value
Emissions (CO, CO_2, O_2, HC, NO_x and PN)	% or ppm	Mean value

The same test database is used by Siemens and LOGE for their respective investigations in order to ensure consistency during the software interface development activities.

2 Methods and results

2.1 In-cylinder process simulation

2.1.1 Heat release modelling

Introduction to the CFM model

The Coherent Flame Model (CFM) is based on the 3D CFD ECFM (Extended Coherent Flame Model) model implemented in 3D CFD codes [3]. The CFM is a combustion model dedicated to the flamelet combustion regime. This approach is well adapted to premixed and partially premixed combustion processes, which represent the main oxidation mechanisms in SI engines. As presented in Figure 2-1, the CFM formalism distinguishes two zones: fresh and burned gases, which are separated by a flame front propagating from the burned gases towards the fresh gases mixture. Chemical reactions of fuel oxidation occur in the flame front, which is a very thin layer compared to all scales of the turbulent flow.

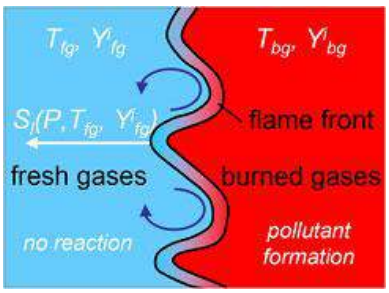


Figure 2-1 The Coherent Flame approach.

The different equations of the model written for 3D simulations were simplified following quasi-dimensional hypothesis to obtain a 0D phenomenological model called the CFM-1D model, as it accounts for the 1D radial propagation of the flame [4]. This reduction of the 3D model is based on several assumptions:

- Both fresh and burned gases are considered as ideal gases
- The mixture composition and temperature are considered as homogeneous in each zone (fresh and burned gases)
- The pressure is the same in the two zones.

To describe the combustion process, the gas in the combustion chamber is described as a mixture of three gases (fuel, fresh air and burned gases). The heat release rate, $\frac{dQ_V}{dt}$, is written as:

$$\frac{dQ_V}{dt} = PCI \,.\, \dot{w}_F,$$

where PCI is the fuel heating value [J/kg] and $\dot{w}_F$ is the rate of fuel consumption [kg/s]. Following the CFM formalism, the rate of fuel consumption depends on the flame surface, S_f, and the fresh gases properties:

$$\dot{w}_F = \rho_{fg} Y_{fg}^f U_l S_f,$$

where ρ_{fg} is the fresh gases density, Y_{fg}^f is the fuel mass fraction in the fresh gases and U_l is the laminar flame speed computed using a given experimental correlation. The fresh gas temperature is obtained using a 0D equation for the fresh gas enthalpy [5]; this temperature allows computing the laminar flame speed according to Metghalchi and Keck's correlation [6]. The flame surface, S_f, see Figure 2-2, is written as the product of a mean surface, S_m, and the flame front wrinkling, Ξ:

$$S_f = \Xi . S_m.$$

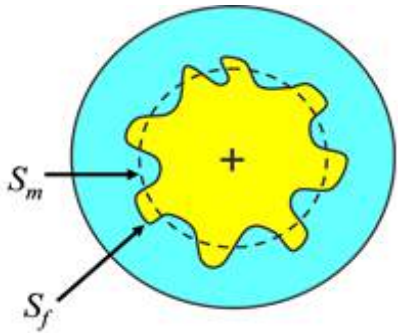


Figure 2-2 Definition of the mean flame surface.

As a first approximation, S_m is computed assuming a spherical flame propagating in a "pan-cake" geometry and which progressively becomes cylindrical when reaching the piston and the cylinder head walls, Figure 2-3.

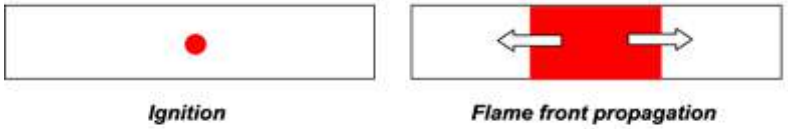


Figure 2-3 Mean flame surface evolution, assuming a pancake geometry for the combustion chamber.

The actual geometry can also be taken into account but that option was not retained for the project activities. A flame wrinkling correlation obtained by reduction of the 3D CFD equation for the flame surface density [7][8] is used:

$$\frac{1}{\Xi}\frac{d\Xi}{dt} = f\left(u', l_t, \tau, U_l, \delta_l, r_{bg}, C_w\right),$$

where l_t is the integral length scale, $\tau = \rho_{fg}/\rho_{bg}$ is the thermal expansion rate, δ_l is the laminar flame thickness, r_{bg} is the current mean radius of burned gases, and C_w is a modelling constant.
Hence, the velocity fluctuation $u' = \sqrt{2/3k}$ must be computed. Accordingly, turbulence computation is required to have access to the turbulent kinetic energy, k.
A 0D turbulence model is used to compute the turbulent kinetic energy, k, which is here correlated to the dissipated kinetic energy, $E_{kin,diss}$:

$$k = C_{turb}.\frac{E_{kin,diss}}{m},$$

where m is the mass in the cylinder and C_{turb} is a modelling constant. $E_{kin,diss}$ is computed using the kinetic energy in the combustion chamber, E_{kin} , according to the following equation:

$$\frac{dE_{kin,diss}}{dt} = \frac{dE_{kin}}{dt} - C_{diss}.E_{kin,diss},$$

with C_{diss} as a modelling constant. Finally, the evolution of the kinetic energy is obtained assuming a linear decrease of the tumble motion from the intake valve closure (IVC) to the top dead center (TDC) by using the following expression:

$$\frac{E_{kin}}{dt} = \frac{1}{8}.m.\omega_{eng}^2.\left[h^2.\frac{dN_{tumble}}{dt} + 2.N_{tumble}.h\frac{dh}{dt}\right],$$

with h the distance between the piston and the cylinder head [m], ω_{eng} the engine speed [rad/s] and N_{tumble} the tumble number at IVC [-].

Calibration process
One generally tunes the combustion chamber model using a simple scheme with the valves closed. It implies that only the compression and combustion strokes are simulated during this initial fitting stage. An overview of the developed calibration process is given in Figure 2-4.

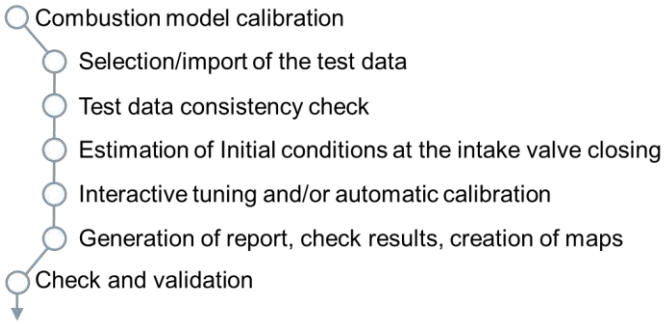


Figure 2-4 Calibration process applied for the CFM model set-up.

From this, the proper initial conditions must be defined at IVC, in terms of pressure, temperature and gas composition. The pressure at IVC can be directly gathered from the measured crank-angle resolved pressure trace. The mass of fuel and air is known from the test data as well. The main difficulty at this stage is to evaluate the residual gas content which corresponds to the amount of burned gas in the chamber at IVC. Indeed, this is a variable that is not normally measured on the engine test bench but has a strong influence on the combustion and pollutant formation processes.

Note: the residual gas content, *Yres,* is expressed as a fraction of the total mass of gas trapped in the cylinder. It is sometimes called IGR for internal gas recirculation (% IGR) or even internal EGR for internal exhaust gas recirculation (% EGR).

On the test side, the residual gas content is estimated by the engine test bench software from other measured variables. The same kind of approach is used by Siemens and an estimation is completed from the

available test data using a dedicated algorithm based on an iterative procedure [8] that stops when convergence is reached (i.e. the difference between the residual gas mass fraction at iteration n and n-1 is inferior to $1e^{-8}$). This method uses the mean pressure and temperature at the intake and exhaust manifolds. The table below shows that the two estimations for the residual gas content. The largest deviations are observed for the highest engine loads.

Table 2-1 Comparison of the estimations of the residual gas content (Siemens vs engine dyno).

Point number	*Yres* estimation (dyno)	*Yres* estimation (Siemens)	deviation [%]
1	0.1518	0.1523	0.328
2	0.1038	0.0917	-13.195
3	0.0791	0.0627	-26.156
4	0.0606	0.0467	-29.764
5	0.1327	0.1550	14.387
6	0.0922	0.0898	-2.673
7	0.0702	0.0604	-16.225
8	0.0570	0.0461	-23.644
9	0.1208	0.1329	9.105
10	0.0828	0.0782	-5.882
11	0.0641	0.0544	-17.831
12	0.0528	0.0425	-24.235

In the past, Siemens developed an application-oriented tool for supporting the calibration of the CFM. This tool is available in the Siemens Simcenter Amesim software and is used for the project execution. The combustion fitting tool is interactive, dedicated to assist the user in setting parameters for the CFM sub-model by comparing simulation and experimental data. Thus, the CFM model parameters can be interactively modified by the user in order to get the best possible fitting between the simulated in-cylinder pressure and experimental ones.

In practice, the calibration process relies on the tuning of a set of model parameters. One of the most critical one is the actual compression ratio that can differ from the one evaluated during the design phase. This is particularly true in the case of a research engine. In the project, we use the so-called thermodynamic compression ratio evaluated from test data, 1 ratio below the “design” value (estimated from the geometry).

For the compression stroke, the main parameters to be handled are the cylinder wall temperatures and the heat exchange correlation coefficients. These values are common for all operating points. Concerning the wall temperature in [K], the correlation proposed by IFPEN [8] for a gasoline case is applied:

$$T_{wall} = \frac{200}{23} . IMEP + 83 + 273.15,$$

which gives a value of 364.8 K at 1 bar and 504 K at 17 bar IMEP.

Two parameters for the heat exchange correlation by Woschni [9] are tuned in order to obtain the right compression stroke. The combustion model parameters used to tune the heat release can be divided into two main groups. The first one represents the parameters specific to each operating point, with tumble and cut-off (turbulent length scale) in particular. The second group contains the CFM parameters common to all operating points, which are the initial flame volume, the gain for flame wrinkling and the gain for flame quenching at walls. For the exhaust stroke, the two remaining parameters of the Woschni heat exchange model are optimized. These parameters are common for the twelve points.

Results from the first optimization can be observed on the following figures for the 12 studied operating points, Figure 2-5.

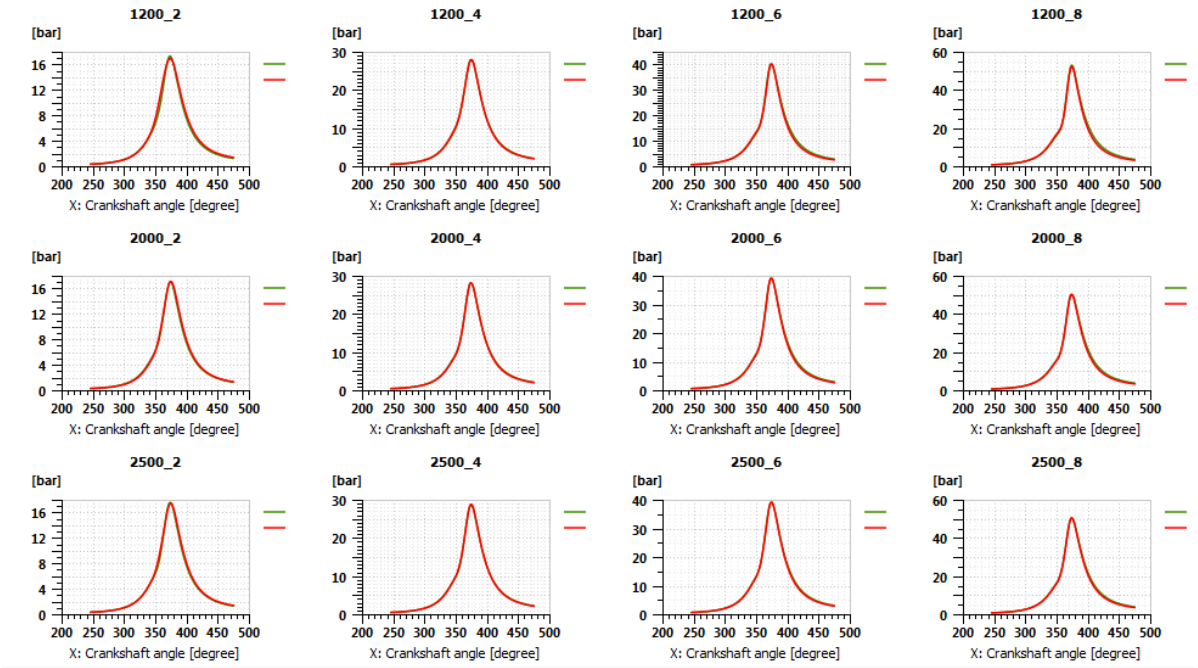


Figure 2-5 Results of the CFM model for the 12 operating points (red = simulation, green = measure).

Looking more in the detail at the results, we can, of course, observe some minor discrepancies between the experimental data and the simulation. This is illustrated in Figure 2-6 for a particular point where we can see some deviations.

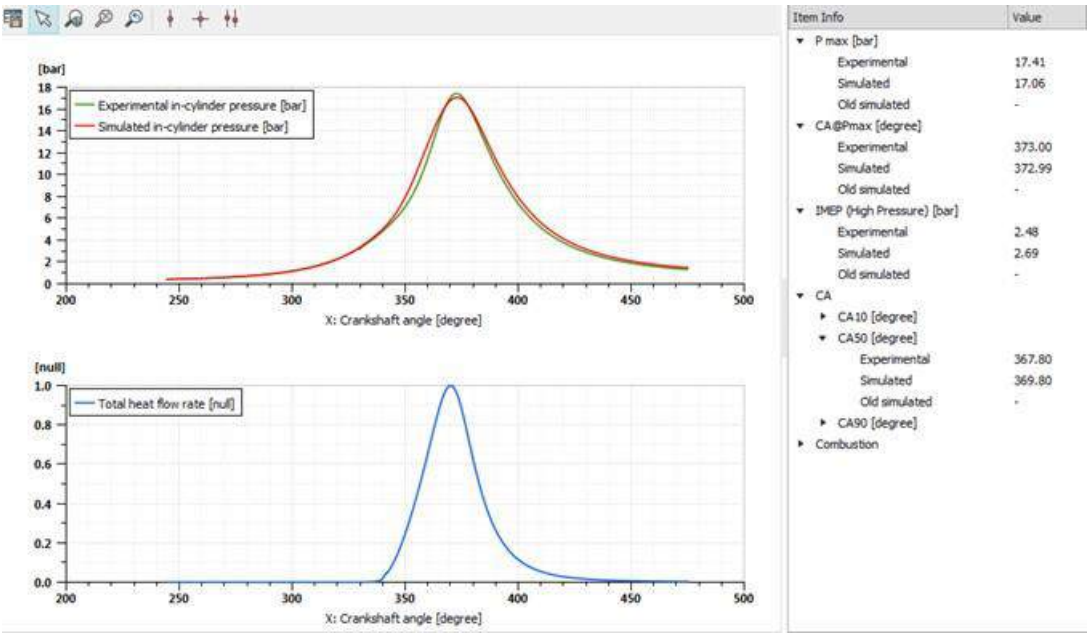


Figure 2-6 Details for the point 1200 rpm, 2 bar (red = simulation, green = measure).

It is interesting is to see that the CFM is able to accurately capture the initiation of the combustion just after the spark advance. This is illustrated in the Figure 2-7 where we see a delay of approximately 10 °CA between the spark and the actual development of the combustion in the chamber.

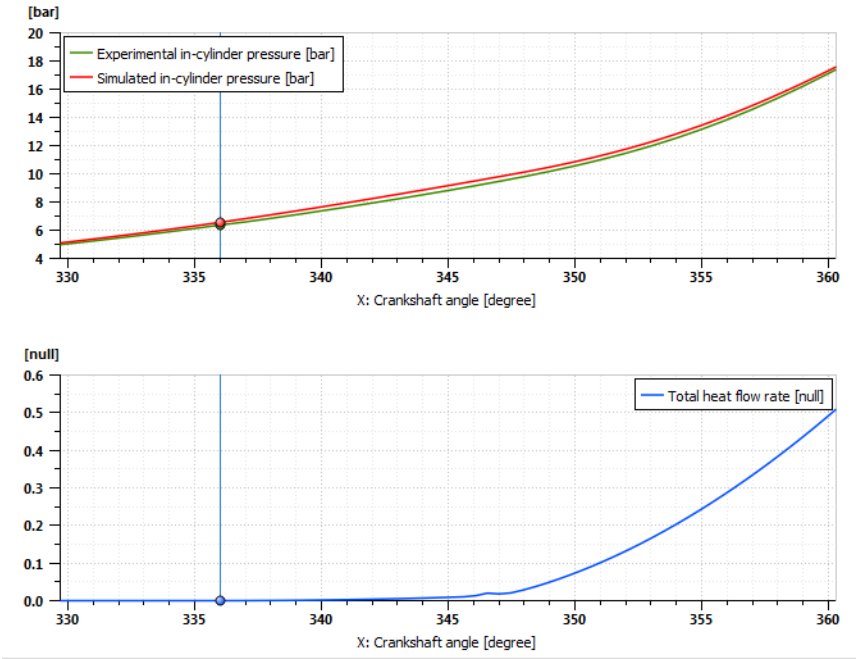


Figure 2-7 Initiation of the combustion, point 1200 rpm, 4 bar (red = simulation, green = measure).

The calibration process leads to the definition of a (tumble, cut-off) set for each of the studied operating points. These two values characterize the turbulence in the combustion chamber for given operating conditions. The tumble is an image of the mean flow in the cylinder and the cut-off characterizes the local turbulence scale.

From the 12 values resulting from the tuning process of the CFM, one can set-up maps defining the tumble value and the integral length scale (cut-off) as a function of the engine speed and the mass of air trapped in the cylinder. This later reflects the engine load. The two maps generated at this stage are illustrated in Figure 2-8. The order of magnitude of the Y axis is consistent with the physics since tumble values are in the range 1-3, and the cut-off can be linked to the distance between the piston and the cylinder-head at TDC (here in centimetres).

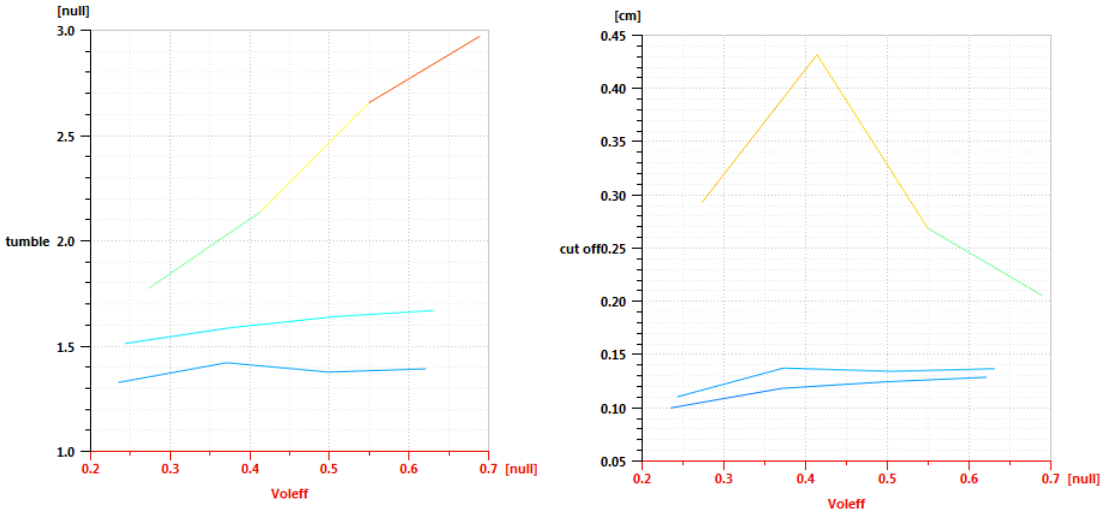


Figure 2-8 Tumble and cut-off maps from the CFM calibration (3 curves for engine speed 1200, 2000 and 25000rpm)

Since these two calibration parameters are associated to actual physical variables, the trends seen on the maps are according to our expectations. These characteristics easily permit us to interpolate or extrapolate values in and out of the tuning zone. In other words, with the CFM, we can have a good confidence in the

predictions of various operating points, when they differ from the 12 calibrated points. This capability will be used in the following to extend the scope of the analysis.

Validation of the CFM

The results given by this first calibration stage of the CFM are illustrated in this chapter. A direct comparison between measurements and simulation is given in the tables below, which show a good agreement.

Table 2-2 Validation of the CFM for the prediction of the pressure peak (engine dyno vs simulation).

Point	Max(Pcyl) test [bar]	Max(Pcyl) simu [bar]	deviation [bar]
1	17.409	17.0590	0.3500
2	28.105	28.1646	-0.0596
3	40.496	40.4756	0.0204
4	53.354	52.6076	0.7464
5	17.166	17.2158	-0.0498
6	28.321	28.2919	0.0291
7	39.329	39.4585	-0.1295
8	50.571	50.6173	-0.0463
9	17.676	17.5448	0.1312
10	28.845	29.0009	-0.1559
11	39.346	39.3985	-0.0525
12	50.859	50.7580	0.1010

All the operating points simulated with the CFM show a deviation to the predicted pressure peak that is below 1 bar.

Table 2-3 Validation of the CFM for the prediction of the peak pressure angle (engine test vs simulation).

Point	Max(Pcyl) angle test [°CA]	Max(Pcyl) angle simu [°CA]	deviation [°CA]
1	373	372.992	0.008
2	374	373.920	0.08
3	373	373.456	-0.456
4	374	373.456	0.544
5	373	373.920	-0.920
6	373	373.456	-0.456
7	373	373.456	-0.456
8	373	372.992	0.008
9	373	373.920	-0.920
10	374	373.920	0.080
11	374	373.456	0.544
12	373	373.456	-0.456

All the operating points simulated with the CFM show a deviation on the predicted maximum pressure angle below 1 °CA, as seen in Table 2-3 above.

Table 2-4 Validation of the CFM for the prediction of indicated mean effective pressure (engine test vs simulation).

Point	IMEP test [bar]	IMEP simu [bar]	deviation [bar]
1	2.4804	2.6919	-0.2115
2	4.2129	4.0941	0.1188
3	5.9879	5.4031	0.5848
4	7.7421	6.8156	0.9265
5	2.5471	2.7519	-0.2048
6	4.2987	4.2115	0.0872

7	6.0554	5.7001	0.3553
8	7.7973	7.1673	0.6300
9	2.5908	2.747	-0.1562
10	4.3945	4.3509	0.0436
11	6.1305	5.8692	0.2613
12	7.9030	7.3831	0.5199

Most the operating points simulated with the CFM show a deviation on the IMEP (image of the indicated torque) below 0.5 bar. The point number 4 (1200 rpm, 8 bar) presents the highest discrepancy in terms of torque production. This might not be related to the modelling of the combustion heat release itself since this seems properly predicted as illustrated in the following table, Table 2-5. This would rather be related to other thermodynamic effects (bad estimation of the wall temperature, error in the estimation of the injected fuel by the control unit etc).

Table 2-5 Validation of the CFM for the prediction of the timing for 50 % fuel burned "CA50" (engine test vs simulation).

Point	CA50 test [°CA]	CA50 simu [°CA]	deviation [°CA]
1	367.8	369.8	0.5438
2	368.8	368.6	-0.0542
3	368.1	367.5	-0.1630
4	368.0	367.4	-0.1630
5	368.5	369.2	0.1900
6	368.4	368.2	-0.0543
7	368.6	367.7	-0.2442
8	368.5	367.4	-0.2985
9	368.2	369.5	0.3531
10	368.8	368.8	0.000
11	368.9	368.5	-0.1084
12	368.7	367.9	-0.2170

All the operating points simulated with the CFM show a deviation on the angle for 50 % fuel burned (CA50) below 0.5 °CA which is a good performance for a phenomenological model.

As a conclusion of the work done by Siemens on the model with valves closed (compression and combustion), the results produced by the CFM are in good agreement with the test data and present a level of accuracy which is in-line with the expectations for a phenomenological combustion model. The main strong point of the CFM is the calibration through the tumble and cut-off maps, which are sufficiently smooth to be applied for interpolated points and extrapolated points.

2.1.2 Simulation using SI-SRM and investigation of possible interfaces

Introduction to the SI-SRM by LOGE

The 0D Spark-Ignited Stochastic Reactor Model (SI-SRM) is based on simulations that have been performed using the software package LOGEengine™ version 3.0 from [10]. The 0D SRM accounts for mixture and temperature inhomogeneity of the cylinder gas due to direct fuel injection, turbulent mixing and heat transfer. The cylinder gas inhomogeneity has a major impact on ignition, flame propagation and emission formation. The 0D SRM has been tested under both spark-ignited and compression-ignited engine conditions and the results are published in several works [10, 11, 12]. In the next section, a brief overview on the underlying theory, as well as the turbulence sub models, is given.

Model Fundamentals

The 0D SRM is a model for physical and chemical processes applicable to simulation of in-cylinder processes in spark-ignited and compression-ignited engines. The 0D SRM considers gas inside the cylinder as an

ensemble of notional particles, which can mix with each other and exchange heat with the cylinder walls. Each particle has a chemical composition, temperature and mass; that is, each particle represents a point in phase space for species mass fraction and temperature. The temperature $T(t)$ and species concentrations $Y_i(t)$ are treated as random variables that can vary within the cylinder and determine the composition of the gas mixture using probability density functions (PDFs). The in-cylinder mixture is thus represented by a PDF in phase space and the particles constitute the realization of this distribution. In practice all stochastic particles in the SRM represent a portion of the in-cylinder mass and rather than a PDF, a mass density function (MDF) is used; the MDF can be considered as a mass-based discretization of the PDF. The solution for the mass fractions and temperature is obtained from the transport equation for the MDF. These data are further used to calculate other engine quantities, such as pressure and heat release rate. The joint vector $\varphi(t)$ of the local scalar variables is defined as $\varphi(t) = (Y_1, \dots, Y_{N_S}, T; t) \equiv (\varphi_1, \dots \varphi_{N_S}, \varphi_{N_S+1}; t)$, where N_S is the number of chemical species in the reaction mechanism. This vector has a corresponding joint scalar MDF that is expressed as $F_\varphi(\psi; t) = F_\varphi(\psi_1, \dots, \psi_{N_S}, \psi_{N_S+1}; t)$ with $\psi_1, \dots, \psi_{N_S}, \psi_{N_S+1}$ being a realization of the random variables $\varphi_1, \dots, \varphi_{N_S}, \varphi_{N_S+1}$. In addition, as proposed in the partially stirred plug flow reactor (PaSPFR) [14], it is assumed that probabilities of all scalar variables are independent of position, i.e. statistical homogeneity applies. This implies that the MDF does not vary spatially within the cylinder. With the defined variables, the time evolution of the MDF can be written as:

$$\frac{\partial}{\partial t}F_\Phi(\psi,t) + \frac{\partial}{\partial \psi_i}\left(Q_i(\psi)F_\Phi(\psi,t)\right) = mixing\ term \qquad (1)$$

The initial conditions are given by $F_\varphi(\psi; 0) = F_0(\psi)$ where $F_0(\psi)$ represents the initial distribution at time $t = 0$. Equation (1) describes the Partially Stirred Plug Flow Reactor (PaSPFR) and also serves as a base for the description of the stochastic reactor models for engine applications [15, 16]. The mixing term on the right-hand side is discussed in the next section. The term Q_i on the left-hand side of equation (1) is, in general, a source/sink operator that depends on the phenomena under consideration. For direct injection engines this term represents the change of the MDF due to 1) chemical reactions, 2) convective heat loss, 3) volume changes due to piston motion, and 4) direct fuel injection. These terms are calculated based on the species and energy conservation equations that for DI engines can be expressed as (for details see, e.g., [17]):

$$Q_i = \frac{W_i}{\rho}\sum_{j=1}^{N_R}\omega_{i,j} + \frac{\dot{m}_f}{m}\left(Y_{i,f} - Y_i\right) \quad i = 1, \dots, N_{Species} \quad ; \quad j = 1, \dots, N_{Reactions} \qquad (2)$$

$$Q_{N_S+1} = \frac{1}{\rho c_p}\frac{dp}{dt} + \frac{h_g A}{m c_p}(T - T_W) - \frac{1}{c_p}\sum_{i=1}^{N_S} h_i \frac{W_i}{\rho}\sum_{j=1}^{N_R}\omega_{i,j} + \frac{1}{c_p \rho}\frac{\dot{m}_f}{V}\sum_{i=1}^{N_S} Y_{i,f}(h_{i,f} - h_i) \qquad (3)$$

In equations (2) and (3) $\omega_{i,j}$ and Y_i denote the molar net rate of formation of species i due to reaction j and the mass fraction of species i respectively. The subscript f refers to the injected fuel. W_i denotes molar mass of species i, ρ is the density, T is the mean temperature of the gas, T_w is the cylinder wall temperature, c_p is the specific heat capacity at constant pressure, h_g is Woschni's heat transfer coefficient, A is the heat transfer area, h_i is the specific enthalpy of species i, p is the pressure and N_R and N_S stand for the number of reactions and species, respectively, and f denotes fuel. In equation (2) the terms on the right-hand side represent changes in composition space due to chemical reactions and fuel injection, respectively. Equation (3) contains terms describing temperature changes caused by work due to piston movement, convective heat transfer, chemical reactions and fuel injection, respectively. The total wall heat transfer is calculated through Woschni's model (for details see, e.g., [916]). The distribution of the heat transfer over the particles follows a stochastic approach, explained by Bhave and Kraft [1717]. The right-hand side of equation (1) represents the time evolution of the MDF in composition and temperature space due to molecular mixing. The right-hand side is modelled using a particle interaction model and a time dependent turbulent mixing time. The next section briefly outlines the concept of the mixing time modelling for the SI-SRM. In addition to the local variables, global quantities are distinguished. These are the total mass (m), volume (V), and mean pressure (p), which are assumed to not vary spatially in the combustion chamber. The volume change, in terms of

crank angle degree, is calculated based on the known engine geometry. The pressure is calculated from the equation of state as $p(t) = \langle\rho(t)\rangle R \langle T(t)\rangle / \langle W\rangle$, where the mean density is calculated as $\langle\rho(t)\rangle = m/V(t)$ and T and W are the mean (angled brackets) temperature and mean molecular mass, respectively. Equation (1) is solved numerically using a Monte Carlo particle method (e.g. Pope [18]) with the operator splitting technique as previously presented by Maigaard et al. [15]. The expression of the mixing term on the right-hand side of equation (1) is presented in equation (4) and described in the next section.

$$mixing\ term = \frac{C_\Phi \beta}{\tau}\left[\int_{\Delta\psi} F_\Phi(\psi - \Delta\psi, t)F_\Phi(\psi + \Delta\psi, t)d(\Delta\psi) - F_\Phi(\psi, t)\right] \qquad (4)$$

C_Φ and β are two model parameters that in the present study have been set to 2 and 1 respectively. The mixing time history, τ in equation (4), is the main input parameter for the SI-SRM. With respect to actual engines, mixing time history can be understood as the inverse of the frequency at which air, fuel and residual gases mix with each other. In the next sections a brief introduction on the mixing time and flame propagation sub-models is give. For more details regarding the chemistry step please refer to [12].

Mean mixing time sub model

In the SI-SRM, the mixing time describes turbulence time scales during the engine cycle. The mixing time governs the intensity of mixing between particles, which in turn influences mixture inhomogeneity in the gas phase for scalars such as species mass fractions and temperature, which have a strong influence on the auto-ignition process, the local rates of heat release and pollutant formation. Hence, to some extent, the mixing time describes the local character of turbulent flow and chemistry interactions; the shorter the mixing time, the higher the intensity of the mixing operations on particles and vice versa. The mean representative profile is optimized during model calibration against experimental data through various parameters (see Figure 2-9**Error! Reference source not found.**).

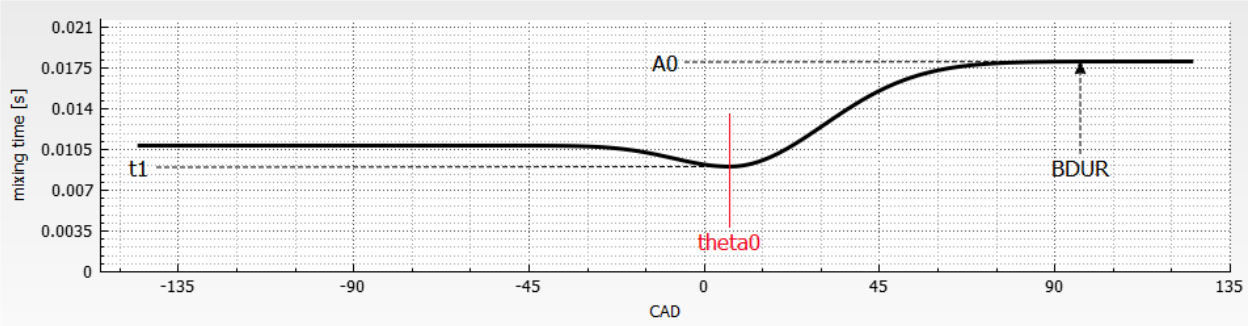


Figure 2-9: Concept of modelling the mean representative mixing time for the SI-SRM simulations of spark-ignited engines with port injection.

A Genetic Algorithm (GA) is employed during model calibration in LOGEengine to calibrate the mixing time model constants (t_1, $A0$, $BDUR$), which controls the shape of the mixing time profile as shown in Figure 2-9. Parameter ($theta_0$) represent the experimental spark-timing.

The modelling of the particle interaction in the 0D SRM governs how the gas-phase particle composition vectors evolve and is needed to mimic the composition change of real fluid parcels due to mixing caused by the turbulence. The dynamic of particle interaction influences mixture inhomogeneity under engine conditions and in turn, affects pollutant formation. In the SI-SRM the particle interaction sub-model strongly affects the complex chemistry of emission formation and describes the local character of turbulent flow and chemistry interaction. In this work, the CURL [19] particle interaction model has been used.

Turbulent flame propagation model

In LOGEengine 3.0 the flame front is assumed to expand approximately spherically, centred at the defined spark plug location and limited by the cylinder walls and the piston. The turbulent flame speed is calculated using a correlation between laminar and turbulent flame speed. The laminar flame speed is calculated based

on a detailed Ethanol Toluene Reference Fuel (ETRF) reaction scheme and pre-compiled in a look-up table. Although the flame volume is calculated in three dimensions, the turbulence is still calculated without spatial resolution, which in turn allows for significantly faster calculations. Enthalpy losses to the cylinder walls are described using Woschni's heat transfer equation. For simplicity it is assumed that the heat transfer did not affect the spherical flame shape, whilst the total heat loss to the walls manifested itself via the temperature dependency in the laminar flame speed library. For the flame geometry calculation, a polygon-based approach is used and in Figure 2-10Figure 2-10 an exemplary visualization of the flame front is presented. The flame sphere was approximated as a set of tetrahedrons, each with an analytically solvable volume. The flame surface is represented as a set of nodes, each of which can propagate outwards from the flame centre with a flame speed defined by local conditions. In this work, statistical homogeneity was assumed, hence the flame propagation speed was hence thought to be equal for all nodes. For more details please refer to [20].

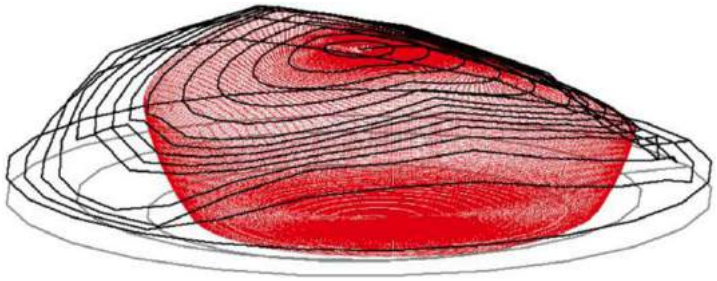


Figure 2-10: Visualization of the flame surface described using a set of nodes at regular angular intervals.

LOGEengine emission look-up table generation

The methodology to create the emission look-up table for the Siemens MVEM consists of multiple steps, as illustrated in Figure 2-11. First, the 0D SRM is calibrated to match the cylinder pressure and exhaust emissions of the BOSCH single-cylinder operating points. Second, the mixing time is parameterized for engine speed and fuel mass. During the engine map simulation, when the operating point is changed, the current mixing time and spark ignition is calculated by the parameterization function and the performance and emissions of the operating point are predicted. Additionally, the 0D SRM is coupled with the tabulated chemistry and laminar flame speed user table of the EU5 E5 gasoline mixture. Third, to automate the process of engine performance map simulations and the creation of the emission look-up table, the 0D SRM is coupled with the CAE tool modeFRONTIER. The fix points of the look-up table are predefined in another look-up table and serve as the input variables of the different operating points:

- Speed
- Fuel mass
- EGR rate
- Spark ignition
- Air-fuel ratio

The valve timings do have a significant impact on the emissions but the modelling approach used by the SI-SRM (simulation valve closed) cannot deal with this degree of freedom. In addition, the injection timing and/or pressure are not taken into account in the maps creation process at this stage. It would be considered later in the project, following the research and development of a liquid film model by LOGE.

The operating points are calculated sequentially and the results for mean effective pressure, maximum cylinder pressure, CA10, CA50, CA90, CO_2, CO, HC, NO_x and soot emissions are stored in the look-up table. Since no experimental data was available for the soot mass, the soot emission parameters are based on best practice values.

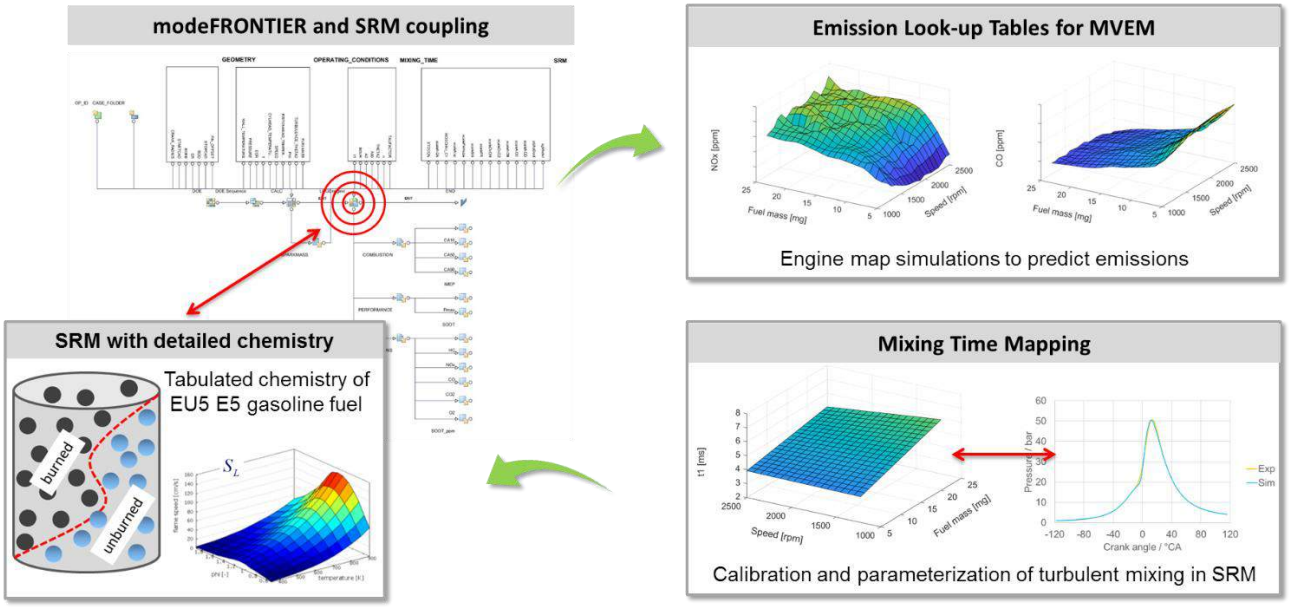


Figure 2-11 Methodology for engine mapping with the SI-SRM.

Emission and combustion look-up table content

LOGE used the data shared by BOSCH and the 12 reference operating points for the calibration of the SI-SRM model. The software is then used to generate an engine mapping i.e. a complete data set including simulation results for various engine operating conditions. The main inputs and outputs of the SI-SRM model are given in the Table 2-6.

Table 2-6 Inputs and outputs of the SI-SRM model for engine mapping.

Input variables	Unit	Values
Engine speed	rpm	1200, 2000, 2500
Air/fuel ratio	-	11.81, 14.17, 17.71
Mass of fuel	mg	From 5 to 25–step 2.5
Spark advance	°CA	-30, -20, -10
Residual mass fraction	%	5, 10, 15, 20

Output variables	Unit
CA10 (10 % fuel burned angle)	°CA
CA50 (50 % fuel burned angle)	°CA
CA90 (90 % fuel burned angle)	°CA
Maximum (Pcyl) angle	°CA
IMEP	bar
NO_x	Yppm
CO	Yppm
CO_2	Yppm
O_2	Yppm
soot	Yppm

With this design of experiment conducted by LOGE, the engine map includes approximately 4500 operating points, covering most of the engine control degree of freedom.

Coupling strategy

At this stage, Siemens starts to investigate several options for interfacing the SI-SRM maps with its CFM. The first option consists in using the emissions and soot models by LOGE in parallel to the combustion heat

release model by Siemens, as illustrated in Figure 2-12. The second option consist of a two steps approach where the output of the CFM would be actually used as inputs to the emissions and soot models, as presented in Figure 2-13.

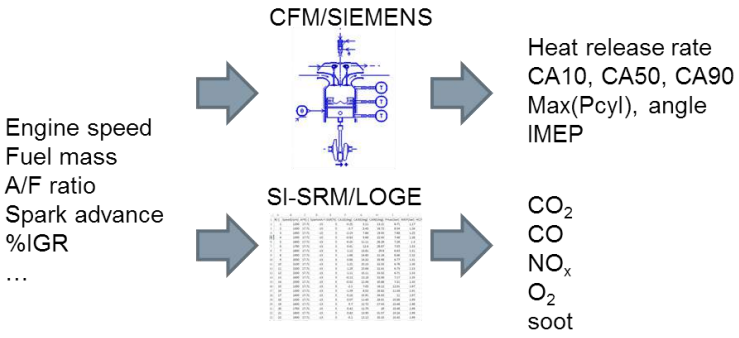


Figure 2-12 Interface using a parallel modelling approach for heat release & emissions.

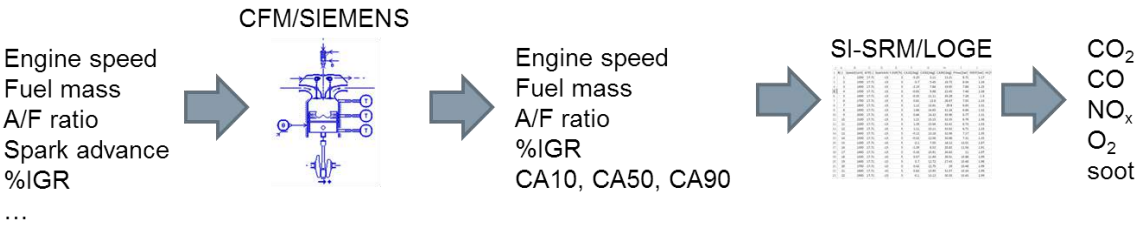


Figure 2-13 Interface using a two steps modelling approach for heat release & emissions.

In practice, the choice is driven by the intrinsic quality and weakness of the two models from LOGE and Siemens. Indeed, a quick analysis of the results from the SI-SRM in terms of combustion heat release prediction, see Figure 2-14, shows significant discrepancies when compared to the test data whereas the CFM is capable of much better accuracies. On the other hand, the LOGE model includes much more complexity for describing the pollutant formation process and soot in particular. Hence, we can consider the parallel approach as the most appropriate way to couple the two approaches. It permits the sum of the discrepancies generated by the two models to be avoided.

Figure 2-14 Comparison between measurement (yellow) and SI-SRM results (blue) for the CA50.

In fact, the analysis and development done on the single-cylinder approach emphasized other technical considerations, which confirm the choice in favour of the parallel approach.

Emissions data consistency

In order to track the pollutants from the combustion chambers, Simcenter Amesim can deal with a mixture of 12 species, instead of the 3 mentioned previously. The 12 gas mixture is then composed of Fuel, N_2, O_2, H_2, H_2O, NO, NO_2, CO, CO_2, HC, NH_3 and soot.

The emissions data from LOGE are adapted for the Simcenter Amesim simulation in order to ensure a consistency in terms of units, mass balance and number of species handled. To do this, we transform the 5

mass fractions given in dry basis by the SI-SRM model, into the 12 mass fractions in humid basis required by the Simcenter Amesim model.

In the LOGE table, we have five species NO_x, HC (unburned hydrocarbons), CO, CO_2, O_2 completed by soot expressed in Yppm (mass fraction in part(s) per million) on dry basis. The first step is to estimate the 5 other species H_2, Fuel, NH_3, H_2O and N_2 and the NO_2/NO ratio in the same dry basis.

First, the Fuel, H_2O and the NH_3 are considered to be zero. By definition in the Simcenter Amesim model, fuel possibly remaining after the combustion (fuel rich operation) is transferred as HC at the engine outlet. As we are in a dry basis, the H_2O fraction is null and there is no NH_3 generated by the combustion process (this species is here to account for the modelling of after-treatment systems). Assuming a constant H_2/CO ratio equal to 0.3 (in mole fraction) and a NO_2/NO_x ratio equal to 0.2 (in mole fraction too), the following equations can be written to evaluate the amount of H_2 and NO_2:

$$y_{H_2} = 0.3 \,.\, \frac{W_{H_2}}{W_{CO}} \,.\, y_{CO}$$

$$y_{NO_2} = y_{NO_x} . 0.2 \,.\, \frac{W_{NO_2}}{0.2 \,.W_{NO_2} + 0.8 \,.W_{NO}}.$$

The mass fraction of N_2 is deduced from the others, in order to have the sum of the mass fraction equal to 1.

We are now able to deduce the mole fraction of the species on a dry basis:

$$x_i = \frac{{y_i}/{W_i}}{\Sigma {y_k}/{W_k}}.$$

The coefficient of conversion from humid to dry basis, noted K_b, is calculated as follows:

$$K_b = \frac{200}{200 + {H}/{C} \,.[CO_2]_{\%dry} + \left({H}/{C} \,.2\,.{H_2}/{CO}\right).\ [CO]_{\%dry}},$$

where ${H}/{C}$ is the ratio between hydrogen and carbon atoms in the fuel, $[CO_2]_{\%dry}$ and $[CO]_{\%dry}$ are respectively the CO_2 and CO volumetric concentration in percent.

Thanks to the evaluation of the coefficient of conversion from humid to dry basis, we can easily compute the mole fraction of the 12 species required by the Simcenter Amesim model, in a humid basis:

$$x_{i,humid} = K_b . x_{i,dry}.$$

And finally deduce the humid mass fraction:

$$y_i = \frac{x_i . W_i}{\Sigma x_k W_k}.$$

Then, we format the SI-SRM data in order to be able to interpolate as a function of the engine speed, the spark advance, the burned gas mass fraction, the air fuel ratio and the mass of fuel.

An example of a table for CO_2 is given Figure 2-15. The same axis can be applied for any pollutant simulated by the SI-SRM model including soot.

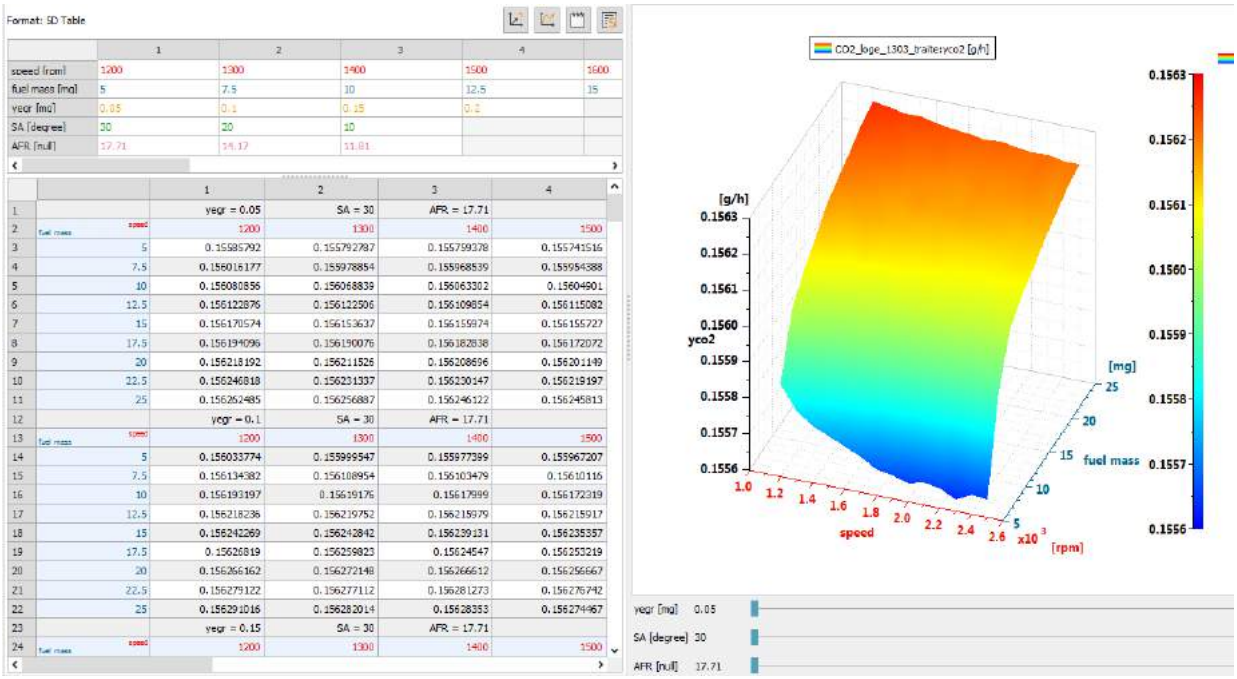


Figure 2-15 Emission table for CO_2 (humid basis) generated by Siemens.

2.2 Single-cylinder simulation

2.2.1 Modelling approach, definition of the boundary conditions and injection

The model created by Siemens for the single-cylinder investigation is illustrated in Figure 2-16. It is composed of a CFM completed with a gas exchange process model, in order to simulate the gas flow in the cylinder head and intake pipes an injector model to pilot the delivery of fuel and pressure sources to define the boundary conditions at the level of the intake and exhaust manifolds.

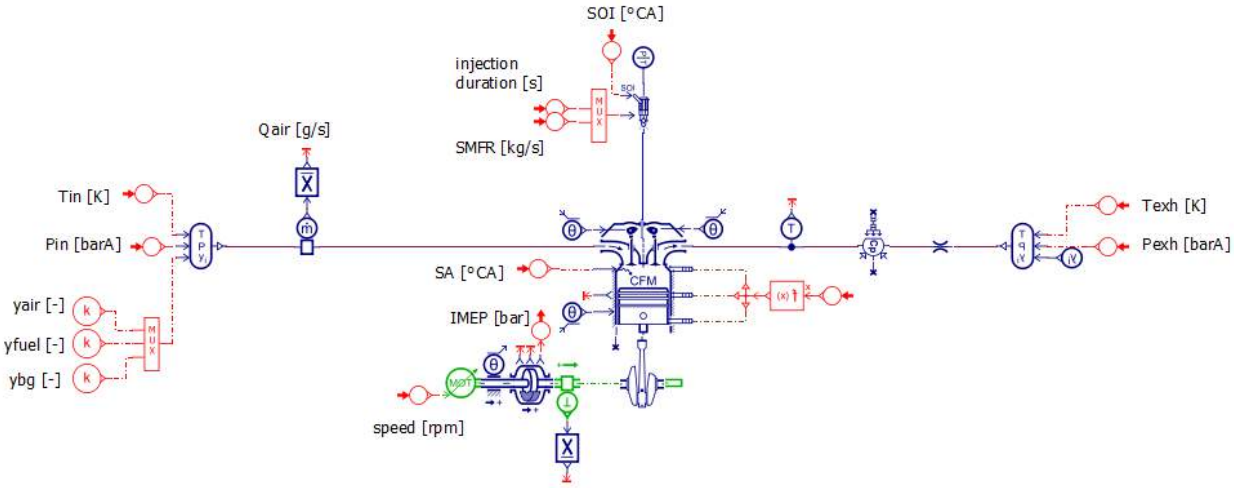


Figure 2-16 Single-cylinder engine model in Simcenter Amesim.

Definition of the boundary conditions

The definition of the boundary conditions at the level of the intake and exhaust manifold models requires a pressure, a temperature and a gas composition.

- Pressure signal

  The pressure applied at the level of the manifold can be either a constant value or a crank-angle resolved signal. Both type of data are available in the test data shared by BOSCH for the modelling activities.

- Temperature signal
  A constant signal is applied on the model.
- Gas composition
  In the model, we take into account for a mixture of 3 gases (air, fuel and burned gas). At this stage, one consider pure air at the intake (direct injection) and pure burned gas at the exhaust.

In practice, the cylinder head component includes a "back-flow" model in order to capture the potential effect of back flows (burned gas going from the cylinder into the intake manifold) on the thermodynamic state of the gases seen upstream the valve port. The main principle of this buffer zone is given below.

- During back flows, as long as the gases go in the backward direction, masses and enthalpy of this buffer zone are inflating and the intake manifold conditions are not affected.
- When the flow goes in the forward direction, as long as the buffer is not emptied, enthalpy and masses that fill the cylinder come directly from the buffer. Once again the intake manifold conditions are not affected.
- Then, when the buffer is empty, enthalpy and masses that fill the cylinder directly come from the intake manifold.

At the exhaust, a simple volume and an orifice element are inserted between the exhaust valves and the boundary condition. It permits to gather from the model, a value for the exhaust gas temperature (evaluated from the engine-out enthalpy flow rate), to be confronted to the measured value applied at the boundary.

The injection process is defined using an injector model that ensures the right delivery of the fuel mass with the right start of injection. The evaporation model is set-up in order to ensure that all the liquid fuel evaporates prior to the intake valve closing.

2.2.2 Physical consistency using imposed mean manifold conditions

Methodology

The way one deals with the boundary conditions in manifolds affects the prediction quality of the gas exchange process and hence the gas state in the combustion chamber at intake valve closing. The best modelling option is to apply crank-angle resolved pressure traces (measurement) as boundary conditions in manifolds, in a high-fidelity single cylinder engine model that can capture all the details of the gas dynamics. By this way, we can expect a fine prediction of the volumetric efficiency and gas composition in the chamber. The major drawback of this approach is that it requires actual intake and exhaust pressure traces for each of the simulated operating point. That is a strong limitation since we only have access to 12 points from the engine test whereas we want to extend the scope of the analysis to any kind of operating conditions, with various intake and exhaust manifold pressure levels. Since our goal is to apply a Design of Experiment (DoE) on the baseline model (single cylinder) in order to generate data to feed a reduced Mean Value Engine Model, we need to simulate many different intake and exhaust conditions which is only possible using constant values applied over the engine cycle.

On the other hand, the crank-angle resolved pressure at the intake and exhaust could have been provided by a full air path system model. However, the methodology proposed by Siemens in PaREGEn is not to develop a full multi-cylinder high-fidelity engine model (which is a common approach in engine 1D software) but rather to explore the reduction to a Mean Value Engine Model (see section 2.3) in order to ease the integration of the modelling approach in a full vehicle context so as to evaluate the engine attributes on real driving cycles including RDE (Real Driving Emissions). This MVEM approach is widely used in the industry, by control engineers in particular [21]. In practice, some engineering teams nowadays require to have simulation running much faster than real time to have a change to test vehicle on hundreds of driving cycles (RDE context) using virtual environments. The crank-angle based approaches cannot match with this strong requirements even if they can be real-time compatible.

Last by not least, Siemens, as other partners in WP1 including LOGE who took part in the software interface development (Section 2.2.2), worked essentially with the data shared by BOSCH for a single-cylinder research engine. Hence, no data were available for describing an actual air path system.

As a conclusion, using constant signals for the pressure in manifolds ease the migration process from a phenomenological crank-angle based model to a mean value model and allows Siemens to develop and possibly exploit a methodology supported by a background already available in its Simcenter Amesim product. The Design of Experiment required for the generation of the appropriate data would be simple to define and the consistency with a mean value model requiring mean values at its boundaries can be insured as detailed in the following.

Consistency of the approach with constant conditions in manifolds

Imposing constant pressure values in the intake runner instead of a detailed pressure trace is however not a straightforward process. Indeed, imposing directly the measured mean pressure signal on a crank-angle based gas exchange process model does lead to discrepancies in terms of air mass flow and volumetric efficiency prediction. That is linked to the impact of the pressure wave propagation and corresponding pressure pulsation upstream the valves that cannot be neglected for a precise prediction of the air mass flow rate and cylinder trapping efficiency. The methodology applied is then to impose at the level of the intake manifold, a constant pressure from measurement corrected by an offset used to ensure a good prediction of the engine filling. The main goal is here to get the right pressure at the intake valve closing, to guarantee a proper evaluation of the compression and then the combustion strokes. This developed methodology should give a reasonable estimation of the gas composition, pressure and temperature in the chamber at IVC.

Some investigations and analysis are conducted at this stage to valid the retained option. The analyses are based on a direct comparison of the results using different modelling approaches. One actually compares 4 four modelling options:

- A model where a corrected constant pressure is imposed at the intake. The correction is defined thanks to a PID controller that sets the intake pressure in order to ensure the right pressure at IVC. This is our reference modelling approach for the project,
- A model where the measured constant value is imposed at the intake,
- A model where the measured crank-angle resolved pressures are imposed at the intake and exhaust,
- A model where the measured crank-angle resolved pressures are imposed at the intake and exhaust and including a modelling of the runners using a 1D CFD approach (see Figure 2-17).

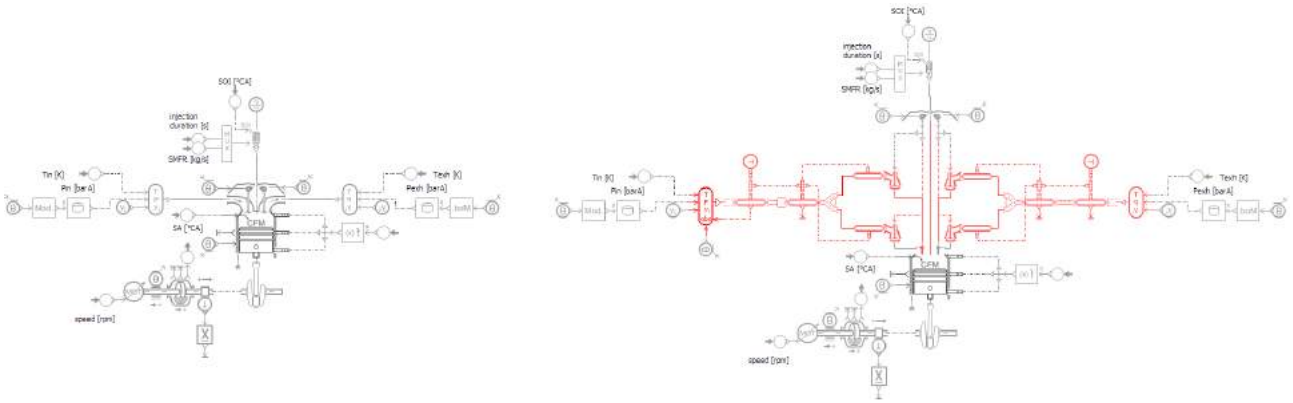


Figure 2-17 Measured pressures imposed at the valves vs at the boundaries of a CFD1D model (red = CFD1D model).

The results of the four approaches are illustrated on the point at 2500 rpm, 2 bar IMEP in Figure 2-18 (the gas (3) in the legend corresponds to the burned gas).

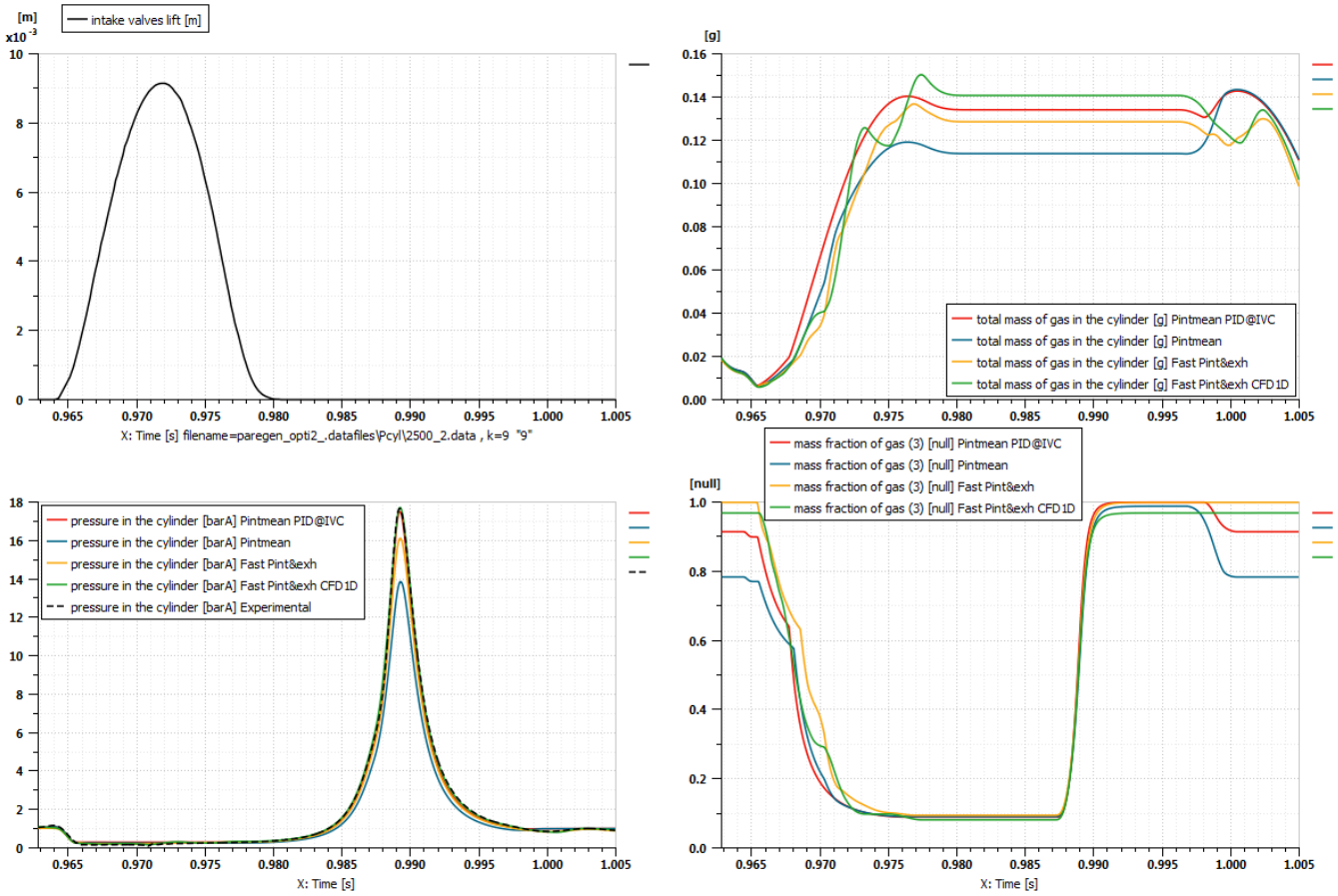


Figure 2-18 Impact of the modelling of the boundary conditions on the in-cylinder process simulation (red = reference model).

The engine filling and resulting mass of gas trapped in the cylinder are sensitive to the way we deal with the boundary conditions. Most of the models give consistent results but we see a significant deviation when the mean pressure from the measurement is directly applied (blue curves). This leads in this case to an under-estimated pressure at IVC resulting in under-estimated pressure in the cylinder. On the other hand, applying a corrected constant value (red curves) permits to have an accurate prediction of the trapping efficiency and hence, the in-cylinder pressure. The interesting point at this stage is that the four modelling approaches deliver approximately the same results in term of residual gas content (burned mass fraction of gas (3)) which give us a good confidence in the estimation of *Yres* given by our reference approach.

2.2.3 Iterative calibration process for the CFM

The calibration process of the CFM in the context of a single-cylinder engine model is introduced in Figure 2-19. It slightly differs from the baseline one illustrated in Figure 2-4 with a new iteration linked to the definition of the initial conditions for the CFM at IVC. Indeed, when inserting a gas exchange model, the conditions at IVC in terms of gas composition and residual gas content in particular are no longer estimations but predictions by the model itself. The CFM must be tuned again accordingly.

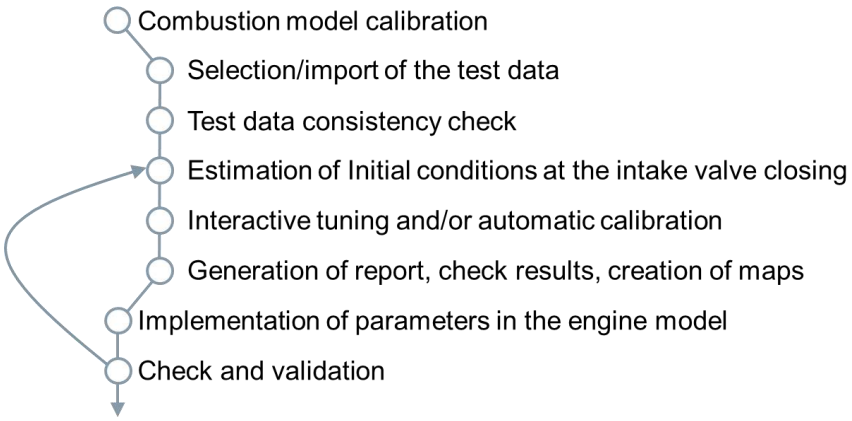


Figure 2-19 Updated calibration process applied for the single-cylinder model set-up.

In practice, a single loop is generally sufficient to get accurate-enough results, as illustrated in the following.

2.2.4 Results of the single-cylinder model

The results of the single-cylinder model are given in this part of the document. We only consider at this stage the simulation of the gas exchange process and combustion heat release. The estimation of the emissions and soot are details in the next chapter.

Overall, the quality of the calibration is very similar than in the case with closed-valves. We cannot see in Figure 2-20 any major deviation when compared to the previous approach (see Figure 2-5).

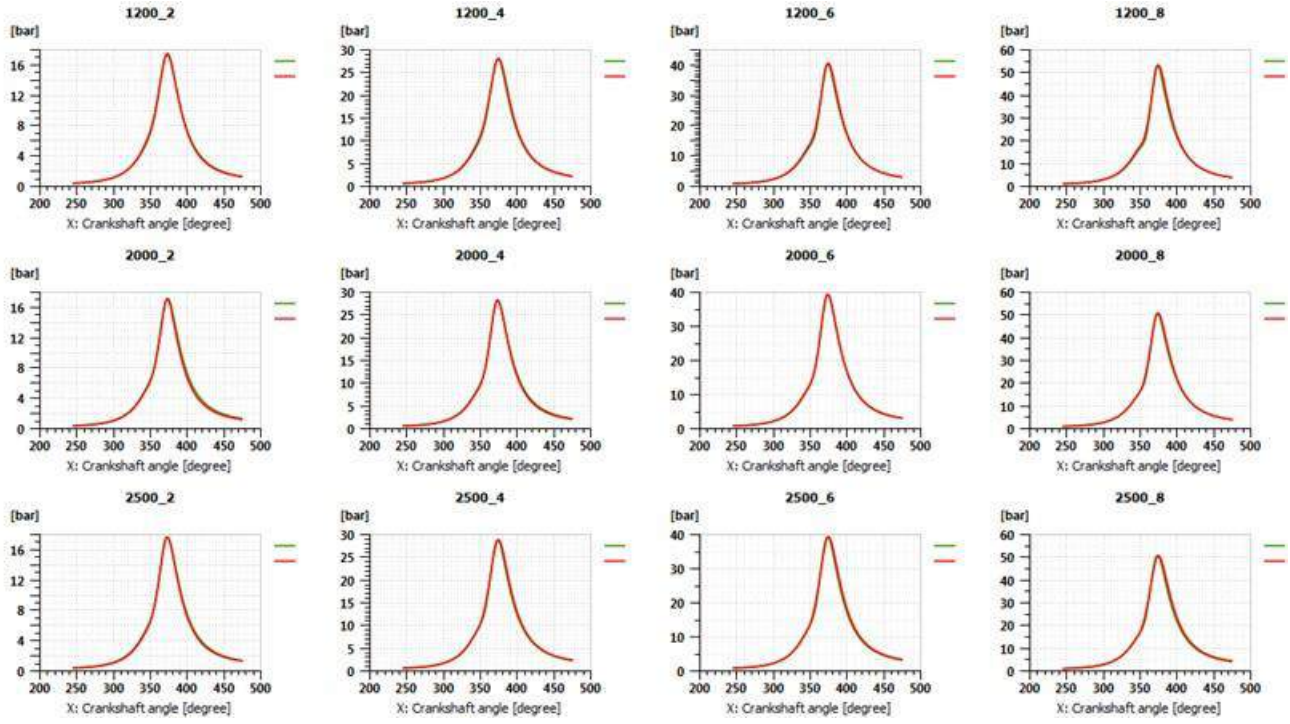


Figure 2-20 Results of the single-cylinder model for the 12 operating points (red = simulation, green = measure).

When checking for the details, we can observe that the single-cylinder model provides estimation for the residual gas content, *Yres**, that are significantly different from the values given by the first round estimation (from simulation and the engine test). The data are given in the table below, Table 2-7, which shows the lower residual amounts with the upgraded model compared to those expected from baseline estimators. This is an interesting outcome of the Siemens activities in WP1.

Table 2-7 Comparison of the estimations of the residual gas content (Siemens vs engine dyno).

Point number	Yres estimation (test)	*Yres* first estimation (Siemens)	*Yres** simu single cylinder (Siemens)
1	0.1518	0.1523	0.0960
2	0.1038	0.0917	0.0615
3	0.0791	0.0627	0.0484
4	0.0606	0.0467	0.0394
5	0.1327	0.1550	0.0991
6	0.0922	0.0898	0.0649
7	0.0702	0.0604	0.0485
8	0.0570	0.0461	0.0389
9	0.1208	0.1329	0.0940
10	0.0828	0.0782	0.0585
11	0.0641	0.0544	0.0450
12	0.0528	0.0425	0.0368

We clearly see a difference between the estimators (from the engine test or from the CFM tool) and the actual simulation of the gas exchange process. That was expected, because some operating points present some significant back-flows at the intake and at the exhaust, resulting in some deviations in the estimators that cannot predict such a phenomena. This assessment is important since we can see that the residual gas content is lower than estimated by the test system. From this, the iterative process for the calibration of the CFM is actually a trigger point for a fine-tuning of the model. The residual gases have a major impact on the heat release and the differences observed between the first guess (CFM tool estimator) and the actual prediction by the single-cylinder model cannot be ignored in the calibration process. The iterative process does address this.

The impact of the residual gas content on the heat release (with a similar turbulence in the chamber) is exemplified in Figure 2-21 where three levels of *Yres* are simulated. We see a major impact here in the combustion process and hence on the phasing of the CA50, the pressure trace.

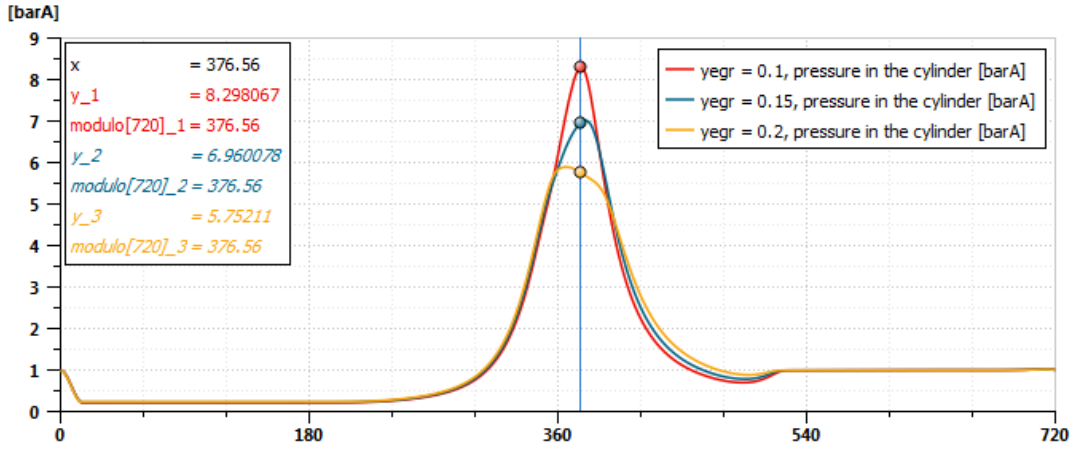


Figure 2-21 Impact of the residual gas content on the combustion heat release (Yres = 0.1, 0.15, 0.2).

A summary of the main results generated by the single-cylinder engine model once the CFM combustion model is fine-tuned is given in the following, Table 2-8.

Table 2-8 Results for the single-cylinder engine model.

Point	Max(Pcyl) [bar]	Max(Pcyl) angle [°CA]	CA50 [°CA]
1	17.40	373.18	369.68
2	28.07	374.45	371.04

3	40.21	374.60	370.56
4	52.85	374.69	370.40
5	16.96	373.25	368.43
6	28.10	373.51	368.54
7	39.14	373.98	368.99
8	50.60	374.17	369.17
9	17.56	373.06	368.09
10	28.71	374.51	369.72
11	39.17	374.68	369.87
12	50.46	374.70	369.76

The single-cylinder engine model permits us to evaluate the air mass flow rate at the intake, which can be compared with the test data. The results are given in Table 2-9 and present a good level of consistency.

Table 2-9 Results for the intake mass flow rate.

Point	Mass flow test [kg/h]	Mass flow simulation [kg/h]	deviation [%]
1	5.19	4.83	-7.453
2	7.88	8.28	4.831
3	10.44	11.39	8.341
4	13.11	14.73	10.998
5	7.65	6.82	-12.170
6	11.81	11.68	-1.113
7	15.95	16.72	4.605
8	19.96	21.88	8.775
9	9.27	8.68	-6.797
10	14.62	15.51	5.738
11	19.67	21.55	8.724
12	24.55	27.84	11.818

Finally, the temperature of the gas at the outlet of the cylinder is also simulated by the model and can be shown in parallel to the measured exhaust temperature, Table 2-10. In this case, we cannot directly compare the values since the temperature of the gas pulses at the exhaust valves present a temperature level higher than the temperature measured in the manifold because of the strong heat exchanges that occurs in the cylinder head.

Table 2-10 Results for the exhaust temperature.

Point	Exhaust temp test [K]	Cylinder-out temp simulation [K]
1	631.561	970.316
2	672.218	986.976
3	735.847	954.066
4	780.822	939.818
5	726.151	1104.636
6	774.334	1097.879
7	843.990	1083.660
8	872.549	1075.834
9	762.190	1188.058
10	823.026	1184.043
11	886.655	1168.193
12	909.605	1151.980

For information, the significant difference observed on the exhaust temperatures above is also present on the SI-SRM model results, as shown in Figure 2-22. In this later case, the discrepancy is even larger because the model only predicts the temperature of the combustion gas at the exhaust valve opening (and not integrated over the complete exhaust stroke as in the Siemens single-cylinder model).

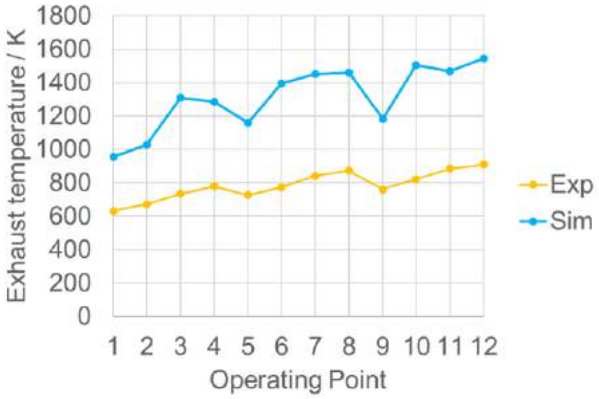


Figure 2-22 Results for the exhaust temperature by the SI-SRM model.

2.2.5 Direct interface with LOGE data using map based model

In the coupling strategy developed in Section 2.1.2, the inputs of the SI-SRM maps are detailed in the Table 2-6. If we consider the interface with the single-cylinder engine model in Simcenter Amesim, we can assess the following:

- The engine speed is an input of the single-cylinder engine model that can be duplicated as an input to the SI-SRM maps,
- The spark advance is also an input from the control that can be shared by the CFM and the SI-SRM maps,
- The mass of fuel injected has to be processed in the Simcenter Amesim model, which includes an injector model but which can be direct transferred to the SI-SRM model.
- The air/fuel ratio has to be evaluated by the single-cylinder engine model, from the air mass flow rate and the amount of fuel injected, and then transferred as an input of the SI-SRM maps,
- The residual/burned gas mass fraction is the most delicate variable to handle for the coupling. Indeed, the investigations completed by Siemens and the comparison between the estimations by BOSCH (used by LOGE for the calibration of its model) and the values given by the model demonstrate the importance to implement a function to make the data consistent. In other words, we need to set-up a basic model to estimate a level for the residual given by estimators, *Yres*, from the levels given by the single-cylinder model, *Yres**.

$$Y_{res} = F(Y^*_{res}).$$

This transfer function is created in the form of a map as a function of the engine speed and the *Yres**. The function implemented on the single-cylinder model is illustrated on Figure 2-23 .

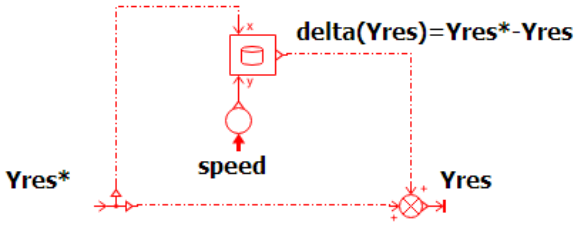


Figure 2-23 Simple conversion function from simulated *Yres to the values used as input of the SI-SRM model *Yres*.**

At this stage, the single-cylinder engine model developed by Siemens is capable of providing the right variables to the SI-SRM maps. From this, a direct interface with the engine-out emission model is possible. The retained approach uses look-up tables with one table for each of the pollutant including soot. The final model generated for the project is illustrated in the Figure 2-24.

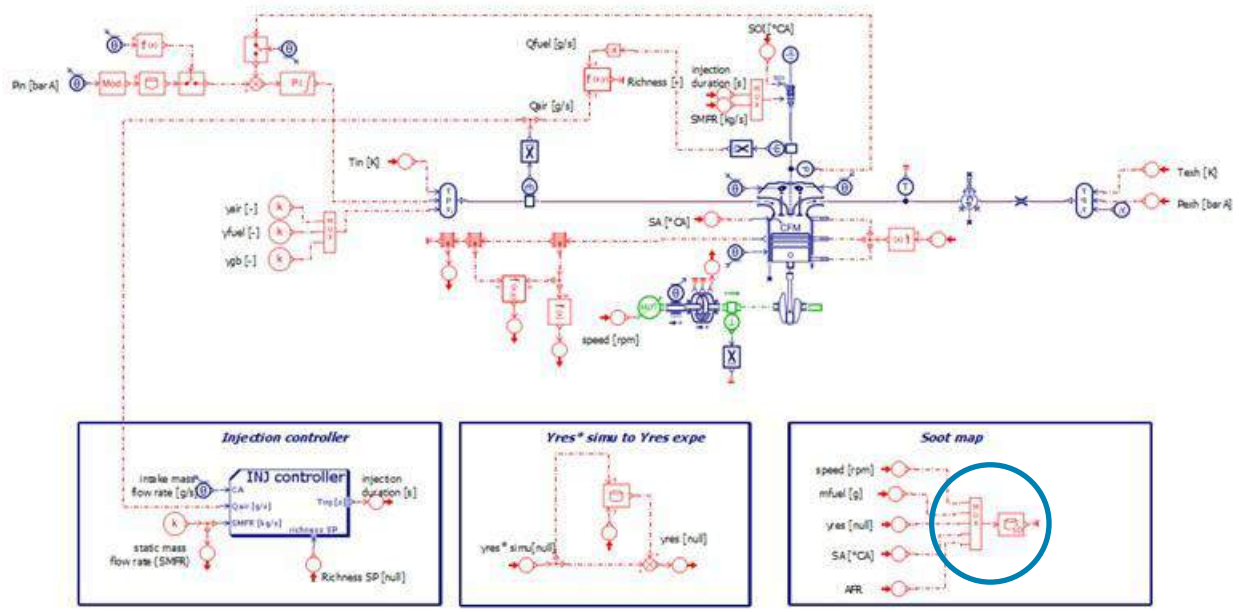


Figure 2-24 Final single-cylinder model including estimation of combustion heat release and emissions (blue circle).

With the model, we can now simulate the impact of the engine control or boundary conditions on the engine trapping efficiency, combustion heat release and engine-out emissions. The results in terms of NO_x emissions are introduced in Figure 2-25. The deviations observed are inherent to the assumptions and modelling approaches retained in the LOGEengine software. The levels and trends are well-captured which is a satisfactory results for a 0D/1D model.

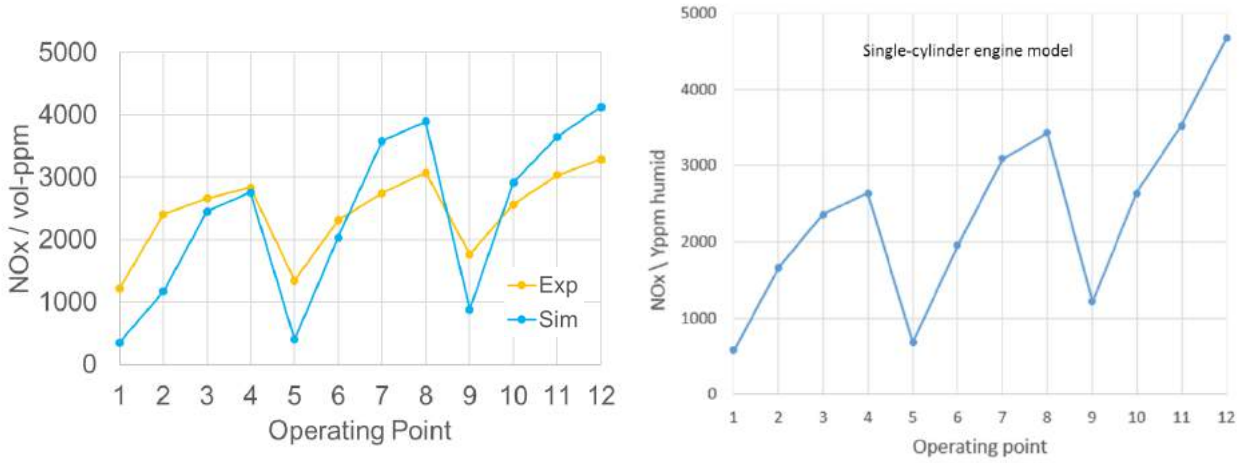


Figure 2-25 Validation of the NO_x emissions by comparing the test data vs SI-SRM (left) and single-cylinder engine model (right).

Illustrations of the capability to simulate the soot mass are given in the following Figure 2-26 and Figure 2-27. Since soot mass is not available from the raw test data delivered by BOSCH, LOGE was not yet able to fine tune its soot model. Hence, the levels predicted by the coupled approach are estimations from model based on LOGE best practices. This aspect would be enhanced during the project. However, we observe than the main trends are properly reproduced by the current approach. The air/fuel ratio and engine load have a major impact on the NOx and soot production.

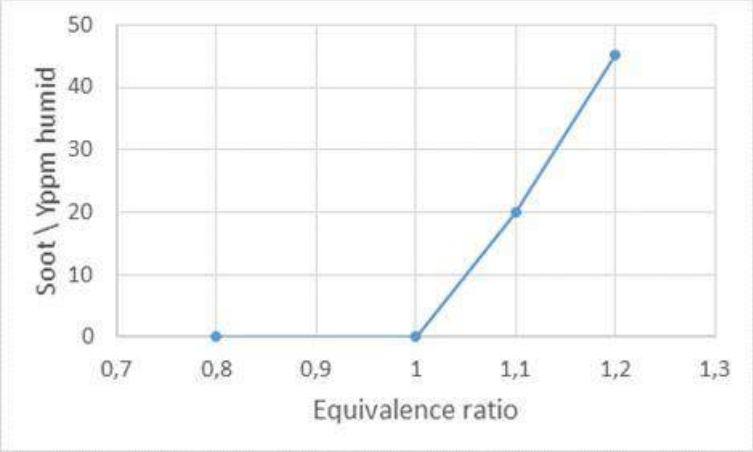


Figure 2-26 Soot emissions for various equivalent ratios at 2000 rpm, 6 bar IMEP.

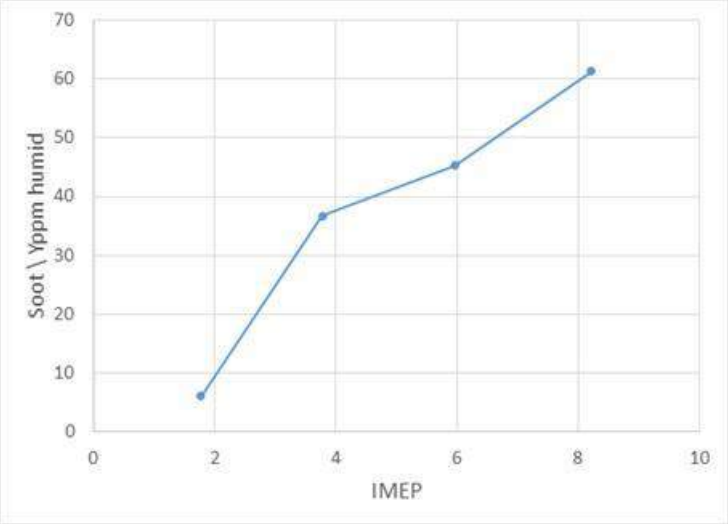


Figure 2-27 Soot emissions in rich conditions (equivalent ratio = 1.2) as a function of IMEP, 2000 rpm.

Unburned hydrocarbons are not modelled using the coupled approach. The simulation of HC is a real challenge for 0D/1D phenomenological models. It is not addressed at this stage.

2.3 Reduced Mean Value Engine Model

2.3.1 Introduction to the MVEM

Mean value models (also known as quasi-linear models) are intermediate models between map-based models and crank-angle based models. Basically, the cylinders are described using energy and mass conservation equations, but complex in-cylinder phenomena such as combustion and heat transfer are described using empirical equations (or efficiency maps). Moreover, the temperature, pressure and mass flows variations in the engine block are averaged over the cycle (hence the “mean value” name). Mean value models tend to represent the engine behaviour with a maximum possible number of physical equations given the “black-box” type representation of the cylinders. They allow for greater simulation speed and compactness while still delivering relatively good insight and accuracy.

The main inputs of the MVEM are:

- The engine speed,
- The intake manifold conditions (pressure, temperature and composition),
- The fuel mass flow rate and enthalpy flow rate,
- The exhaust conditions (mainly pressure),

- The engine coolant temperature.

The main calculated outputs are:

- The combustion heat release,
- The indicated torque,
- The intake mass flow rate,
- The exhaust mass flow rate, enthalpy flow rate,
- The heat rejection.

The in-cylinder process is modelled using several efficiency maps or values. The intake mass flow rate is evaluated using a volumetric efficiency map, η_V:

$$dm_{intake} = \rho_{in} . \eta_V . \frac{\omega}{4\pi} . C,$$

Where C is the engine displacement [m^3], ω is the engine speed [rad/s] and ρ_{in} is the density of the intake gases.

The mean combustion heat release, dh_{comb}, is directly linked to the injection mass flow rate. In order to be as accurate as possible, a combustion efficiency, η_{comb}, is introduced as below:

$$dh_{comb} = dm_{fuel} . Q_{hv} . \eta_{comb},$$

where dm_{fuel} is the injected mass flow rate [kg/s] from direct or indirect injection and Q_{hv} the fuel heating value.

The combustion heat flow rate is handled using an energy balance (Figure 2-28) and converted into:

- Mechanical power at the crankshaft (indicated power since the frictions are handled outside of the component),
- Thermal power lost in the exhaust gas,
- Thermal power transferred to the cylinder walls (heat rejection).

Each of these conversions is characterized by a dedicated efficiency.

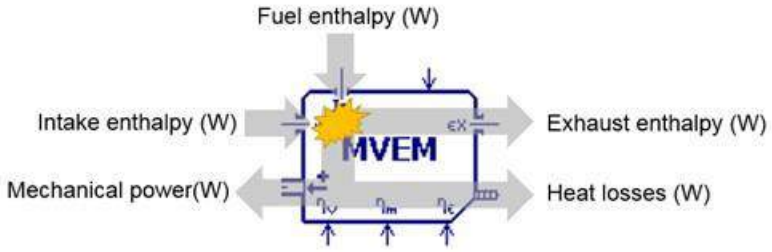


Figure 2-28 Cylinder energy balance in the MVEM.

A corrected indicated efficiency map is used inside the model to take into account the pumping losses, which have a major impact on the transient behaviour of the system in particular during tip-out conditions (an injection cut-off leads to motored conditions/engine brake) on turbocharged engines. The pumping losses are expressed in the form of an indicated mean effective pressure using a correlation from the Ecole Centrale de Nantes that combines the effects due to the low pressure loop and the high pressure loop:

$$IMEP_{motored} = -(P_{exh} - P_{int}) . \left(1 - \frac{N}{N_{max}}\right) - P_{exh} . \left(\frac{N}{N_{max}}\right)^2 - 0.35\, P_{int}.$$

From this, one can generate an equation for a corrected indicated efficiency, including the pumping losses:

$$\eta_{ind}^{corr} = \frac{T_{ind}.\omega - W_{Pump}}{dm_{inj}.Q_{hv}.\eta_{comb}}.$$

To determine the complete energy balance, an exhaust efficiency map is used to compute the fraction of heat losses send to the exhaust. The following equation is used:

$$\eta_{exh} = \frac{dh_{exh} - dh_{inj} - dh_{int}}{dm_{inj}.Q_{hv}.\eta_{comb}}.$$

Where dh represents enthalpy flow rates. Finally, the energy losses through the cylinder walls are deduced from the energy balance.

2.3.2 Introduction to the migration workflow

The methodology to switch from a baseline HF model to the corresponding MVEM is presented here. The basic principle of the migration process applied to a multi-cylinder engine is given in Figure 2-29. Only the "cylinders" are impacted by the migration process. In other words, we replace the CFM and the cylinder head model (gas exchange process) by a single component that modelled the engine block. The final objective when developing a MVEM is to keep the air path system unchanged. This ensures that the final model will be able to capture the main engine time responses that are related to the turbocharging system (the so-called turbo lag) and the manifold filling/emptying processes.

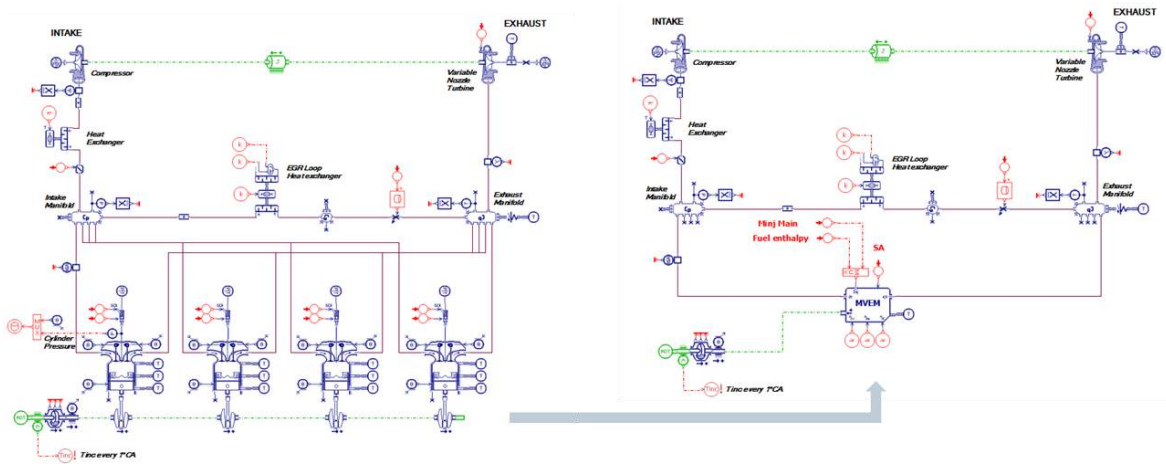


Figure 2-29 Migration from a crank-angle resolved model to a Mean Value Engine Model.

The generation of the results from the reference model, in order to create the MVEM data, is supported by a "MVEM Tool" which is a standard feature in Simcenter Amesim. This tool makes use of the MVEM equations mentioned in the report in order to evaluate engine efficiencies from the simulated variables. The process is illustrated in Figure 2-30. The principle is to apply a Design of Experiment (DoE) on the validated reference model (in our case the single-cylinder engine model) so as to generate a full set of data that are post-processed to create the data and maps that feed the MVEM component.

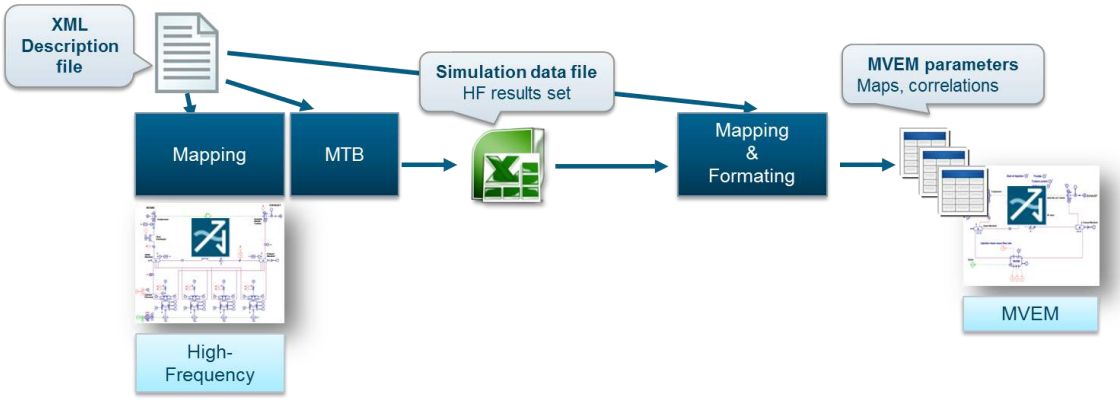


Figure 2-30 Migration workflow by the MVEM tool.

2.3.3 Application of the methodology for the PaREGEn project

The single-cylinder engine model is used to generate the data required by the MVEM component. In a first step, we focus on the 12 baseline operating points in order to develop and then validate the process. In a second step, we generate a full DoE to be able to cover a various degree of freedom of the engine.

At this stage, we apply some signals to control the single-cylinder engine model and collect the results required for the data processing and MVEM set-up. The controls of the reference model are identified on the sketch of the model in Figure 2-31.

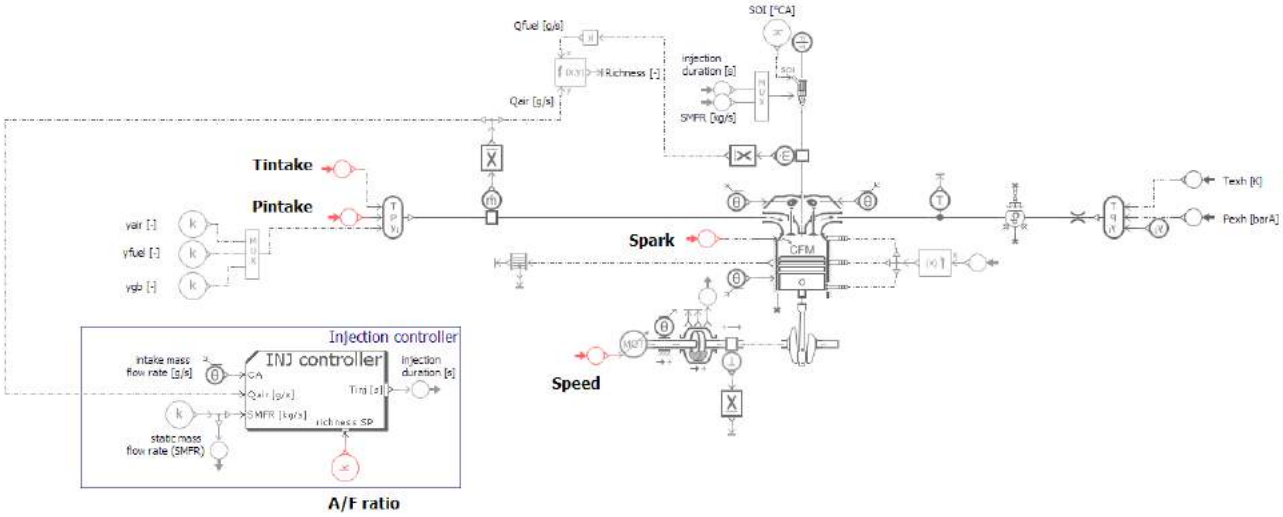


Figure 2-31 Control of the single-cylinder engine model.

The outputs of the model used for the processing of the data are given in the Table 2-11.

Table 2-11 Outputs of the single-cylinder engine model for data processing.

Input variables	Unit
Air mass flow rate	g/s
Exhaust temperature	K
Residual mass fraction	-
Indicated mean effective pressure	bar

The equivalent MVEM model presents some similar inputs (see Figure 2-32) except for the control of the injection which is no longer a stroke to stroke process but replaced by a mean fuel flow to be consistent with the "mean" value modelling. The MVEM includes a map providing a value for the *Yres* (residual mass fraction)

whatever the operating conditions, in order to allow the interface with the map-based emissions model. In practice, this map is generated using the same process as for the MVEM efficiencies in the MVEM tool.

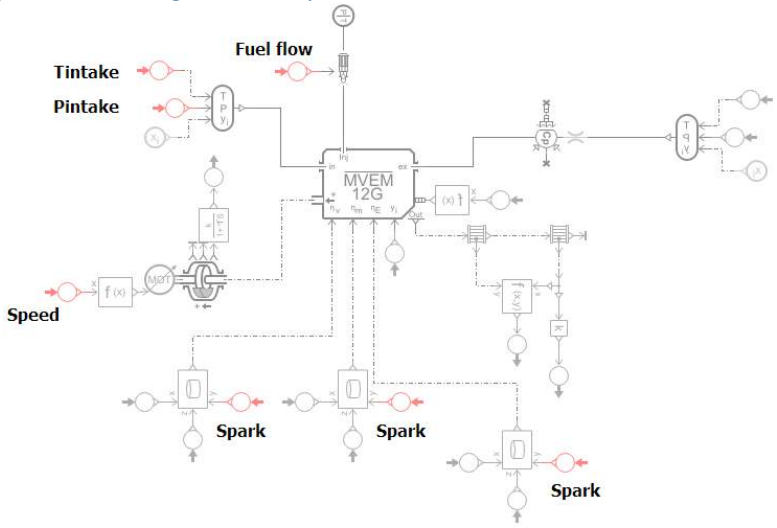


Figure 2-32 Control of the MVEM equivalent model.

As mentioned above, the validation process consists in the completion of the migration process using the 12 reference operating points. The results given by the MVEM must be consistent with the results generated by the reference crank-angle resolved model. In practice, the air mass flow rate is perfectly handled by the process (Table 2-13) and the IMEP as well (Table 2-12Table 2-14). There are reasonable discrepancies observed on the exhaust temperature evaluation (Table 2-14) since the data processing workflow (in the MVEM tool) includes some assumptions related to the handling of the gas properties. It leads to minor deviations, once the estimated exhaust efficiency data are applied in the MVEM component.

Table 2-12 Comparison between the MVEM and reference model for the IMEP production.

Point	IMEP MVEM [bar]	IMEP reference [bar]	deviation [bar]
1	1.89	1.87	-0.019
2	4.04	4.11	0.069
3	6.04	6.13	0.091
4	8.20	8.33	0.132
5	1.80	1.79	-0.016
6	3.81	3.81	0.002
7	5.97	6.01	0.031
8	8.22	8.27	0.057
9	1.96	1.97	0.006
10	4.33	4.40	0.065
11	6.51	6.56	0.054
12	8.79	8.85	0.053

Table 2-13 Comparison between the MVEM and reference model for the air mass flow rate.

Point	MFR MVEM [g/s]	MFR reference [g/s]	deviation [g/s]
1	1.344	1.344	0.000
2	2.301	2.299	-0.002
3	3.166	3.163	-0.003
4	4.093	4.090	-0.003
5	1.900	1.894	-0.006
6	3.246	3.242	-0.005
7	4.649	4.643	-0.005

8	6.081	6.076	-0.005
9	2.394	2.410	0.016
10	4.274	4.308	0.034
11	5.957	5.986	0.030
12	7.710	7.733	0.023

Table 2-14 Comparison between the MVEM and reference model for the exhaust temperature.

Point	Texh MVEM [K]	Texh reference [K]	deviation [K]
1	1004.2	977.8	-26.5
2	1010.9	1020.9	10.0
3	986.9	982.0	-4.9
4	969.1	968.4	-0.7
5	1128.8	1145.6	16.8
6	1117.6	1129.4	11.8
7	1103.2	1112.4	9.2
8	1095.0	1103.4	8.4
9	1209.5	1228.6	19.2
10	1199.5	1211.1	11.6
11	1184.4	1191.0	6.6
12	1171.4	1175.7	4.2

Since the MVEM model reflects accurately the behaviour of the reference single-cylinder engine model, the emissions prediction model gives the same pollutant levels and the discrepancies are negligible as for the air mass flow rate or IMEP evaluation as illustrated above.

3 Discussion and Conclusions

3.1 Discussion and future works

The soot modelling activities at LOGE might lead to the development of new approaches or enhancements. The methodology developed by Siemens and detailed in the present document is then subject to possible change during the PaREGEn project. In particular, the handling of the emissions in Simcenter Amesim, based on a simple map-based approach would evolve with additional degree of freedom to be considered like the injection pressure or other variables related to the actual operation of the engine. However, these possible upgrades of the soot model by LOGE could be quickly inserted in the workflow researched and developed by Siemens. The enhanced results could be then reported by Siemens to the PaREGEn partners.

In the scope of the PaREGEn project, Siemens will also generate a demonstrator for a full vehicle model evaluated on a real driving cycle. For this, an air path system model will be implemented on the validated MVEM model. The next step will be to include the multi-cylinder engine model into a powertrain and vehicle model piloted by a driver model. The final goal is to develop the capacity to simulate the full vehicle on a RDE cycle.

3.2 Conclusion

The activities conducted by Siemens in the Work Package 1 and reported in the present document were largely supported by the other partners, including BOSCH and LOGE. On one hand, BOSCH generated and shared the raw data used for the 0D/1D modelling tasks by LOGE and Siemens in particular. On the other hand, LOGE strongly collaborated for the definition and development of the interface between their SI-SRM model and the Siemens modelling approach. Thanks to this collaborative environment, Siemens was able to research and develop an efficient workflow based on a phenomenological combustion model (CFM) coupled with a map-based model for the engine-out emissions including soot. The migration process towards a MVEM approach is a trigger point for an extension of the activities in the domain of vehicle simulation. The objective is actually to be able to implement the findings of the WP1 activities for soot estimation in a system model that permits the evaluation of the approaches in a vehicle context over real driving cycles.

4 Deviations and Risks

4.1 Deviations

4.1.1 Description of work related to deliverable in GA Annex 1 – Part A

The work done is related to Task 1.6 Exploitation of simulation models and Sub-Task 1.6.1 Phenomenological high frequency to mean value models (Task lead: SIEMENS; Partners: ETH, LOGE) [M1-M18].
The goal of this sub-task will be to ensure the continuity between research SI-SRM simulation (LOGE) and commercial 1D simulation software, in that case Siemens Simcenter Amesim. The first goal will be to prototype the coupling of SI-SRM simulator with a standard crank-angle (CA) Simcenter Amesim engine model using, as far as possible, standardized interfaces and reproducible methods, from strong coupling to model reduction. The integration of Simcenter Amesim injection models as complementary to advanced SI-SRM boundary conditions will also be investigated, due to the injection impact on pollutants formation. Prototypes will be progressively validated up to full engine model validation. Full engine variability modelling will also be investigated in order to improve results representativeness. To improve computational performances, the crank angle engine model integrating SI-SRM will be reduced to a new MVEM. This model will especially extend its current capacity regarding particulate matter sizes and distribution prediction. The impact of the reduction on the prediction levels will also be evaluated in order to ensure the fidelity of the MVEM model to the CA model, on the largest operation range possible. The MVEM prediction results will also be evaluated versus engine measurements to assess the achieved accuracy.
Inputs: SI-SRM and its reduction, engine data and measurement.
Outputs: Tools and methods enabling industrial exploitability of SI-SRM and derived models.

4.1.2 Time deviations from original planning in GA Annex 1 – Part A

There are no deviations with respect to timing of this deliverable

4.1.3 Content deviations from original plan in GA Annex 1 – Part A

There is no significant deviation in terms of content.

4.2 Risk Register

Risk No.	What is the risk	Probability of risk occurrence*1*	Effect of risk*2*	Solutions to overcome the risk
WP1.6	Low quality of the prediction of soot emissions from simulation	2	3	The modelling workflow developed by Siemens can be easily updated when enhanced prediction are available in the PaREGEn project and implemented in the LOGE SI-SRM models in particular.

[1] Probability risk will occur: 1 = high, 2 = medium, 3 = Low

[2] Effect when risk occurs: 1 = high, 2 = medium, 3 = Low

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Appendix A – Acknowledgement

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Project partners:

#	Partner	Partner Full Name
1	RIC	RICARDO UK LIMITED
2	DAI	DAIMLER AG
3	JLR	JAGUAR LAND ROVER LIMITED
4	BOSCH	ROBERT BOSCH GMBH
5	FEV	FEV EUROPE GMBH
6	JM	JOHNSON MATTHEY PLC
7	HON	HONEYWELL, SPOL. S.R.O.
8	JRC	JOINT RESEARCH CENTRE – EUROPEAN COMMISSION
9	UNR	UNIRESEARCH BV
10	IDIADA	IDIADA AUTOMOTIVE TECHNOLOGY SA
11	SIEMENS	SIEMENS INDUSTRY SOFTWARE SAS
12	LOGE	LUND COMBUSTION ENGINEERING LOGE AB
13	ETH	EIDGENOESSISCHE TECHNISCHE HOCHSCHULE ZUERICH
14	UDE	UNIVERSITAET DUISBURG-ESSEN
15	RWTH	RWTH AACHEN UNIVERSITY
16	UFI	UFI FILTERS SPA
17	UOB	UNIVERSITY OF BRIGHTON
18	GARR	GARRETT–ADVANCING MOTION

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Appendix B – Quality Assurance

The following questions should be answered by all reviewers (WP Leader, peer reviewer 1, peer reviewer 2 and the technical coordinator) as part of the Quality Assurance Procedure. Questions answered with NO should be motivated. The author will then make an updated version of the Deliverable. When all reviewers have answered all questions with YES, only then the Deliverable can be submitted to the EC.
NOTE: For public documents this Quality Assurance part will be removed before publication.

Question	WP Leader	Peer reviewer 1	Peer reviewer 2	Technical Coordinator
	Andreas Manz (BOSCH)	Andrea MATRISCIANO (LOGE)	Bastian MORCINKOWSKI (FEV)	Simon EDWARDS (Ricardo)
1. Do you accept this deliverable as it is?	Yes	Yes	Yes	Yes
2. Is the deliverable completely ready (or are any changes required)?	Yes	Yes	Yes	Yes
3. Does this deliverable correspond to the DoW?	Yes	Yes	Yes	Yes
4. Is the Deliverable in line with the PAREGEN objectives?	Yes	Yes	Yes	Yes
a. WP Objectives?	Yes	Yes	Yes	Yes
b. Task Objectives?	Yes	Yes	Yes	Yes
5. Is the technical quality sufficient?	Yes	Yes	Yes	Yes

Abbreviations and Nomenclature

CFM	Coherent Flame Model
EGR	Exhaust gas recirculation
HF	High Fidelity
IMEP	Indicated Mean Effective Pressure
IVC	Intake Valve Closing
MVEM	Mean Value Engine Model
RDE	Real Driving Emissions
SI	Spark Ignited
SRM	Stochastic Reactor Model