Identification of Emission Models in a Spark Ignition Engine for Control Applications

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Abstract

A procedure for the identification of emission models for the design of optimal control of spark ignition engines is presented. The procedure is based on a decomposition technique for the definition of optimal model structure with limited number of parameters.
A two step scheme has been built: in the first step the available physical models, based on a multi-zone thermodynamic model with emission sub-models, are parametrized and an intermediate model, based on Taylor approximation, is derived in order to describe the non linear influence exerted by the physical parameters; in the second step the physical parameters are modeled by means of non linear regression, taking into account the effect of operating engine variables, and the optimal parameters obtained via stepwise approach. The features of the identification technique and preliminary results over a set of more than 300 experimental data are presented.

General

Many mathematical models have been developed for the design of automotive engine control strategy, with different structure and complexity. They range from input-output black-box models, mostly oriented to control design, to gray-box mean-value models, embedding a simplified description of the most relevant physical processes [1,2,3], up to complex 3-D fluid-dynamic models, which could in principle offer a detailed prediction of geometry and control strategy on engine operation [4,5]. These models substantially differ in terms of computational time and experimental data required: for the validation of the simplest black-box models, hundreds or thousands of engine data could be needed to compensate for the lack of physical information, resulting in lower model flexibility; on the opposite side, the computational cost of the detailed 3-D models is not compatible with most control applications.
In some cases, a mixed approach is adopted in order to combine the advantages of various kind of models. An example of hierarchical modelling structure, developed by the authors for the optimal design of control strategies, is shown in fig.1 [6]. A gray-box mean-value model is embedded within a computer code for control simulation and optimization [7,8,9], which is now in use by Magneti Marelli: at higher level, phenomenological models [10,11] and experimental design techniques [12] are employed to reduce the recourse to experiments.

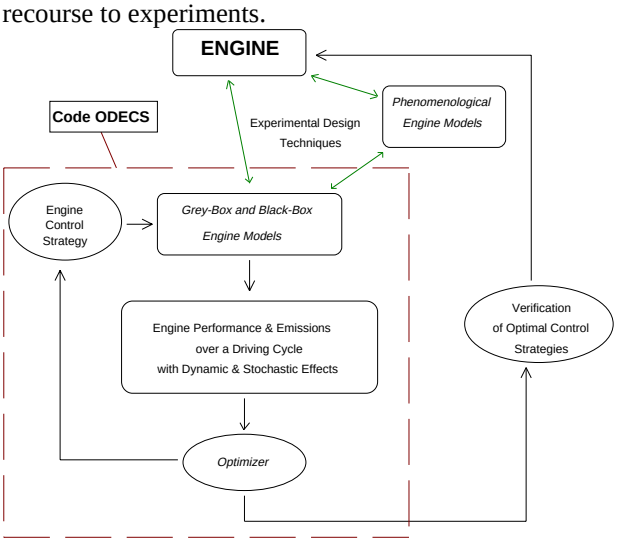

Fig.1 - A hierarchical model structure for engine control design.

An important task for control applications is represented by the prediction of engine emissions. At this moment, fully predictive emission models suitable for the optimal design of engine control strategies, which requires extensive computations, are not yet available. Therefore, a certain number of model parameters must be identified by comparison with experimental data, and their relationships with operating variables determined, in order to use the model for prediction. Several problems arise in the identification phase, due to i) presence of non-linearity, ii) unknown functional relationships between model parameters and engine variables and iii) possible over-parametrization, which imply larger demand of experimental data for model validation.
A conventional approach would therefore require repeated trial and error recourse to non-linear numerical Least Square or Maximum Likelihood techniques, each time that a different functional structure of model parameters were analyzed, with high computational cost.

In the following chapters, a systematic procedure for parameter identification based on decomposition approach is proposed, in order to overcome these problems and to reduce the number of engine experimental data for model validation. The procedure has been applied to the identification of phenomenological emission models quoted in fig.1, synthetically described in next chapter.

Engine and Emission Models

Engine pressure cycle is computed by a classical two-zone thermodynamic model [13]. The heat release law is specified by a Wiebe function. A correlation between combustion time and operating variables, with ten parameters, has been determined, starting from optimal values of combustion time computed by numerical least square techniques, over a set of more than 300 steady-state experimental data [10,11]. A multi-zone model is then used to estimate temperature gradients in burned gases. The key features of the emission models are summarized in the following table:

Model	Mechanism
NOx	Thermal formation through Zeldovich kinetic mechanism [4];
CO	Kinetic equation [4,5];
HC	Adsorption and desorption in lubricant film; Inflow and outflow from then crevices; Post-flame oxidation. [11,14]

Tab.I - Features of the emission models

A model for mechanical losses has also been developed and validated. A detailed description of these models is not compatible with the space constraints of this paper. For further information, the reader is addressed to recent papers of the authors [10,11].

Model Identification

A general non-linear "physical" model (subscript ph) expresses the output variable *y* (i.e. HC, CO or NOx emissions) as function of engine operating variables ν and of a vector of parameters *p*:

$$(1)\quad y_{ph,i} = f\left(p_i, \nu_i\right)$$

where subscript i refers to given engine operating conditions (i.e. engine torque and speed, mixture ratio, spark advance, manifold pressure). The parameters *p* can represent physical quantities used in the model, as kinetic rates, number of zones to account for temperature stratification in burned gases, various coefficients. In many cases, their values could not be considered constant over the entire operational range of the engine. Therefore, they are in turn expressed as a function of the engine operating variables ν, by means of *N* further parameters β, in order that the model could be used in predictive way over the whole operational range:

$$(2)\quad y_{ph,i} = f\left(p_i\left(\beta, \nu_i\right), \nu_i, \beta\right)$$

A direct approach would require the following steps:

i) specification of the parameters *p* of the physical model;
ii) specification of functional structure of the relationships *p(*β,ν*)*;
iii) determination of the optimal values of the *N* parameters β by comparison of computed and observed values over the set of *M* experimental conditions, solving a non linear regression problem:

$$(3)\quad \min_{\beta} S(\beta) = \sum_{i=1}^{M}\left(y_{ph,i}\left(p_i\left(\beta, \nu_i\right), \nu_i, \beta\right) - y_i^*\right)^2$$

iv) estimation of statistical significance of the solution.

It has to be noticed that step iii) involves repeated model evaluation over the entire set of experimental data. For real cases, (i.e. *N*=10÷50, *M*≈300), many thousands of model evaluations would be therefore required, with very high computational cost. Moreover, the entire process from ii) to iv) should be repeated each time that a different functional structure *p(*β,ν*)* has to be assumed, since most of the information achieved to arrive at the solution of the previous problems (3) can not be utilized and is therefore lost.

Decomposition approach

In order to overcome these problems, a two-phases decomposition approach is proposed.
The first phase would require the following steps:

a) specification of the parameters *p* of the physical model;
b) determination of an intermediate model $y_t(p)$ (i.e. 2nd order Taylor approximation) to describe the influence of the physical parameters *p* which exert a non linear influence on the model:

$$(4)\quad y_{t,i}(p) = y_{ph}(p_0) + \sum_{j=1}^{N}\left(p_j - p_{0j}\right)\frac{\partial y_{ph}}{\partial p_j} + \frac{1}{2}\sum_{k=1}^{N}\sum_{j=1}^{N}\left(p_j - p_{0j}\right)\left(p_k - p_{0k}\right)\frac{\partial^2 y_{ph}}{\partial p_j \partial p_k}$$

c) for each i-th operating condition, numerical computation of gradient and Hessian, and their storage in data files;
d) evaluation of the approximation errors $\varepsilon_{i,j}$ for finite variations of each parameter around its nominal value $p_{0,j}$ (*k*=1.1):

$$(5)\quad \varepsilon_{i,j} = y_i^* - y_{ph,i}\left(p_{0,1}, .. p_{0,j-1}, kp_{0,j}, p_{0,j+1}, .. p_{0N}\right)$$

The total approximation error ε_i can then be estimated by a linear model:

(6) $$\varepsilon_i = \frac{1}{\alpha}\sum_{j=1}^{P}\varepsilon_{i,j}\frac{p_j - p_{0,j}}{p_{0,j}}$$

The second phase is composed of the following steps:

e) specification of a functional structure $p(\beta,\nu)$; the following general polynomial relationship has been used:

(7) $$p_{i,k} = \sum_{j=1}^{N}\chi_{j,k}\beta_j\prod_{l=1}^{L}v_{i,l}^{\phi_{j,k,l}}$$

where the actual functional form is determined by the matrices ϕ and χ; this latter assumes 0 or 1 values, and can be changed according to the stepwise procedure to include or exclude some terms in eq.(7);

f) determination of the optimal values of the parameters β by solving a non linear constrained minimization problem (8,9), using the Taylor approximation; constraints (9) are introduced to avoid that unfeasible solutions could be proposed, where the estimated approximation error is larger than a given limit ε_{max}:

(8) $$\min_{\beta} S(\beta) = \sum_{i=1}^{M}\left(y_i\left(p_i(\beta,\nu_i),\nu_i,\beta\right) - y_i^*\right)^2$$

(9) $$\varepsilon_i(\beta) \le \varepsilon_{\max} \qquad i = 1, M$$

the optimization problem has been solved by Augmented Lagrangian approach [17], using the Powell conjugate directions algorithm [18];

g) estimation of the limits of confidence regions at level of probability $(1-\alpha)$ for parameters β, by numerical solution of the following equation:

(10) $$S(\beta) = S(\beta^*)\left[1+\frac{N}{M-N}F(N, M-N, 1-\alpha)\right]$$

where $S(\beta^*)$ represents the sum of squares corresponding to the solution of problem (8,9), and F is the Fisher distribution with N parameters, M observations at $(1-\alpha)$ probability [15].

h) elimination of the less significant parameters β, by zeroing the corresponding χ values in eq.(7);

i) check of the termination criteria (i.e. considering the ratio between the larger and smaller confidence intervals) and repetition of steps f and g (backward stepwise regression).

This procedure offers the following advantages:

- Only the first phase requires a full model evaluation on the entire data set (step c) to compute gradient and Hessian. This information can be stored and easily updated if further parameters would be added to the model.
- Each iteration of the regression technique (step f) is much more faster since it operates on polynomial approximations rather than on the full model.
- The resulting objective function is quadratic, with linear constraints, and very fast convergence can be achieved by classical optimization techniques.
- The entire process can be easily iterated for each different model parametrization, and a stepwise approach can be followed in order to determine the most significant model parameters.
- As final result, an entire class of models with a decreasing number of parameters is obtained, and a trade-off between number of parameters and fitting precision can be achieved.

Results

The three models have been validated over a set of 336 experimental data, measured at Laboratories of Istituto Motori in Naples, in steady-state conditions. The experimental apparatus has been described in previous papers [16]. The following model structure has been adopted:

(11) $$y = p_1(\beta,\nu) + p_2(\beta,\nu)y_T\left(p(\beta,\nu)\right)$$

Besides the parameters p included in the Taylor model y_T, further two terms p_1 and p_2 have been introduced. In case of NOx model, two "physical" parameters have been considered, consisting of kinetic rates in the first two equations of Zeldovich mechanism [4,10,11]. For the HC and CO model, only the first two components of p have been considered. This choice is due to the fact that this analysis has been mainly directed to verify the capabilities of the identification technique, rather than to check the best model performance, which could be certainly improved by a more careful and detailed parametrization. The maximum number of parameters β to be identified is equal to 28 for CO and HC, and to 50 for NOx. Computation of gradient and Hessian has been performed only for the components of p included in the model y_T.

Model	Number of parameters p (P)	No. of physical parameters	Max No. of parameters β (N)
HC	2	0	28
CO	2	0	28
NOx	4	2	50

Tab.II - Number of parameters for the three models

A vector of six engine variables ν has been considered, as described in next table:

1 - Engine speed (rpm)	4 - Air Flow Rate (kg/s)
2 - Air/Fuel Ratio (/)	5 - Ambient Pressure (Pa)
3 - Engine Torque (Nm)	6 - Spark Advance (deg)

Tab.III - Set of engine operating variables

The ambient pressure has been used as dummy variable, to check the capability of the procedure in discarding

the less significant terms. Three separate analyses have been performed for HC, CO and NOx, because their parameters were independent.

The global results are summarized in fig.2 and in tab.IV. For each model, various solutions of the optimization problem (8,9) are reported, for different number of parameters *N*. On y axis of fig.2, the relative model error is plotted (i.e. the ratio of actual value of optimal sum of squares S over the value obtained by the physical model with nominal parameters p_0). On the abscissa, the current number of parameters *N* is reported. Since a backward stepwise approach has been adopted, the entire set of parameters is first included in the model, and in subsequent iterations the less significant of them are excluded. The relative error should generally be a decreasing function of *N*. In a first phase, where the less significant parameters are excluded, the error is almost constant. In some cases, a slight reduction of the error after the first steps may be also noticed, due to the increasing precision obtained in the subsequent numerical solutions of the problem (8,9).

For the NOx model, the relative error is almost constant passing from 50 to about 20 parameters, while it increases from 0.6 to about 0.7 by reducing the number of parameters from 20 to 10. In any cases, a significant improvement of model precision with respect to the starting physical model is achieved (fig.2, 3a-b).

For the HC model, the improvement with respect to the original model is much higher (fig.2, 4a-b), being relative error equal to about 0.30 for *N* ranging from 28 to 10; a relevant error reduction (about 0.44) can be still achieved even with a very small number of parameters.

For CO model, the relative error is higher than in the other two cases, ranging from about 0.65 to 0.70 when *N* passes from 28 to about 10 (fig.2, 5a-b). It must be also remarked that, when the physical models are used without further parametrization (N=0), poor precision levels are usually achieved (fig.3a, 4a, 5a, tab.IV).

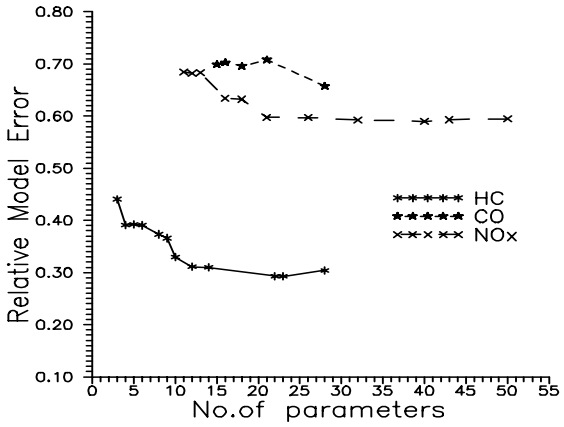

Fig.2 - Relative model error vs. number of parameters for the three physical emission models

HC		CO		NO_x	
N	R^2	*N*	R^2	*N*	R^2
0	0.273	0	0.775	0	0.418
10	0.663	16	0.862	15	0.754
28	0.716	50	0.878	28	0.784
(*) 288	0.893	(*) 288	0.871	(*) 288	0.905

Tab.IV - Number of parameters and correlation index for physical and black-box(*) models.

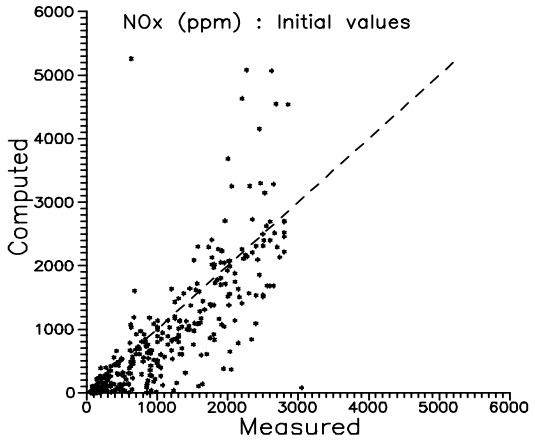

Fig.3a - Computed vs. measured NOx - N=0

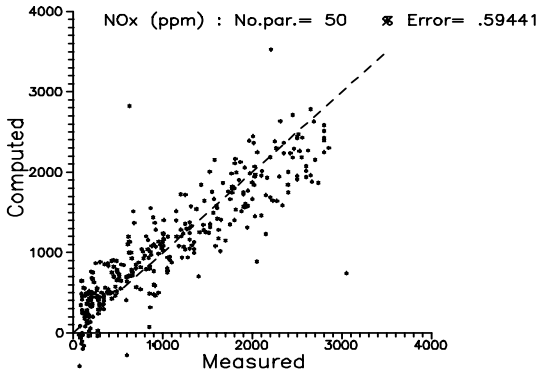

Fig.3b - Computed vs. measured NOx - N=50

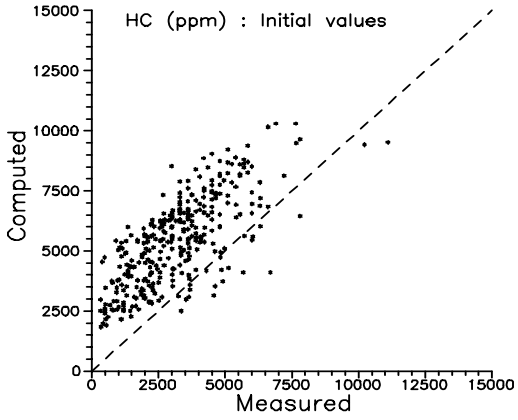

Fig.4a - Computed vs. measured HC - N=0

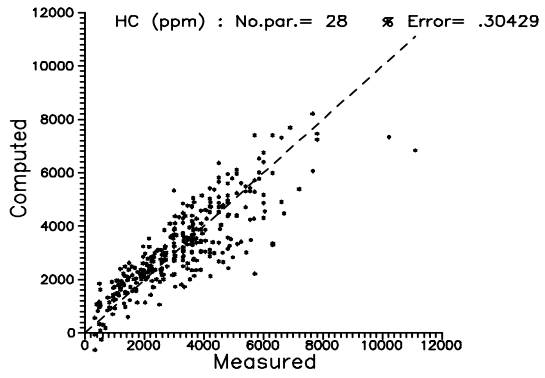

Fig.4b - Computed vs. measured HC - N=28

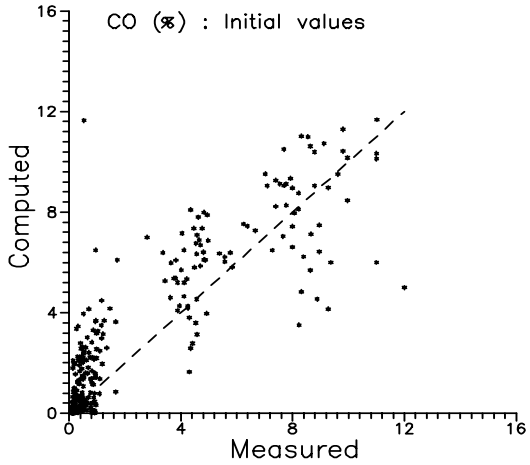

Fig.5a - Computed vs. measured CO - N=0

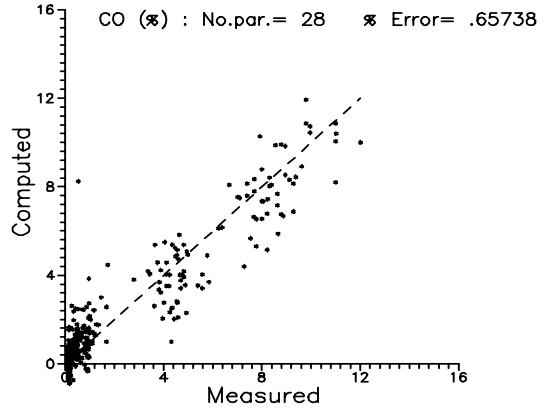

Fig.5b - Computed vs. measured CO - N=28

Finally, the results obtained by physical models can be compared with the ones achieved, on the same data, by a black-box approach, using polynomial regression. For each of the 18 points of the operating plane (Torque, rpm), a third order polynomial in two variables (air/fuel ratio and spark advance) with 16 coefficients has been used. Thus, 288 parameters would be needed for each model. By comparing these results with the previous ones (tab.IV), it can be observed that the determination coefficient among measured and computed values is not much higher than in the best results obtained by physical models, which instead need a number of parameters much lower. Therefore, this would imply that the number of experimental data for model validation can be drastically reduced, of more than one order of magnitude, by the combined use of physical models with the proposed identification technique. Finally, it has to be noticed that, at this stage of the work, attention has been mainly paid on development and implementation of the identification technique, rather than in the absolute precision of the physical models, outlier detection and specification of model parameters. Therefore it is reasonable to expect that further improvements could be achieved in next future by more careful analysis of such aspects.

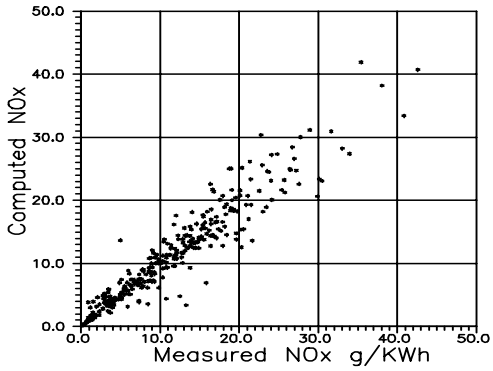

Fig.6a - Black-box model - NOx

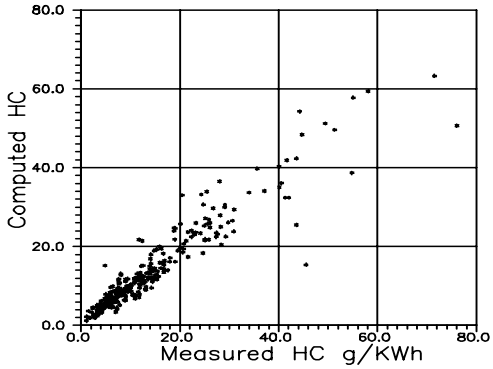

Fig.6b - Black-box model - HC

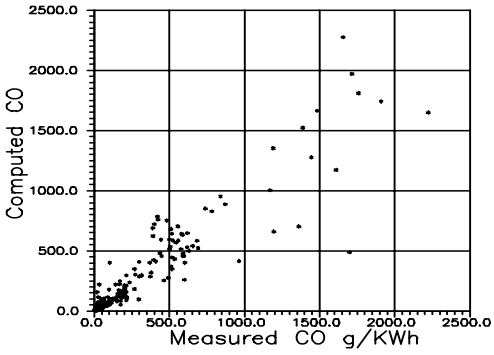

Fig.6c - Black-box model - CO

Conclusions

A procedure for the identification of emission models for spark ignition engines based on a decomposition technique has been proposed. The technique allows to determine the best model parametrization starting from a non-linear physical model, with limited computational time. A trade-off between model precision and number of parameters is also easily obtained.

The preliminary results, obtained over a large set of experimental data, show that model precision can be comparable with that obtained via conventional mapping procedures using black-box models, but with a drastic reduction of the experimental analysis with respect to these latter.

This approach can be therefore very attractive for the development of hierarchical models with limited computational and experimental demand for engine control design.

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Legende

ε	approximation error
ν	engine operating variables
β	model parameters
F	Fisher distribution
M	number of experimental observations
N	number of model parameters
P	number of physical parameters
p	parameters of the physical model
y	computed value
y*	measured independent variable
y_{ph}	physical model
y_T	2nd order Taylor approximation

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