

CFD Analysis of Combustion and Knock in an Optically Accessible GDI Engine

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ABSTRACT

The occurrence of knock is the most limiting hindrance for modern Spark-Ignition (SI) engines. In order to understand its origin and move the operating condition as close as possible to onset of this potentially harmful phenomenon, a joint experimental and numerical investigation is the most recommended approach. A preliminary experimental activity was carried out at IM-CNR on a 0.4 liter GDI unit, equipped with a flat transparent piston. The analysis of flame front morphology allowed to correlate high levels of flame front wrinkling and negative curvature to knock prone operating conditions, such as increased spark timings or high levels of exhaust back-pressure.

In this study a detailed CFD analysis is carried out for the same engine and operating point as the experiments. The aim of this activity is to deeper investigate the reasons behind the main outcomes of the experimental campaign. A tabulated knock model is presented, based on detailed chemical mechanism for the surrogate gasoline. Combustion and knock simulations are carried out in a RANS framework through the use of validated models and the results are compared with cycle-resolved acquisition from the test-bed. The results of the CFD analysis explain the experimentally observed flame behavior and allow to proficiently understand the reasons of the sensitivity to knock of the analyzed unit.

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INTRODUCTION

The recent trend in the design of internal combustion engines is increasingly driven by the limitation of tailpipe pollutant emissions such as CO, NO_x and UHC, combined with a renewed and strong focus paid on CO₂. Promising ways to reduce overall fuel consumption and fulfil the mentioned limitations are the "downsizing" and "down-speeding" strategies, consisting in a progressive reduction of the displaced volume and of the revving speed [1, 2]. In order to preserve the low-load/low-rpm performance, the specific engine output needs to be increased through turbocharging and higher compression ratios.

Both these strategies lead to an increased risk of air-fuel autoignition in spark-ignition (SI) units, also known as "engine knock", which constitutes the major barrier to the achievement of even higher specific performance [3]. Knock is the consequence of the autoignition of a portion of unburnt fuel-air charge before the main

propagating flame front regularly consumes it. It induces a set of high-frequency pressure waves which are responsible for damaging mechanisms of the solid components facing the combustion chamber, such as metal erosion and lubricant film removal, leading to a rapid engine failure for heavy knocking conditions [4, 5].

In order to obtain the maximum allowable specific performance, modern SI units need to operate as close as possible to those promoting engine knock, without incurring in the harmful knock onset. This task is even more complex given the highly stochastic nature of engine flows, leading to cycle-to-cycle variability (CCV) and to the random cycle-dependent knock occurrence [6].

In this framework, the need for accurate and robust tools able to predict fuel autoignition and its dependence on local conditions is a fundamental requirement in the design of modern SI units. Advances in 3D CFD models for spark-combustion and autoignition allow to investigate and identify the reasons for autoignition onset to level which would not be possible with experimental techniques alone,

which are usually confined to laboratory engines [7]. On the other side, numeric models need a thorough validation which can be verified only on instrumented engines.

The most rigorous way to simulate the fuel-air autoignition is the complete resolution of all the forward and backward reactions that are present in the chemical mechanism. In this case the accuracy of the result is completely based on the validation of the native chemical model and on numerical tolerances, especially regarding time discretization. The advantage of a numerically exact result collides with the unaffordable CPU cost of this kind of simulations, especially when complex geometries are investigated with actual fuels, whose chemistry needs typically hundreds of intermediate species for a complete oxidation pathway and the resolution of a transport equation is needed for each of these. Moreover, they assume the fluid cell as a laminar chemical reactor: this makes this approach intrinsically not correct when the simulation of a turbulent flame is needed, since any turbulence-flame interaction is neglected. All the mentioned complications motivate the need for simpler approaches as an essential step.

As for this second approach, the most consolidated practice consists in the use of autoignition (AI) delay times as global indicators of the fuel-air mixture reaction rate. These are usually fitted as a function of local physical conditions and a relevant work is the study by Douaud and Eyzat [8] or similar analyses by other authors [9, 10]. This kind of modelling is CPU-efficient, since the reaction rate is modelled by an algebraic expression, although the modelling accuracy is usually guaranteed on a limited validation range.

An alternative procedure consists in the tabulation of AI delay times as simulated by a chemical solver. These can be calculated for a wide range of physical conditions and stored in a dedicated database (look-up table), which can be addressed during the calculation given that ad-hoc interrogation and interpolation strategies are developed. This approach is promising as in principle it allows to preserve the accuracy of the original chemical mechanism. This is motivated by the calculation of the AI delay times based on a detailed chemical mechanism, and at the same time a good CPU-efficiency can be guaranteed, since no chemical reactions are solved during the CFD run and no additional transport equations are solved for the chemical species. An in-house developed knock model based on this concept is modelled and will be presented in the next Section.

The present work is organized as follows. This study is the numerical counterpart of an experimental study conducted at the Istituto Motori of CNR on an optically accessible version of a currently produced DISI engine, with unitary displacement equal to 399 cm³. [7]. Numerical simulations for the same engine and conducted in a RANS framework with the aim of confirming the outcomes of the experimental campaign and to gain a deeper understanding of the registered trends of combustion and knock onset. As for the GDI spray modelling, a validation activity against experiment will be presented. Spark-ignition and combustion development are simulated through consolidated models and an in-house developed knock model is presented in details

and applied, both against fully resolved chemistry in a test case and against experimental results in the actual engine. The engine knock tendency experimentally measured through the Maximum Amplitude of Pressure Oscillation (MAPO) and IMPO knock severity indices is compared with the CFD results in terms of local and average in-cylinder pressure traces. Finally, in order to simulate the influence of combustion CCV on knock onset, artificially perturbed simulations are carried out in order to impose (not simulate) the maximum level of cyclic variability measured on the real engine. A comparative analysis of both flame kernel development and knock onset confirm the accuracy of the proposed modelling framework.

KNOCK MODELLING

The traditional modelling of knock in SI engines relies on empirical correlations for the autoignition (AI) delay time τ_d . This is defined as the temporal interval between the imposition of constant pressure and temperature to a given mixture (i.e. to a fixed air/fuel/EGR ratio) before the main heat release occurs. This approach was first proposed by Livengood and Wu [11] where the knowledge of the pre-knock chemical reaction rate can be neglected if a global delay time to autoignition is available. The main difficulty in knock prediction in internal combustion engines is that the physico-chemical conditions are continuously changing. Typical examples are:

- Pressure and temperature vary due to piston movement and energy release due to combustion;
- Reactant ratio is extremely varying in DI engines, with region of pure air and other saturated by fuel vapour; in-between the continuous range of air-fuel ratios is present;
- EGR mixing from the previous cycle can potentially add a further degree of mixture quality stratification.

In their work Livengood and Wu [11] proposed a simple relationship between the AI delay and the knock onset as in [Eq. 1](#).

$$I = \int_{t_0}^t \frac{1}{\tau_d} dt \quad (1)$$

In the [Eq. 1](#), t_0 is a conventional time where chemical reaction rate becomes relevant for the analysed case, which in this study is assumed as half of the compression stroke, where pressure and temperatures are such that chemical kinetics of the air-fuel mixture still presents an extremely slow reaction rate. [Equation 1](#) is integrated in time as calculation proceeds and the unknown is the instant t where the unity value is reached. The crank angle corresponding to this condition is the knock onset angle. If in-cylinder conditions are such that the $I < 1$ is verified during all the combustion period, then the unburnt mixture is sufficiently knock resistant and autoignition does not occur. Conversely, if $I = 1$ condition is verified autoignition occurs and the integral function loses any physical meaning for $I > 1$. Therefore, the Livengood-Wu Integral is a synthetic way to model the pre-knock reactions based only on the global AI delay time. The main advantage is that pre-knock chemical reactions are not modelled in the CFD code, with an evident saving of CPU cost.

An alternative formulation for an integral knock function was proposed by Lafossas et al. [12] where a two-species framework was proposed. A knock precursor species is expressed by its concentration Y_{IG} , whose value is initially null. Its rate of increase is given by Eq. 2, which is dependent on the local autoignition delay time τ_d through Eq. 3:

$$\frac{dY_{IG}}{dt} = Y_{TF} \cdot F(\tau_d) \quad (2)$$

$$F(\tau_d) = \frac{\sqrt{\tau_d^2 + 4(1 - \tau_d)^{Y_{IG}/Y_{TF}}}}{\tau_d} \quad (3)$$

In Eq. 2 and 3 Y_{TF} is the fuel tracer mass fraction, i.e. the fuel as a passive non-reactive species. In the Lafossas et al. model it represents the local concentration threshold for the Y_{IG} knock precursor species: when the equality $Y_{IG} = Y_{TF}$ is verified, then the autoignition delay time τ_d is reached and knock is triggered. Several comparative tests were carried out between the Livengood-Wu integral function and the Lafossas et al. model for the same autoignition delay time τ_d . The results were in close agreement.

Both the integral formulations presented are based on the AI delay τ_d . This framework depicts the need of a detailed knowledge of the autoignition delay τ_d for a large variation of pressure, temperature, equivalence ratio and residuals. To this aim an empirical correlation was proposed by Douaud and Eyzat [8], which is reported in Eq. 4:

$$\tau_d = 0.01931 \cdot \left(\frac{OI}{100}\right)^{3.4017} \cdot \left(\frac{p_{[bar]}}{1 + X_{res}}\right)^{-1.7} \cdot \exp\left(\frac{3800}{T_u}\right) \quad (4)$$

In Eq. 4 OI represents the Octane Index of the analysed fuel, X_{res} the fraction of residual gases and T_u the temperature of the unburnt gases; the autoignition delay time τ_d is calculated in [s]. The Douaud and Eyzat correlation is used to calculate the autoignition delay based on local and instantaneous conditions, which can be used in both the integral methods previously presented (Livengood-Wu Integral or the knock precursor model proposed by Lafossas et al.).

An in-house developed knock model is proposed with the aim to overcome the use of empirical correlations such as the one by Douaud and Eyzat or similar. To this aim a variation of the synthetic Lafossas et al. knock model is developed based on an extended tabulation of autoignition delays for the adopted fuel. The aim of such a model are:

- Preserve the computational efficiency proper of a 2-species model (i.e. knock precursor Y_{IG} and fuel tracer Y_{TF}), where no chemical reactions are directly solved by the CFD solver.
- Improve the calculation of AI delay times with respect to empirical correlations. Each fuel/blend presents specific non-Arrhenius behaviours, a relevant example of this is the Negative Temperature Coefficient (NTC) region. A fitting of these fuel-specific distinctive features would be necessary in case of empirical correlations. In the framework of a tabulation technique, these features are intrinsically described by the look-up table.

- Decoupling from any flamelet combustion model. The physical variables governing the autoignition delay time (i.e. pressure, temperature, equivalence ratio and residual level) are not related to a specific combustion model and/or their implementation in the CFD code. The coupling with the in-use combustion model is operated through a progress variable of combustion, which is common in most flamelet combustion models.

The model is based on an extended set of off-line calculated constant pressure AI delay calculations performed by a chemical kinetics solver. The results are used to define a look-up table of ignition times, which will serve as a database of calculated chemical conditions. During the CFD calculation, this is recalled for each fluid cell at every iteration and an interpolated autoignition delay is calculated based on the closest physical conditions stored in the look-up table. The CFD solver is not invoked in the preliminary stage. The chemical kinetics software used for the look-up table construction is the DARS-Basic software. The range of physical conditions (i.e. pressure, temperature, equivalence ratio and EGR) must cover the entire design space of these physical variables which is experienced by the end-gases during the mixing and compression processes. The look-up table resolution should be as high as possible, in order to limit the interpolation job and to reduce the related error. A preliminary sensitivity analysis led to typical steps for each variable, which are:

- Pressure: 10 bar;
- Temperature: 20 K;
- Equivalence ratio: 0.1;
- EGR: 2%;

The number of calculated cases is generally in the range of 10^4 to 10^5 . However as it will be later shown the indexing technique used for the quest of reference conditions allows the use of such large look-up tables without affecting the CFD overall elapsed time.

Once a set of discrete conditions is defined by the user, the deputed chemical kinetic software calculates a constant pressure reactor case for each (p,T,Φ,EGR) vector. The autoignition delay time is conventionally assumed for each case as the time of the maximum OH concentration. A look-up table is created containing the 4-dimensions hyperspace of physical conditions. For each (p,T,Φ,EGR) vector an autoignition delay time is available from the chemical kinetics solution. A predefined order is applied for the data storage in the look-up table, which is needed in order to be able to operate a fast neighbour data recovery during the CFD calculation. In the proposed model a series of nested loops of physical conditions is adopted, in particular:

- Pressure: 1st level loop (i.e. outermost loop);
- Equivalence ratio: 2nd level loop;
- Temperature: 3rd level loop;
- EGR: 4th level loop (i.e. innermost loop).

Given such choice, when the index (or position) of the AI delay for a stored (p,T,Φ,EGR) vector is desired it is immediate to retrieve it by means of the following relationship Eq. 5:

$$I_{\tau_d} = (I_p - 1) \cdot (n_T \cdot n_{\Phi} \cdot n_{EGR}) + (I_{\Phi} - 1) \cdot (n_T \cdot n_{EGR}) + (I_T - 1) \cdot n_{EGR} + I_{EGR} \quad (5)$$

In Eq. 5 the I terms are the indexes relative to the calculated states whose physical conditions are the closest to the exact local ones: these are the *neighbour states* defined after. For each of them the position in the look-up table is determined by the knowledge of the data storage criterion. This indexing technique allows the efficient handling of very large look-up tables with no evident increase in CPU cost. With the developed technique an overall increase limited to 5% of the total CPU time is measured when compared to the use of empirical correlations.

Neighbour States and Interpolation

A fluid cell in the unburnt gases is characterized by a generic $(p^*, T^*, \Phi^*, EGR^*)$ vector, whose values are given by the CFD solver. In principle the generic $(p^*, T^*, \Phi^*, EGR^*)$ vector can be stored in the look-up table as a set of calculated physical coordinates: in this case the autoignition delay would be immediately available from the database itself. Although theoretically possible, this is a singular case and it is not of relevant interest. The most common situation that is verified is that the $(p^*, T^*, \Phi^*, EGR^*)$ vector is not present itself in the database, although autoignition delays for close conditions are. These are called *neighbours states* (or *neighbours conditions*). Since the look-up table stepping is known to the CFD code (from look-up table heading coordinates), an immediate variable bounding procedure is performed as reported in Table 1.

Table 1. Bounding variables for the generic $(p^*, T^*, \Phi^*, EGR^*)$ vector.

Generic Variable (input data)	Lower Calculated Value (output data)	Upper Calculated Value (output data)
p^*	p_{inf}	p_{sup}
T^*	T_{inf}	T_{sup}
Φ^*	Φ_{inf}	Φ_{sup}
EGR^*	EGR_{inf}	EGR_{sup}

Other parameters immediately available are the exact coordinate positioning within the look-up table hyperspace, e.g. the number of pressure discrete steps to find the calculated p_{inf} and p_{sup} values. This defines the I_p parameter needed in Eq. 5. The same applies to the other coordinates in Eq. 5, i.e. to calculate the I_T , I_{Φ} and I_{EGR} parameters. The problem consists in identifying 16 *neighbours states* bounding the generic $(p^*, T^*, \Phi^*, EGR^*)$ vector. For each *neighbour state* the pre-calculated τ_d is available in the look-up table. The only requirement is the knowledge of the exact position of the *neighbour states* within the table. This is the scope of Eq. 5 addressing the exact line of each state.

Once the 16 *neighbour states* and their respective τ_d are found in the database, the problem moves to the calculation of the autoignition delay time τ_d^* related to the generic $(p^*, T^*, \Phi^*, EGR^*)$ vector. This is the final result of the model, as it is the global indicator of the local end-gas reactivity and knock tendency. As the problem is defined

starting from 4 independent variables, a 4-dimension interpolation procedure is necessary in order to calculate the interpolated delay time τ_d^* .

A procedure based on multiple linearly interpolating operations is defined. For the sake of clarity just the basic operations are described in detail, while for the repetitions just the modification in initial conditions is underlined. At first, Φ and EGR are fixed to their lower calculated states, i.e. Φ_{inf} and EGR_{inf} . A bi-linear interpolation is then carried out on the free variables (temperature and pressure). This is represented in the lower-left part of Figure 1. After the linear interpolation on the exact cell-values T^* and p^* , a first delay is calculated in point 1. The same sequence of operations is repeated for fixed Φ_{sup} and EGR_{inf} , and a second delay is calculated in point 2. The AI delays represented in 1 and 2 are interpolated over p and T , while bound values are imposed for Φ and EGR. The interpolation over Φ is carried out based on the cell value Φ^* , and an updated AI delay is calculated in A. All the operations performed to this point are at a fixed lower bound EGR_{inf} value. These are repeated from the beginning for the upper bound EGR_{sup} value: an AI delay in 3 is calculated for Φ_{inf} (analogous to the AI delay in 1), another is calculated for Φ_{sup} in point 4 (analogous to the AI delay in 2) and interpolation over equivalence ratio is performed to obtain the AI delay in point B. Finally, linear interpolation over EGR is performed and the final τ_d^* is calculated. This represents the reactivity of the end-gas for the exact cell values $(p^*, T^*, \Phi^*, EGR^*)$. All the conditions reported in the look-up table come from a chemical kinetics simulation. The overall numeric error given by interpolation can be strongly limited by using high-resolution look-up tables. The accuracy of the generic (not calculated) τ_d^* delay benefits from high-resolution data, as this increase the physical proximity of the calculated conditions to the unknown target one.

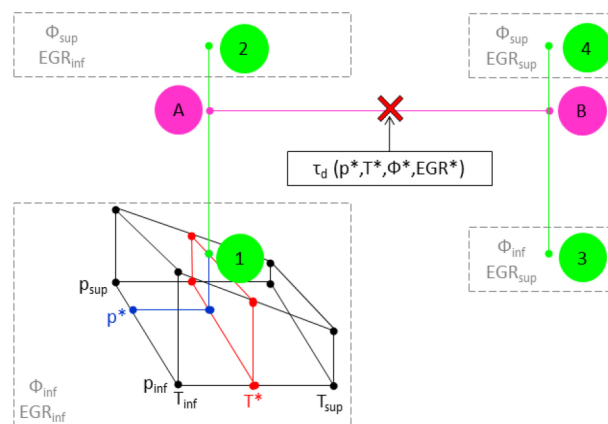


Figure 1. Multi-linear interpolation technique for the AI delay time for the inhouse developed knock model.

Comparison of Empirical and Look-Up Table Interpolated AI Delays

In this section the empirical correlation for autoignition delay τ_d (Eq. 4) is compared with the tabulated approach based on look-up table interpolation. In Figure 2 a comparison is carried out for a RON98 fuel and a comparison between the calculated AI delays and the values predicted by the empirical correlation are reported for various pressure and EGR levels.

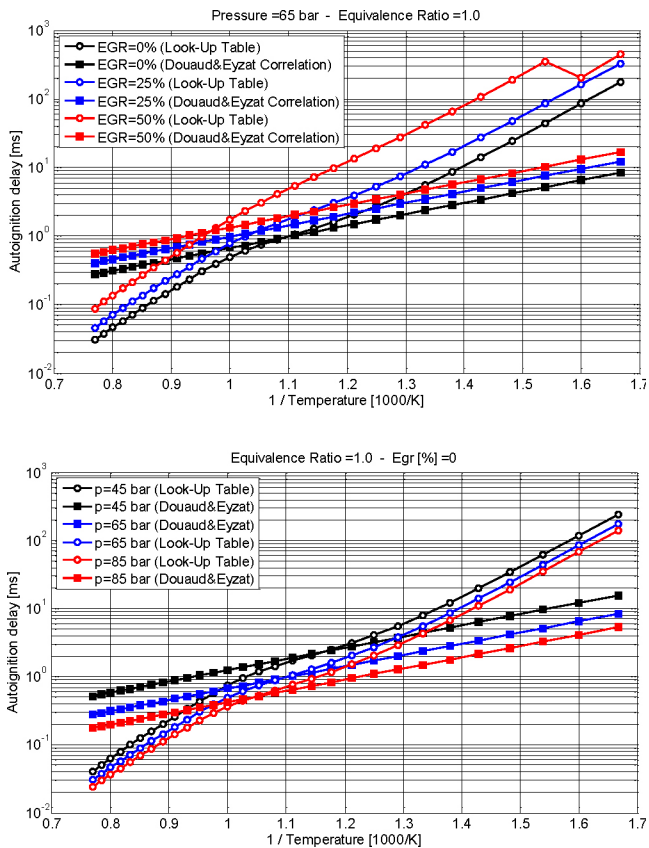


Figure 2. Comparison of AI delay times for engine-relevant conditions between the Douaud and Eyzat correlation and the look-up table interpolation for a RON98 fuel. (a), top: sensitivity to EGR; (b), bottom: sensitivity to absolute pressure.

Two separate behaviours are observed when comparing the AI delays predicted for the same conditions by the two methods. A first tendency is identified at temperatures higher than 1000 K, where the output from the look-up table shows lower AI delays than those predicted by the empirical correlation. This states an underestimation of the chemical kinetics rate for the Douaud and Eyzat correlation which would delay the autoignition onset. However, the range of involved temperatures is rarely found in internal combustion engines since end-gases are rarely subjected to compression levels such as their unburnt temperature exceeds 1000 K. A second and more relevant trend is verified at temperatures lower than 1000 K, where the chemically calculated AI delays are systematically higher than the corresponding values from the Douaud and Eyzat formula. This states an overestimation of the autoignition chemical kinetics rate for the empirical correlation case in this range. This tendency is more important since it comprises all the unburnt mixture heating process due to piston compression. The chemical pathway experienced by the reacting mixture is comprised in this range and an evident delay in autoignition onset is to be predicted when adopting a chemically tabulated method for this reason. The path to autoignition is strongly and erroneously accelerated by the empirical correlation. Although several improvements to the original Douaud and Eyzat correlations are proposed in literature, such as three-zones splitting of the same with ad-hoc coefficients, these are not of general use over all the interesting physical range for a given fuel.

Knock Model Validation Against Detailed Chemistry

A test case is analysed in order to evaluate the knock model response against a CFD case with fully resolved chemistry. The case consists of a planar domain bounded by adiabatic walls, where a variety of initial conditions is imposed with the aim of simulating the combination of possible physical realizations that are potentially experienced by unburnt mixture in a stratified internal combustion engine. A linear variation of temperature, equivalence ratio and residuals mass fraction is imposed through user-coding, as illustrated in the sketch in Figure 3.

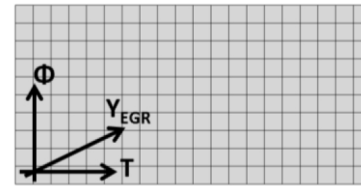


Figure 3. Sketch of initial field for the comparison between the tabulated knock model and fully resolved detailed chemistry.

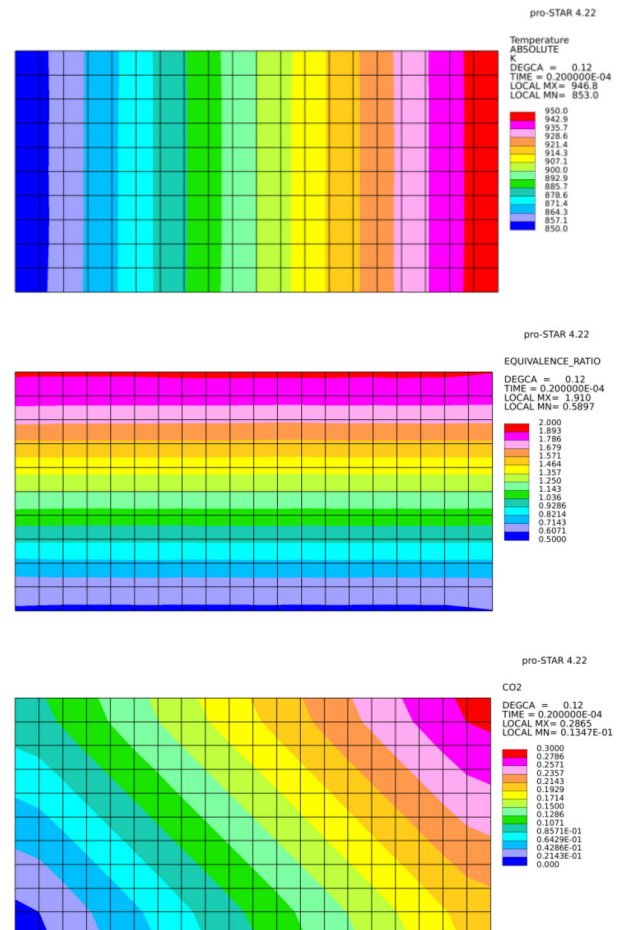


Figure 4. Initial conditions for the test case between the tabulated knock model with the fully resolved detailed chemistry. (a), top: temperature field; (b), middle: equivalence ratio field; (c), bottom: residual concentration field.

The physical range where the autoignition behaviour is investigated is carefully chosen to be engine-relevant, i.e. unburnt temperature variation is between 850 K and 950 K, equivalence ratio between 0.5 and 2.0 and EGR mass fraction from 0% to 30%. As for this last, a pure