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# A methodology based on reduced schemes to compute autoignition and propagation in internal combustion engines

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**Abstract**

The prediction of autoignition (AI) delay is an essential prerequisite to account for abnormal combustions (e.g. knock or super knock) that can appear in Internal Combustion (IC) engines. In this paper, a simple model called Ignition to Propagation Reduced Scheme (IPRS) is proposed to add AI predictions in reduced chemical schemes, which are classically used to compute in-cylinder combustion in the context of Large Eddy Simulations (LES). The IPRS principle is to use a single two-reaction reduced scheme and adapt the pre-exponential factor of the fuel oxidation reaction as a function of the temperature: one value is used at low temperatures to correctly predict AI delays and an other one can be used at higher temperatures, where heat release occurs, to keep the flame propagation properties of the chemical scheme. After a first section that introduces the model, Perfectly Stirred Reactors and 1D flames simulations are used to verify that: (1) the modification of the pre-exponential constant of the Arrhenius law at low temperature does not alter the propagation properties of the reduced scheme and (2) this modification is sufficient to accurately predict AI delays. The IPRS model captures autoignition times exactly like a full chemical scheme in a compressed zero dimensional test case representative of engine compression. In the last section this model is applied to 1D single hot spot simulations to investigate the modes of reaction after autoignition.


*Keywords:* LES; Knock; Autoignition; Internal combustion engine; Reduced scheme

## 1. Introduction

During the last decade engine downsizing has revealed to be a useful path to improve the efficiency of Internal Combustion (IC) engines. This technique allows to operate engines in a zone of higher efficiency by reducing the cylinders size and by increasing the pressure inside the chamber thanks to turbo chargers. It is commonly used in the industry up to a downsizing level of about 25%. Beyond this level abnormal combustions such as knock or super knock start occurring due to the high pressure and temperature conditions inside the cylinder. Understanding abnormal combustions is a main field of research inside the IC engine

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community in order to reach higher levels of downsizing. Previous studies [1–3] proved that LES is a powerful tool able to reproduce unsteady phenomena occurring in piston engines. However, to study abnormal combustion in IC engines, a model able to accurately predict Auto-Ignition (AI) delays has to be added to the LES solver. Because of the complexity of low temperature kinetics [4–7], most modeling approaches rely on tabulation of ignition delays obtained from zero dimensional ignition computations [8] or from representative 1D flamelets [9]. Some reduced schemes compatible with LES (limited to a few reactions and species) for the primary reference fuels are also available [10,11] but they are limited to the AI delay prediction and have to be associated to other models for high temperature reactions. Here an alternative solution is explored: a single two-step reduced scheme is used to describe both AI and propagation. It is called IPRS (Ignition to Propagation Reduced Scheme). The scope is not to reproduce the complex path of chemical reactions leading to AI but only to tune the reduced scheme reactions such that the AI delay is the same as the one obtained with complex chemistries. The model is introduced in the next section and validated on AI cases and 1D premixed flames. Homogeneous zero dimensional flow elements representative of IC engine are then simulated where complex chemistries AI delays are available to assess the accuracy of the IPRS model. In the last section the model is applied to non-homogeneous cases where autoignition phenomena can lead to detonation. The paper focuses on two fuels (pure isooctane and a gasoline surrogate called Sur95t in Pera et al. [12]) but the methodology can be extended to other fuels.

## 2. Predicting autoignition delay with a two-step chemistry

In reactive LES the source terms $\dot{\omega}_T$ and $\dot{\omega}_k$ in the energy and the species conservation equations have to be closed. For a mechanism including $M$ reactions between $N$ reactants and with $W_k$ the molar weight of species $k$:

$$\dot{\omega}_k = \sum_{j=1}^{M} \dot{\omega}_{kj} = W_k \sum_{j=1}^{M} \nu_{kj} Q_j \tag{1}$$

where $\nu_{kj} = \nu''_{kj} - \nu'_{kj}$ is the global stoichiometric coefficient of species $k$ in reaction $j$. The progress rate $Q_j$ is defined by:

$$Q_j = K_{f,j} \prod_{k=1}^{N} \left(\frac{\rho Y_k}{W_{kj}}\right)^{\nu'_{kj}} - K_{r,j} \prod_{k=1}^{N} \left(\frac{\rho Y_k}{W_k}\right)^{\nu''_{kj}} \tag{2}$$

In this relation $\rho$ is the density, $Y_k$ represents the species mass fractions and $K_{f,j}$ (respectively $K_{r,j}$) is the forward (respectively reverse) rate of reaction $j$ obtained with the Arrhenius law:

$$K_{f,j} = T^{\beta_j} A_{f,j} \exp\left(-\frac{E_{a,j}}{\mathcal{R}T}\right) \tag{3}$$

with $R$ the perfect gas constant, $T$ the temperature, $A_{f,i}$ the pre-exponential constant, $E_{a,j}$ the activation energy and $\beta_j$ the temperature exponent. For propagating flames the most important parameters that have to be accurately predicted by the source term closure are the laminar flame speed $S_L^0$, the flame thickness $\delta_L^0$ and the adiabatic flame temperature $T_{ad}$. Single-step chemical schemes can provide an accurate description of flame propagation process but they can not predict the burned gas temperature over a wide range of equivalence ratios because it depends on the species enthalpies. A simple solution to this problem has been used in the gas turbine community [13,14] by adding a reversible reaction between CO and $CO_2$. This is sufficient to capture both flame speed and adiabatic temperature over all relevant compositions. The resulting two-step schemes family can be written:

$$C_xH_{2x+2} + \left(x + \frac{x+1}{2}\right)(O_2 + aN_2) \rightarrow \quad xCO_2 + (x+1)H_2O + \left(x + \frac{x+1}{2}\right)aN_2 \tag{4}$$

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 \tag{5}$$

Table 1 summarizes the Arrhenius coefficients of the two-step mechanism classically used to compute isooctane/air flames propagation. The reaction exponents differ from the stoichiometric coefficients and are adjusted to obtain the right dependence of the flame speed in pressure. This scheme was designed to reproduce the Hasse et al. experiments [15]. Reduced schemes are widely used and several authors point out their accuracy in a wide range of configurations [2,16]. However they obviously fail to capture AI delays which are driven by low temperature chain reactions and the chemistry of radicals such as alkylperoxy or hydroperoxyalkyl [4–7]. All studies show a correlation between the AI delay $\tau_{AI}$ and the pre-exponential of the Arrhenius law:

$$\tau_{AI} \sim \frac{1}{A_{f,j}} \exp\left(\frac{E_{a,j}}{\mathcal{R}T}\right) \tag{6}$$

Table 1
Arrhenius parameters for the $C_8H_{18}$/air scheme.

| | $C_8H_{18}$ oxidation | | $CO$–$CO_2$ equilibrium | |
|---|---|---|---|---|
| $E_a$ [cal/mol] | $3.6 \cdot 10^4$ | | $1.4 \cdot 10^5$ | |
| A [$cm^3$/mol] | $5.443 \cdot 10^{12}$ | | $2.0 \cdot 10^5$ | |
| $\beta_j$ [−] | 0.1 | | 0.0 | |
| Reaction exponents [−] | $n_{C_8H_{18}}$ | 1.1 | $n_{CO}$ | 1.00 |
| | $n_{O_2}$ | 0.54 | $n_{O_2}$ | 0.50 |

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