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Jet Ignition Prediction in a Zero-Dimensional Pre-Chamber Engine Model

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Abstract

This paper presents a multi-chamber, multi-zone engine model to predict the ignition of a lean main chamber by a pre-chamber. The two chambers are connected by small cylindrical holes: the flame is ignited in the pre-chamber, hot gases propagate through the holes and ignite the main chamber through Turbulent Jet Ignition (TJI). The model original features are: i) separate balance equations for the pre- and main chambers, ii) a specific model for temperature and composition evolution in the holes and iii) a DNS-based model¹ to predict the ignition of the main chamber fresh gases by the burnt gases turbulent jets exiting the holes. Chemical reactions during TJI are the result of two competing mixing processes: (1) the hot jet gases mix with the fresh main chamber to produce heated zones and (2) at the same time, these hot gases cool down. (1) increases combustion and leads to ignition while (2) decreases it and can prevent ignition. The overall outcome (ignition or failure) is too complex to be modelled simply and the present model relies on recent DNSs of TJI¹ which provided a method to predict the occurrence of ignition. Incorporating this DNS information into the engine model allows to predict whether ignition will occur or not, an information which is not accessible otherwise using simple models. The resulting approach is tested on multiple cases to predict ignition limits for very lean cases, effects of H₂ injection into the pre-chamber and optimum size for the holes connecting the two chambers as a function of equivalence ratio.

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Keywords

turbulent jet ignition, pre-chamber ignition, internal combustion engine, multi-zone engine model

1 Introduction

2 Transport relies today mainly on Internal Combustion Engines (ICEs) burning
3 petroleum-derived fuel. One way to improve ICEs is to use homogeneous
4 lean combustion: engines operating under these conditions can have very low
5 pollutant emissions and very high efficiency². However, burning homogeneous
6 lean mixtures and meeting the demands of practical combustion systems
7 is complicated by low reaction rates, extinction, instabilities and mild heat
8 release associated to very lean mixtures which can cause misfires and partial-
9 burns, decrease engine efficiency and increase unburnt hydrocarbon emissions
10 and combustion instabilities, thereby preventing proper operation using Spark
11 Ignition (SI) in the main chamber³⁻⁵.

12 The Pre-Chamber Ignition (PCI) strategy can enable fast combustion under
13 all operating conditions by igniting the flow in a small semi-confined volume (the
14 pre-chamber) connected to the main chamber by small holes. The hot turbulent
15 jets issuing from these holes enter the main chamber and provide multiple
16 ignition sites for the homogeneous lean mixture⁶. In addition to ensuring
17 ignition, the high speed jets also increase the turbulence level in the main
18 chamber and therefore, the combustion speed, allowing to use leaner mixtures.
19 In practice, air/fuel mixture flows from the main chamber to the pre-chamber
20 during the compression stroke and is ignited inside the pre-chamber with a
21 spark plug. When the pre-chamber is ignited, the first gases leaving it and
22 entering the main chamber are unburned. Later the pre-chamber combustion
23 products cross the holes and enter the main chamber where they must ignite
24 the lean mixture and promote turbulence. This process is often referred to as
25 Turbulent Jet Ignition (TJI) and results in an overall increase of the main

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chamber burning rate in comparison with SI. The pre-chamber can contain the homogeneous premixed mixture available in the main chamber, or also be fueled using an auxiliary injection inside the pre-chamber. This allows to decouple the equivalence ratios in the two chambers and for example, to burn richer mixtures in the pre-chamber.

Attard et al.^{7,8} have demonstrated the capability of the PCI concept, increasing the air dilution limit above $\lambda = 2.0$ while maintaining very high levels of engine efficiency. This has been confirmed in more recent studies^{9,10}. However, experiments also reveal that the design of the pre-chamber is critical: Sadanandan et al.¹¹ show that, in a divided chamber academic configuration, the size of the pre-chamber orifices determines the injection speed and temperature of the jets. During TJI, two mechanisms compete: (1) mixing is necessary to create zones where the fresh gases of the main chamber and the hot gases of the jet are mixed so that chemical reactions are accelerated but (2) this mixing also decreases temperature so that chemical reactions are slowed down. One might think that smaller holes are always beneficial since they generate more vigorous jets causing faster combustion. Actually, when the size of the holes decreases, the pressure drop increases which can indeed generate higher injection speeds, but can also inhibit ignition beyond a certain speed due to excessive mixing rate in a finite rate chemistry environment¹. In addition, reducing the size of the holes increases the cooling of the gases as they pass through, resulting in lower jet temperature and chemical reaction rates.

Engine performance models have been used for a long time in all types of engines, including pre-chamber engines¹²⁻¹⁸. However, as yet, no model includes submodels to take into account the thermal effects in the ducts connecting pre- and main chambers, nor to predict the result of the main chamber jet ignition attempts. They assume an automatic ignition of the main chamber and some of them even impose a combustion law like the well-known Wiebe law¹⁹. As a consequence, they miss an important part of the problem and cannot be used near the jet ignition limit.

In the present work, a zero-dimensional pre-chamber engine model (called PEMIP for Pre-chamber Engine Model with Ignition Prediction) is derived to include both duct thermal effects and jet ignition prediction (Figure 1). It uses a multi-zone approach, similar to usual engine models, to obtain the speed, temperature and composition of the jets entering the main chamber. At this point, a model for TJI (the COR model, derived during previous work using Direct Numerical Simulation (DNS)¹) is used to predict whether main chamber

Figure 1. Graphical view of the use of three-dimensional numerical simulations to construct the engine model.

63 ignition by TJI occurs. Due to the integration of the COR ignition model,
 64 PEMIP is limited to cases where the ignition of the main chamber takes place
 65 in the vortex of the jets issuing from the pre-chamber. Ignition concepts where
 66 the main chamber is seeded with quenched radicals to trigger a volume ignition
 67 such as APIR^{20,21} are therefore excluded.

68 The PEMIP governing equations (third section) include model constants
 69 that are set using Large Eddy Simulation (LES) data from Ref.²² (fourth
 70 section) performed for TJI in a real engine. Thereafter, PEMIP is used for other
 71 operating points and compared with other LES data to check its capabilities,
 72 for example to predict ignition failure. PEMIP applications are given in the fifth
 73 section: for example, it is used to predict the optimum hole size for ignition as
 74 a function of the equivalence ratio of the main chamber.

75 Engine Configuration

76 Figure 2 shows a sketch of the Groupe Renault engine used here. The four-
 77 holes pre-chamber design comes from the work of Müller et al.²³. Table 1 lists
 78 the geometric quantities of the divided combustion chamber engine. vcr is the
 79 volumetric compression ratio, V_{pc} and V_{mc} are the volume of the pre- and main

chamber, respectively, and d_i is the i^{th} duct diameter (the 4 ducts do not have the same diameter). The temperature of the engine walls is assumed to be at a constant value of 420 K (specified by the engine manufacturer). A premixed propane-air mixture is used to fill the engine during the intake phase.

Figure 2. Sketch of the divided combustion chamber engine used.

Bore [m]	Stroke [m]	vcr [-]	V_{mc}^{TDC}/V_{pc} [-]	$d_{1,3}$ [m]	$d_{2,4}$ [m]
$76 \cdot 10^{-3}$	$90 \cdot 10^{-3}$	15.72	26.73	$1.2 \cdot 10^{-3}$	$0.9 \cdot 10^{-3}$

Table 1. Engine geometric properties.

Zero-Dimensional Engine Model

Modelling Approach

The global model is decomposed into four open systems that exchange mass with each other and heat with the outside. These systems are called zones and are namely: the pre-chamber fresh gases zone (pcf), the pre-chamber burnt gases zone (pcb), the main chamber fresh gases zone (mcf) and the main chamber burnt gases zone (mcb) (Fig. 3). Inside these gaseous zones, the temperature, the pressure and the mixture are supposed to be homogeneous. The pressure P is uniform inside the pre-chamber (pc)

$$P^{pc} = P^{pcf} = P^{pcb} \quad (1)$$

and inside the main chamber (mc)

$$P^{mc} = P^{mcf} = P^{mcb}. \quad (2)$$

Evolution of the Thermodynamic State of the Zones

$N + 3$ state variables are required for the description of each zone

- P , the pressure of the zone;
- m_k for $k = 1$ to N , the mass of the N species present in the mixture;
- a state variable describing the energy of the system, here the temperature T ;
- V , the volume of the zone.

The corresponding $N + 3$ equations required for each zone are given by ideal gas law, species mass balance, energy balance and volume variation laws. The mass m inside each zone reads

$$m = \sum_k^N m_k \quad (3)$$

and the species mass fractions

$$Y_k = \frac{m_k}{m} \text{ for } k = 1, N. \quad (4)$$

Figure 3. Sketch of PEMIP zones and submodels.

105 **State Equation** The N species gaseous mixture that fills the four zones is
 106 supposed to be ideal so that the equation of state reads $PV = m\mathcal{R}T/W$ or
 107 in its derived form

$$P \frac{dV}{dt} + V \frac{dP}{dt} - \frac{\mathcal{R}}{W} T \frac{dm}{dt} - \frac{\mathcal{R}}{W} m \frac{dT}{dt} - \mathcal{R} T m \sum_k^N \frac{1}{W_k} \frac{dY_k}{dt} = 0, \quad (5)$$

108 where $\mathcal{R}$, t , W and W_k are the universal ideal gas constant, the time, the mean
 109 molecular weight and the molecular weight of the k^{th} species, respectively. For
 110 clarity, the specific zone suffixes (*pcf*, *pcb*, *mcf* and *mcb*) are omitted when the
 111 equation is valid for the four zones of PEMIP.

112 **Species Mass Balance** The four zones have multiple inlets and outlets. Gases are
 113 supposed to exit the zones at the outlets with the mean state of the zones. The
 114 rate of change in the mass of each species then reads

$$\frac{d(m_k)}{dt} = \sum_i \dot{m}_i Y_{k,i} - \sum_o \dot{m}_o Y_k, \quad (6)$$

115 where $Y_{k,i}$ is the mass fraction of the k^{th} species of the mixture entering the
 116 zone through the i^{th} inlet, $\dot{m}_i$ and $\dot{m}_o$ are the mass flow rates entering the
 117 zone through the i^{th} inlet and leaving the zone via the o^{th} outlet, respectively.
 118 Summing Eq. 6 over all species, the total mass variation reads

$$\frac{dm}{dt} = \sum_i \dot{m}_i - \sum_o \dot{m}_o. \quad (7)$$

119 **Energy Balance** The balance equation for the total internal energy U reads

$$\frac{dU}{dt} = -P \frac{dV}{dt} + \dot{Q}_w + \sum_i \dot{m}_i h_i - h \sum_o \dot{m}_o, \quad (8)$$

120 where $\dot{Q}_w$ is the rate of heat transfer through the walls, h_i the enthalpy per unit
 121 mass of the mixture entering the zone through the i^{th} inlet, and h the enthalpy
 122 per unit mass. For an ideal gas, the total internal energy can be rewritten in
 123 terms of mass fractions and temperature

$$U = m \sum_k^N Y_k u_k(T) \quad (9)$$

or, in its derived form

$$\frac{dU}{dt} = u \frac{dm}{dt} + m C_v \frac{dT}{dt} + m \sum_k^N u_k \frac{dY_k}{dt}, \quad (10)$$

where u is the total internal energy per unit mass, C_v the heat capacity at constant volume per unit mass, and u_k the total internal energy per unit mass of the k^{th} species. Substituting the corresponding derivatives and using $h = u + PV/m$ yields a balance equation for temperature

$$m C_v \frac{dT}{dt} + P \frac{dV}{dt} = \dot{Q}_w + \sum_i \dot{m}_i \left(h_i - \sum_k^N u_k Y_{k,i} \right) - \frac{PV}{m} \sum_o \dot{m}_o. \quad (11)$$

Volume Variation The volume variation of the zones inside the constant volume pre-chamber follows

$$\frac{dV^{pcf}}{dt} + \frac{dV^{pcb}}{dt} = 0. \quad (12)$$

In the main chamber, the volumes change due to the piston motion

$$\frac{dV^{mcf}}{dt} + \frac{dV^{mcb}}{dt} = \frac{dV^{mc}}{dt}, \quad (13)$$

with

$$\frac{dV^{mc}}{dt} = \left[\frac{\frac{1}{4}s \cos(\Omega)}{\sqrt{c^2 - (\frac{1}{2}s \sin(\Omega))^2}} + \frac{1}{2} \right] s \dot{\Omega} \sin(\Omega) \pi \frac{b^2}{4}, \quad (14)$$

where s , c , b , Ω and $\dot{\Omega}$ are the engine stroke, connecting rod length, bore, crank angle and angular rotation speed, respectively.

Wall Heat Losses

The rate of heat transfer through the walls of both chambers is computed as

$$\dot{Q}_w = A_w h_w (T_w - T), \quad (15)$$

where A_w is the wall surface area, h_w the wall heat transfer coefficient, and T_w the wall temperature supposed to be spatially uniform and constant during the whole engine cycle. The heat transfer coefficient is estimated using a specific

correlation for four-stroke engines²⁴

$$\mathfrak{h}_w = \frac{\kappa}{L} C_{\mathfrak{h}_w} \left(\frac{\rho \overline{U}_p L}{\mu} \right)^{0.7}, \quad (16)$$

where κ is the gas thermal conductivity, $C_{\mathfrak{h}_w}$ a constant which depends on the engine geometry, ρ the gas density, μ the gas dynamic viscosity, L a characteristic length that equals the pre-chamber diameter d^{pc} for the pre-chamber zones and the engine bore b for the main chamber zones, and $\overline{U}_p$ is the mean piston speed defined as

$$\overline{U}_p = s \frac{\dot{\Omega}}{\pi}. \quad (17)$$

The wall surface of each zone is estimated using pre- (A_w^{pc}) or main chamber wall surface (A_w^{mc}) weighted by the zone filling volume fraction, which compares the volume of the specific zone to the volume of the chamber to which it belongs, such that

$$A_w^{pcf} = A_w^{pc} \frac{V^{pcf}}{V^{pcf} + V^{pcb}}, \quad (18)$$

$$A_w^{pcb} = A_w^{pc} \frac{V^{pcb}}{V^{pcf} + V^{pcb}}, \quad (19)$$

$$A_w^{mcf} = A_w^{mc} \frac{V^{mcf}}{V^{mcf} + V^{mcb}}, \quad (20)$$

and

$$A_w^{mcb} = A_w^{mc} \frac{V^{mcb}}{V^{mcf} + V^{mcb}}, \quad (21)$$

with

$$A_w^{mc} = A_w^p + A_w^h + \pi b \left[\frac{1}{2} s (1 - \cos(\Omega)) + c - \sqrt{c^2 - \left(\frac{1}{2} \sin(\Omega) \right)^2} \right], \quad (22)$$

where A_w^p and A_w^h are the surface area of the piston and the head of the engine, respectively.

Submodel for the Connecting Ducts

Due to the pressure difference between the two chambers, a mass flow from one of the two chambers (called the upstream chamber, *up*) to the other (called the downstream chamber, *ds*) occurs (the flow can go both ways: from *pc* to *mc* but also vice versa). Gases first expand at the duct inlet (*in*) from P^{up} to P^{in}

before flowing into the constant cross section duct, exchanging heat through the walls (Fig. 4). The heat exchange can cause the temperature at the duct outlet (*out*) T^{out} to be significantly different from the temperature at the duct inlet (*in*) T^{in} ^{22,25}. This must be taken into account because the temperature of the burnt gases jets is one of the key parameters controlling the ignition of the main chamber¹.

Holes Inflow Properties The inflow properties are estimated at the inlet of the holes assuming an isentropic expansion at a constant heat capacity ratio γ equal to the heat capacity ratio of the upstream chamber γ^{up} . The critical pressure ratio between upstream and downstream chambers from which the flow is choked is defined as

$$P_{r,cr} = \left(\frac{\gamma^{up} + 1}{2} \right)^{\frac{\gamma^{up}}{\gamma^{up}-1}}. \quad (23)$$

Therefore, the pressure ratio between the upstream chamber and the inlet of a duct which acts as a throat reads

$$P_r^{in} = \min \left(\frac{P^{up}}{P^{ds}}, P_{r,cr} \right). \quad (24)$$

The temperature at the duct inlet is estimated from isentropic changes as

$$T^{in} = T^{up} P_r^{in \frac{1-\gamma^{up}}{\gamma^{up}}} \quad (25)$$

and the mass flow of the j^{th} duct as

$$\dot{m}_{d,j} = C d_j A_{d,j} P^{up} \sqrt{\frac{2\gamma^{up}}{\gamma^{up}-1} \frac{W^{up}}{\mathcal{R}T^{up}} \left(P_r^{in - \frac{2}{\gamma^{up}}} - P_r^{in - \frac{\gamma^{up}+1}{\gamma^{up}}} \right)}, \quad (26)$$

Figure 4. Sketch of a flow through a duct following an expansion from an upstream chamber to a downstream chamber.

where $A_{d,j}$ is the cross section of the j^{th} duct and Cd_j the discharge coefficient of the j^{th} duct estimated using the correlation of Ashimin et al.²⁶

$$Cd_j = \left[1.23 + 58 \left(\frac{\dot{m}_{d,j} d_{d,j}}{A_{d,j} \mu^{in}} \right)^{-1} \frac{l_{d,j}}{d_{d,j}} \right]^{-1}, \quad (27)$$

where $d_{d,j}$ and $l_{d,j}$ are the diameter and length of the j^{th} duct, respectively. The mixture composition is assumed not to change during the expansion from the upstream chamber to the inlet of a duct (i.e. $Y_k^{up} = Y_k^{in}$).

Duct Outflow Properties In the ducts, the gases exchange heat through the walls: their temperature changes and potentially their chemical composition varies too. Both control TJI and must be considered. Here, a Lagrangian approach is used to determine the temperature and composition of the gas flowing in the ducts.*

Inside the ducts, pressure is assumed to be homogeneous such that

$$P^{in} = P^{out} = \frac{P^{up}}{P_r^{in}}. \quad (28)$$

The residence time t_{res} of a fluid element that goes through the j^{th} duct is estimated as

$$t_{res,j} = l_{d,j} \frac{\rho^{in} A_{d,j}}{\dot{m}_{d,j}}. \quad (29)$$

From $t = 0$ at the inlet to $t = t_{res,j}$ at the outlet of the j^{th} duct, the evolution of the bulk thermochemical variables of the flowing mixture can be described by Ordinary Differential Equations (ODEs). Temperature is given by

$$\frac{dT}{dt} = \frac{1}{\rho C_p} \left[\frac{4}{d_d} \mathfrak{h} (T_w - T) - \sum_k^N \dot{\omega}_k h_k \right], \quad (30)$$

where C_p is the heat capacity at constant pressure per unit mass, $\mathfrak{h}$ the heat transfer coefficient, d_d the duct diameter, $\dot{\omega}_k$ and h_k are the chemical source term and the enthalpy per unit mass of the k^{th} species, respectively. Species mass fractions are determined by

$$\frac{dY_k}{dt} = \frac{1}{\rho} \dot{\omega}_k. \quad (31)$$

*For this model, the duct wall temperature T_w is supposed to be constant over the whole engine cycle.

Equations 30 and 31 are integrated from $t = 0$ to $t = t_{res,j}$ thanks to a SciPy²⁷ wrapped ODE solver. Thermodynamic and kinetic parameters are computed using Cantera²⁸. The chemical scheme used for the LES is also used in Cantera. Data from LES of the real engine ignition sequence of Ref. ²² are used to assess whether the composition has time to change. The data was extracted for one of the smallest ducts (duct no. 2) at the crank angle when the residence time is the shortest during the burnt gases injection period. In this way, if the mixture reaches equilibrium in this situation (high temperature losses and short residence time) then it would be possible to assume that the mixture reaches equilibrium in all cases. Initial thermodynamic properties are extracted from the LES, initial mixture composition is set to equilibrium. The convective heat transfer coefficient h is adjusted so that the final temperature $T(t = t_{res,2})$ equals the outlet temperature of the LES. Figure 5 shows that under these conditions which are typical of a real engine, the residence time is too short for the mixture to reach equilibrium but long enough for the mixture to have time to react so that the composition changes. It is then impossible to assume equilibrium, nor frozen chemistry during the flow of burnt gases. The evolution of chemistry must be resolved if a precise description of the composition at the outlet of the duct is required.

A slight variation in the burnt gases composition may have an effect on the ignition of the main chamber but has a negligible contribution to the thermodynamic properties of the zones. Thus, to reduce computational cost, an analytic expression for the temperature neglecting chemical reactions is used

Figure 5. Temperature and species mass fraction evolution of burnt gases losing heat in a given time compared to corresponding equilibrium composition. Heat losses and end time are set to match LES data of Ref. ²² at the shortest residence time for the duct no. 2.

when the mixture does not react or when a slight variation in the burnt gases composition does not matter, i.e. during fresh gases flow or during burnt gases flow, once the main chamber has been ignited.

Assuming that the mixture does not react and that thermodynamic properties do not change from the inlet to the outlet of the j^{th} duct, the outlet temperature can be analytically estimated as²⁹

$$T_j^{\text{out}} = T_w + (T^{\text{in}} - T_w) \exp \left(- \frac{\pi d_{d,j} l_{d,j} h_j^{\text{in}}}{\dot{m}_{d,j} C p^{\text{in}}} \right). \quad (32)$$

Equation 32 is used during the whole engine cycle except during the burnt gases jet ignition period, where Eqs 30 and 31 are integrated to know the exact composition of the jets of burnt gases. In all cases, the convective heat transfer coefficient is evaluated at the inlet of the ducts and equals h_j^{in} , estimated using Sieder and Tate³⁰ correlation multiplied by a correction factor $1 + \left(\frac{d_{d,j}}{l_{d,j}} \right)^{2/3}$ to take into account the effect of a non-developed temperature profile following a sudden contraction in a short duct³¹

$$h_j^{\text{in}} = \frac{\kappa^{\text{in}}}{d_{d,j}} 0.027 \left(\frac{4 \dot{m}_{d,j}}{\mu^{\text{in}} \pi d_{d,j}} \right)^{0.8} \left(\frac{\mu^{\text{in}} C p^{\text{in}}}{\kappa^{\text{in}}} \right)^{1/3} \left(\frac{\mu^{\text{in}}}{\mu_w^{\text{in}}} \right)^{0.14} \left[1 + \left(\frac{d_{d,j}}{l_{d,j}} \right)^{2/3} \right]. \quad (33)$$

Submodel for Turbulent Jet Ignition (TJI)

Now that the temperature, speed and composition of the gases exiting the holes are known, a model is needed to predict whether these gases ignite the main chamber. For that, the DNS-based COR (for Convected Open Reactor) model is used¹. COR consists in following an open reactor—small enough to be homogeneous—initially full of burnt gases, convected into the chamber (Fig. 6): these hot burnt gases mix at a certain rate with the cold fresh gases of the main chamber within this open reactor and chemistry inside the reactor can be tracked using an ODE solver with complex chemistry. In this approach, the mixture fraction between the hot jet and the cold gases ξ in the open reactor changes according to a mixing rate θ defined as

$$\theta = \frac{\dot{m}_{\text{in}}}{m}, \quad (34)$$

where m is the reactor mass, $\dot{m}^{in}$ is the mass flow entering the reactor (i.e. that comes from the flammable atmosphere). The mixture fraction ξ in the open reactor starts at $\xi = 1$ in the injected burnt gases jet and goes to $\xi = 0$ as the reactor is convected inside the chamber and mixes with the fresh gases. The details of the convection movement are unimportant once the evolution of ξ is specified. Based on DNS results, θ is modelled by a parabolic function¹

$$\theta = \theta_0 4\xi(1 - \xi), \quad (35)$$

where θ_0 is the maximum mixing rate supposed to scale as the inverse of a jet flow time scale such that

$$\theta_0 = K^{COR} \frac{U^{out}}{d_d}, \quad (36)$$

with $K^{COR} = 0.3$, and where U^{out} is the speed at the outlet of the duct.

For the application of this ignition model to the complete pre-chamber engine model PEMIP, the jets of hot burnt gases are considered as a succession of quasi-steady states, each generating an infinite number of ignition sites having the same aerothermochemical properties. As a consequence, a single ignition site can be used as a representation of the multiple ignition attempts. Figure 7 shows guidelines for using the COR model which is coupled to the thermal model for the connecting ducts. In this work, the potential shocks that can be generated at the outlet of the ducts are supposed not to be responsible for ignition and are therefore not modelled.

Figure 6. Sketch of the COR ignition model¹.

Figure 7. Flowchart showing the practical use of the COR model, from Ref.¹.

Turbulence

Turbulence kinetic energy in the pre- and main chambers is modelled using a simple phenomenological approach¹⁵. Turbulence is supposed to be only due to the inflowing duct jets so that in each chamber

$$\frac{dm\mathfrak{K}}{dt} = \sum_j \dot{m}_{d,j} \frac{U_j^{out2}}{2} - m\varepsilon, \quad (37)$$

where $\mathfrak{K}$ is the turbulence kinetic energy per unit mass, U_j^{out} is the j^{th} duct outlet velocity in the event that the ducted flow transfers into the chamber (pc or mc) and ε is the rate of dissipation of the turbulence kinetic energy defined as

$$\varepsilon = \frac{(2\mathfrak{K}/3)^{3/2}}{l_t}, \quad (38)$$

with $l_t = \overline{d_d}$, the mean duct diameter defined as

$$\overline{d_d} = \sqrt{\frac{1}{n_d} \sum_j d_{d,j}^2}, \quad (39)$$

where n_d is the number of ducts.

Flame Surface

Combustion inside pre- and main chambers is modelled by a flame surface A_f that sweeps across the chambers consuming the fresh gases. A simple closed balance equation for the flame surface density Σ may be derived from heuristic arguments following Marble et al.³² and Darabiha et al.³³, assuming that Σ is homogeneous

$$\frac{d\Sigma}{dt} = C_{A_f^{+,t}} \frac{\varepsilon}{\mathfrak{K}} \Sigma - C_{A_f^-} S_L^0 \frac{\Sigma^2}{1 - bf}, \quad (40)$$

where $C_{A_f^{+,t}}$ and $C_{A_f^-}$ are two model constants and $\varepsilon/\mathfrak{K}$ represents the flame stretch generated by the turbulence. The first term in the Right Hand Side (RHS) expresses the flame surface production due to the stretch rate acting on the flame surface, the second term expresses the flame annihilation, assumed to be proportional to the mean reaction and inversely proportional to the available reactants per unit of flame area. S_L^0 is the only chemical parameter appearing in the balance equation. It is computed and tabulated using Cantera²⁸ before being read according to the thermochemical conditions of the fresh gases.

Integrating Eq. 40 over the pre-chamber volume, a balance equation for the pre-chamber flame surface is obtained

$$\frac{dA_f^{pc}}{dt} = C_{A_f^{+,t}}^{pc} \frac{\varepsilon^{pc}}{\mathfrak{K}^{pc}} A_f^{pc} - C_{A_f^-}^{pc} S_L^{0pc} \frac{A_f^{pc2}}{1 - bf^{pc}}, \quad (41)$$

which describes the flame surface evolution after having been initiated at spark Ignition Timing (IT) as a sphere of radius 1.5 mm.

In the main chamber, when burnt gases injection occurs and ignition has been realized, the production of flame surface by the jet injection of burnt gases is taken into account by an additional production term estimated as $C_{A_f^{+,jet}}^{mc} \sum_j \pi d_{d,j} U_j^{out}$ (Fig. 8). The main chamber flame surface balance equation therefore reads

$$\frac{dA_f^{mc}}{dt} = C_{A_f^{+,t}}^{mc} \frac{\varepsilon^{mc}}{\mathfrak{K}^{mc}} A_f^{mc} - C_{A_f^-}^{mc} S_L^{0mc} \frac{A_f^{mc2}}{1 - bf^{mc}} + C_{A_f^{+,jet}}^{mc} \sum_j \pi d_{d,j} U_j^{out}. \quad (42)$$

Figure 8. Sketch of flame surface production by a cylindrical jet of burnt gases.

Mass Transfer

The zones can exchange mass with each other by combustion (fresh gases zone to burnt gases zone) and by transfer through the ducts. During combustion, the rate of mass transfer from fresh gases to burnt gases in each chamber reads

$$\dot{m}_{f \rightarrow b} = \rho_f S_L^0 A_f, \quad (43)$$

where ρ_f is the density of the fresh gases that the flame is consuming. Before hot burnt gases issue into the main chamber, the mixture flowing from the main chamber to the pre-chamber is made up of fresh gases. When combustion occurs in the pre-chamber, fresh gases are first pushed out before burnt gases reach the inlet of the ducts and are pushed out in turn. This transition from fresh gases to burnt gases ejection is controlled by BF_{thr}^{pc} , the pre-chamber Burnt Fraction (BF) threshold from which burnt gases are ejected through the ducts. After that burnt gases ejection starts, if a backflow from main to pre-chamber occurs due to the combustion in the main chamber, it is assumed that this flow is made up of burnt gases only.

Resolution of the Set of Ordinary Differential Equations

The set of ODEs comprises $2 \times (3 + 2 \times (2 + N)) = 14 + 4 \times N$ equations where N is the number of species (Table 2). There are also $14 + 4 \times N$ unknown variables (Table 3) so that the problem is closed. The model description has eight constants, namely:

- $C_{h_w}^{pc}$ and $C_{h_w}^{mc}$, the wall heat transfer constants (Eq. 16);
- $C_{A_f^{+,t}}^{pc}$ and $C_{A_f^{+,t}}^{mc}$, the flame surface production by flame stretch constants (Eqs 41 and 42);
- $C_{A_f^{+,jet}}^{mc}$, the flame surface production by jet injection constant (Eq. 42);
- $C_{A_f^-}^{pc}$ and $C_{A_f^-}^{mc}$, the flame surface destruction constants (Eqs 41 and 42);

- 317 - BF_{thr}^{pc} , the pre-chamber Burnt Fraction threshold from which burnt gases
318 are ejected from the pre-chamber.

319 The set of ODEs can be written in a matrix form such as

$$\mathbf{A} \frac{d}{dt} (\boldsymbol{\psi}(t)) = \mathbf{f}(\boldsymbol{\psi}(t)), \quad (44)$$

320 where $\mathbf{A}$ is the matrix that contains the coefficients in front of the derivatives
321 of the ODEs and $\boldsymbol{\psi}$ is the vector of unknown variables. By inverting the matrix
322 $\mathbf{A}$, all the time derivatives can be expressed as a function of the instantaneous
323 variables

$$\frac{d}{dt} (\boldsymbol{\psi}(t)) = \mathbf{A}^{-1} \mathbf{f}(\boldsymbol{\psi}(t)). \quad (45)$$

324 Euler's method is then used to approximate the solution over time, using linear
325 approximation over a short time step dt

$$\boldsymbol{\psi}(t + dt) = \boldsymbol{\psi}(t) + \mathbf{A}^{-1} \mathbf{f}(\boldsymbol{\psi}(t)) dt. \quad (46)$$

mc, pc	volume		Eqs 12/13
	turbulence kinetic energy		Eq. 37
	flame surface		Eqs 41/42
	f, b	ideal gas law	Eq. 5
		species mass balance	Eq. 6
		energy balance	Eq. 11

Table 2. List of the $14 + 4 \times N$ ODEs.

mc, pc	$P, A_f, \mathfrak{R}$		
	f, b	V, m_k, T	

Table 3. List of the $14 + 4 \times N$ variables.

326 Calibration and Validation of PEMIP

327 The engine model PEMIP is now applied to the pre-chamber engine introduced
328 in the second section. First, the model constants are calibrated using the LES
329 data from Ref. 22 which uses the same engine. Then, the results of PEMIP are
330 compared to other LES cases to check its capabilities. The chemical kinetics
331 used for LES 22 is used in PEMIP so that complex chemistry effects are taken
332 into account in the COR ignition model.

Calibration of the Model Constants

Operating Point The operating point of Ref.²² used to calibrate PEMIP corresponds to a typical engine operation at 3000 rpm. Propane is used as fuel for both intake lean premixed mixture and pre-chamber additional fuelling. Gaseous fuel injection inside the pre-chamber starts immediately after Intake Valve Closing (IVC) = -108.0 Crank Angle Degree (CAD) at the beginning of the compression phase and stops at End Of Injection (EOI) = -70.0 CAD so as to have a mean stoichiometric mixture inside the pre-chamber when igniting the pre-chamber at IT = -10.0 CAD. The mean pressure and temperature inside the engine at IVC are equal to 2.6 bar and 373 K, respectively. The air-fuel equivalence ratio λ of the intake premixed mixture is equal to $\lambda_{in} = 1.5$. This operating point is labelled # $\lambda 1.5$ IT-10 throughout this work.

Non-Reactive Case Unfired non reactive compression and expansion strokes are first used to calibrate wall heat transfer constants before calibrating the combustion model using fired strokes. The only unset model constants for non reactive (unfired) cases are the two wall heat transfer constants $C_{\mathcal{R}_w}^{mc}$ and $C_{\mathcal{R}_w}^{pc}$, since the six other constants relate to the combustion model. These constants are calibrated to match the pre- and main chamber mean temperature of an unfired LES under the same operating conditions as # $\lambda 1.5$ IT-10 (Fig. 9). Other zone state variables are in good agreement, the pre-chamber equivalence ratio differs during the piston downward phase because of mixture stratification in the pre-chamber²² that is not solved by PEMIP: the mixture that escapes first is located at the bottom of the pre-chamber, this is the lean mixture that came from the main chamber during the piston upward phase. Making it escape thus increases the fuel-air equivalence ratio ϕ . Duct quantities are in good agreement.

Reactive Case The pre-chamber Burnt Fraction (BF) threshold from which burnt gases are ejected through the ducts BF_{thr}^{pc} is set using the LES data, computing the BF inside the pre-chamber at the moment when the mean progress variable at the outlet of the ducts exceeds 0.5 (2.35 CAD, $BF^{pc} = 0.73$). The remaining constants of the flame surface models are calibrated to match the fired LES data (Fig. 10). First, pre-chamber flame surface constants are tuned in order to match the flame surface of the LES. For the main chamber, the flame surface computed from the LES cannot be targeted as part of the combustion takes place in a well dispersed combustion regime where no flame front clearly consumes the charge²². Both pressure and combustion duration are targeted instead. The

Figure 9. Temperature, pressure and fuel-air equivalence ratio inside pre- and main chambers (upper row) and duct mass flow, outlet speed and outlet temperature (bottom row) for both unfired PEMIP and LES (operating conditions from #λ1.5 IT-10).

jet ignition model predicts an instantaneous ignition for all ducted jets. Duct quantities can only be compared before that main chamber combustion induces a backflow into the pre-chamber. From this point, the backflow is supposed to correspond to burnt gases in PEMIP while the composition changes depending on the position of the flame in the actual engine²². Before this backflow, duct quantities are in good agreement. Outlet temperature is slightly over estimated because of the pre-chamber mixture homogeneity assumption that does not hold in the actual engine: lean burnt mixture is first pushed out of the pre-chamber²² that produces cooler jets than stoichiometric burnt gases. In addition, the drop in temperature through the ducts is a little overestimated during the first moments of TJI (Fig. 11). Final model constants are shown in Table 4.

$C_{\mathcal{R}_w}^{mc}$	$C_{\mathcal{R}_w}^{pc}$	$C_{A_f^{+,t}}^{mc}$	$C_{A_f^{+,t}}^{pc}$	$C_{A_f^{+,jet}}^{mc}$	$C_{A_f^-}^{mc}$	$C_{A_f^-}^{pc}$	BF_{thr}^{pc}
0.445	0.2	0.45	1.2	10.0	2.0	3.6	0.73

Table 4. Model constants calibrated to match the LES data from Ref. ²².

Figure 10. Pressure, flame surface and burnt fraction inside pre- and main chambers (upper row) and duct mass flow, outlet speed and outlet temperature (bottom row) for both fired PEMIP and LES (#λ1.5IT-10). The CAD of the pre-chamber (pc^{ign}) and main chamber ignition (mc^{ign}) and the TJI period predicted by PEMIP are superimposed.

Figure 11. Drop of temperature through the ducts for both fired PEMIP and LES (#λ1.5IT-10). The TJI period predicted by PEMIP is superimposed.

Validation Using Engine LES Data

Now that PEMIP has been calibrated, it is used for other operating points and compared with LES data to check its ability to predict ignition limits. The operating points used for validation are summarized in Table 5 alongside the reference case #λ1.5IT-10 (used for calibration). They differ from the reference case by a change of IT (−10 CAD or −30 CAD), intake premixed propane-air mixture air-fuel equivalence ratio λ_{in} (1.5 or 2.0) or pre-chamber additional fuel

type (propane or hydrogen). In all cases, the additional fuel injection is adjusted to keep a mean stoichiometric mixture inside the pre-chamber at IT.

label	IT [CAD]	λ_{in} [-]	pc add. fuel
# λ 1.5 IT-10 (ref.)	-10.0	1.5	propane
# λ 1.5 IT-30	-30.0	1.5	propane
# λ 2.0 IT-10	-10.0	2.0	propane
# λ 2.0 H ₂ IT-10	-10.0	2.0	hydrogen

Table 5. Variant parameters of the different operating points.

Ultra-Lean $\lambda_{in} = 2.0$ Case PEMIP with an ultra-lean $\lambda = 2.0$ intake premixed mixture (# λ 2.0 IT-10) does not predict any ignition during the TJI period (Fig. 12). This is consistent with the LES results (Fig. 13) which show large, dispersed, weakly reactive zones which do not transition to healthy flame fronts. Pressure traces—evidence of the Heat Release Rate (HRR) in the chambers—slightly differ.

In the pre-chamber, the overpressure observed with PEMIP is probably due to the mixture homogeneity assumption: in PEMIP, the mixture is burnt close to stoichiometry whereas in the actual engine, pre-chamber combustion starts in a rich mixture trapped at the top of the pre-chamber²².

In the main chamber, although the burnt gases jets do not give rise to healthy flame fronts in the LES, diffuse reaction zones, during the TJI period, consume some of the main chamber charge without giving rise to self-sustained flames (Fig. 13). These phenomena are not taken into account in PEMIP which only gives a 'yes or no' answer to the main chamber ignition. PEMIP main chamber BF then remains very low, only supplied by the burnt gases coming from the pre-chamber (Fig. 12).

Figure 12. Pressure and burnt fraction inside pre- and main chambers for both PEMIP and LES (# $\lambda_{2.0}$ IT-10). The CAD of the pre-chamber ignition (pc^{ign}) and the TJI period predicted by PEMIP are superimposed (PEMIP does not predict any main chamber ignition).

Figure 13. Plane cut normal to the x axis (left), y axis (right) intersecting the ducts by their axis and coloured by the normalized HRR with three isolines of temperature (LES, # $\lambda_{2.0}$ IT-10)

405 *Ultra-Lean $\lambda_{in} = 2.0$ Case With Hydrogen Addition* For the case with hydrogen
 406 pre-chamber fuelling (# $\lambda_{2.0}$ H₂IT-10), the propane pre-chamber injection
 407 is replaced by hydrogen injection. The premixed laminar flame speeds are
 408 tabulated as a function of an additional variable: the hydrogen fuel mass ratio

$$\xi_{H_2} = \frac{Y_{H_2}}{Y_{H_2} + Y_{C_3H_8}}. \quad (47)$$

409 For this case, PEMIP agrees with LES data and predicts that the main
 410 chamber ignition occurs during the TJI phase (Figs 14 and 15), giving rise
 411 to established flame fronts. Unlike # $\lambda_{1.5}$ IT-10 where main chamber ignition
 412 occurs at the same time for all the jets, here the jets issuing from the largest
 413 holes ($d_{1,3}$) ignite the main chamber before the jets issuing from the smallest

holes ($d_{2,4}$). This is consistent with what can be observed using LES (Fig. 15): at 5 CAD the ignition of the main chamber by the jets of $d_{1,3}$ occurred while it is necessary to wait until around 10 CAD to observe main chamber ignition from $d_{2,4}$ jets. This is due to a combined effect of temperature and mixing rate: when duct diameter decreases, temperature loss and jet mixing rate increase (Fig. 16), which disadvantages jet ignition.

LES shows that even if main chamber ignition is successful, the ultra lean flame consumption rate is such that the main chamber charge is very slowly consumed and this is correctly retrieved by PEMIP (Fig. 14). The pre-chamber charge is consumed slightly faster in the LES. This is again due to the mixture homogeneity assumption of PEMIP which models a homogeneous stoichiometric combustion in the pre-chamber without taking into account the equivalence ratio stratification. Here, the rich C_3H_8/H_2 -air mixture actually trapped at the top of the pre-chamber in the LES burns faster than a stoichiometric C_3H_8/H_2 -air mixture initially made up of the same C_3H_8 -air mixture as it is assumed in PEMIP.

Figure 14. Pressure and burnt fraction inside pre- and main chambers for both PEMIP and LES ($\lambda 2.0 H_2$ IT-10). The CAD of the pre-chamber (pc^{ign}) and main chamber ignition (mc^{ign}) and the TJI period predicted by PEMIP are superimposed. Jet ignitions from duct no. x are annotated d_x .

Figure 15. Plane cut normal to the x axis (left), y axis (right) intersecting the ducts by their axis and coloured by the normalized HRR with three isolines of temperature (LES, #λ2.0 H₂ IT-10)

Figure 16. Jet maximum mixing rate θ_0 (Eq. 36) and duct outlet temperature for both PEMIP and LES (#λ2.0 H₂ IT-10). The CAD of the main chamber ignition (mc^{ign}) and the TJI period predicted by PEMIP are superimposed. Jet ignitions from duct no. x are annotated d_x .

430 $\lambda_{in} = 1.5$ *Early Ignition Case* An IT of -30 CAD (#λ1.5 IT-30) is used in both
 431 PEMIP and LES, for propane injection, to assess the capability of PEMIP to
 432 model the effects of a change in IT. The main chamber ignition occurs in both
 433 the LES and PEMIP (Fig. 17). PEMIP predicts a pre-chamber combustion a
 434 little earlier but this does not affect the main chamber ignition outcome.

Figure 17. Pressure and burnt fraction inside pre- and main chambers for both PEMIP and LES (#λ1.5IT-30). The CAD of the pre-chamber (pc^{ign}) and main chamber ignition (mc^{ign}) and the TJI period predicted by PEMIP are superimposed.

Application Examples

Examples of parametric studies using PEMIP are now given in to illustrate the capacities of the model to explore new operating conditions and designs. For simplicity, in this section, the four ducts have the same diameter d_d .

Variation of the Intake Premixed Mixture Equivalence Ratio

Starting from the operating point #λ1.5IT-10, equivalence ratio of the intake premixed mixture that fills the engine λ_{in} is varied from 1.3 to 1.7 (Fig. 18). The diameter of the four ducts is maintained at $d_d = 1$ mm. Because this lean mixture fills the pre-chamber during the compression phase, the additional fuel injection duration is adjusted to keep the same equivalence ratio in the pre-chamber at IT.

As expected, the increase in λ_{in} causes lower pressures and longer combustion durations in the main chamber (Fig. 19) due to a combined effect of lower heat release and lower consumption speeds. The combustion duration increases almost linearly until $\lambda_{in} = 1.7$ where the main chamber fails to be ignited by the jets of hot burnt gases, giving the air dilution limit to avoid misfires.

Variation of the Diameter d_d of the Ducts

Still starting from the operating point #λ1.5IT-10, the diameter d_d of the four ducts is varied from 0.7 to 1.2 mm. Changing d_d induces a variation in permeability which influences the filling of the pre-chamber by the main chamber

Figure 18. Pressure inside pre- and main chambers for multiple equivalence ratios of intake premixed mixture λ_{in} , $d_d = 1$ mm. Main chamber jet ignition occurrences are indicated by gold coloured circles.

Figure 19. Crank angle difference between $BF^{mc} = 0.1$ and $BF^{mc} = 0.9$ for multiple equivalence ratios of intake premixed mixture λ_{in} , $d_d = 1$ mm.

premixed flow. The additional fuel injection duration is then adjusted to keep the same equivalence ratio in the pre-chamber at IT.

Decreasing d_d has two effects: i) it creates more vigorous jets because of higher pressure difference (Fig. 20) and ii) it causes earlier hot burnt gases ejection because of higher pre-chamber burning rate and therefore earlier main chamber ignition and combustion (Fig. 21). These combined effects act in favour of faster main chamber combustion, until jets are too vigorous and/or too cold to ignite the main chamber. The failed ignition when d_d reaches 0.7 mm proves that there is a limit in decreasing the diameter to enhance turbulent motions in the main chamber. An optimal d_d range to induce rapid main chamber combustion (optimizing engine efficiency) would be $0.75 \leq d_d \leq 0.9$ mm.

Figure 20. Pressure inside pre- and main chambers for multiple duct diameters d_d , $\lambda_{in} = 1.5$. Main chamber jet ignition occurrences are indicated by gold coloured symbols.

Figure 21. Crank angle at which $BF^{mc} = 0.1$ ($CA10^{mc}$) and $BF^{mc} = 0.9$ ($CA90^{mc}$), and crank angle difference between $BF^{mc} = 0.1$ and $BF^{mc} = 0.9$ for multiple duct diameters d_d , $\lambda_{in} = 1.5$.

Pre-Chamber Ignition Combustion Diagram

The influence of intake equivalence ratio λ_{in} and duct diameter d_d was studied independently. PEMIP allows to actually perform a two-dimensional parametric study of these parameters to delineate a PCI combustion diagram. For this exercise, the diameter of the ducts and the intake equivalence ratio sweep the range $0.7 \leq d_d \leq 1.3$ mm and $1.3 \leq \lambda_{in} \leq 1.9$, respectively. Combustion durations are given in Fig. 22 using a d_d - λ_{in} diagram. Main chamber combustion durations longer than 20 CAD are considered to be too long to result in efficient engine operation and are excluded from proper engine operating range. This map provides a clear view of where the engine could be operated based on the hole design. It also highlights a hole size d^* for which maximum air dilution in the

main chamber can be achieved based on the choice of a maximum main chamber combustion duration of 20 CAD.

Figure 22. Crank angle difference between $BF^{mc} = 0.1$ and $BF^{mc} = 0.9$ in a d_d - λ_{in} diagram with limits of ignition and combustion duration ($CA10-90^{mc} \leq 20$ CAD). The face colour of the markers corresponds to the main chamber combustion duration $CA10-90^{mc}$.

Conclusion

A zero-dimensional multi-zone engine model called PEMIP has been derived to predict the ignition of a main chamber by a pre-chamber. The approach includes submodels for i) the thermal effects of the ducts connecting pre- and main chambers and ii) the ignition of the main chamber by the jets of hot burnt gases (built during previous work using DNS¹). The unknown constants appearing in the governing equations of PEMIP have been calibrated using previously published LES data from Ref. ²² (reference case # $\lambda 1.5IT-10$). Finally, PEMIP predictions have been assessed under other operating conditions by comparing them to other LES cases sharing the same engine baseline: results are in good agreement.

From the reference case # $\lambda 1.5IT-10$, variations of the equivalence ratio of the intake premixed mixture λ_{in} and the diameter of the ducts d_d have been performed to illustrate possible applications of PEMIP. Results allow to identify the lean limit of the intake equivalence ratio λ_{in} above which main chamber ignition does not occur, a crucial information for engine calibration. PEMIP also describes the effects of the duct diameter d_d connecting pre- and main chambers. It provides a diameter range for which main chamber combustion is

the fastest (maximizing engine efficiency) for a given air dilution. Varying both λ_{in} and d_d , a PCI combustion diagram is obtained, with ignition and combustion duration limits as design boundaries.

More generally, PEMIP provides an assessment of the engine performances of a given configuration at a low computational cost. This opens promising perspectives for design of experiment applications. After that, once a PCI system has been optimally designed targeting a few operating points, PEMIP can be used to check that the engine design can be used under all the operating conditions encountered during the use of the ICE.

As such, PEMIP is a great demonstration of the potential of integrating a submodel for jet ignition into a PCI engine model. Although PEMIP agrees with the LES performed, it would benefit from being compared to engine tests and could be corrected accordingly. A model for air intake and exhaust phases could also be added if information on the performance of an entire engine cycle is required.

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Declaration of Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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