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## A simplified mechanism for the prediction of the ion current during methane oxidation in engine-like conditions



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### ABSTRACT

This paper outlines a simplified mechanism for methane oxidation for modelling the ion current in internal combustion engines. The mechanism was used to simulate a laminar flame at elevated pressures and equivalence ratios typical of a spark-ignited engine. The predicted flame speed was found to be accurate between equivalence ratios of 0.9 and 1.1 at pressures of 10 atm and 20 atm. Good agreement was found between published experimental results and numerical results for the flame composition of atmospheric laminar flames at different equivalence ratios.

Experimental results of the ion current and chamber pressure are presented for the combustion of methane in a constant volume chamber at different initial pressures and equivalence ratios. The experimental data obtained were used to validate the mechanism developed. The prediction of chamber pressure and ion current timing were found to be accurate, while there were some inaccuracies in the prediction of the ion current's magnitude.

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### 1. Introduction

The ion current produced during hydrocarbon oxidation is a useful indicator of combustion, containing information on the combustion process that is otherwise difficult to obtain. Ion sensors give localised information on flames and are robust and cheap to manufacture, making ion sensors useful in the analysis of combustion events, particularly in areas where there are large degrees of uncertainty in the combustion process, such as in internal combustion engines.

An ion sensor was used to sense lean blowout in an aircraft engine combustor and was found to perform satisfactorily [1]. Ion sensors have also been installed in spark-ignition engines to predict quantities such as air–fuel ratio [2–5], peak pressure position [6] and in-cylinder pressure [7]. They have also been used to control spark advance timing [8] and knock [9]. In HCCI engines, ion sensors have been shown to be able to estimate CA50, the point at which 50% of the total heat release has occurred [10], and to differentiate between different fuels [11]. In compression-ignition engines, the time derivative of the ion current has been used to detect and control the start of combustion [12]. The ion sensor

has also been proved able to predict engine-out torque [13] and to detect combustion resonance [14]. Given the close relationship between the combustion process and the ions developed, an understanding of the ion formation process in engines may allow insight into engine performance and emissions.

Analytical research studies into the ion current produced in internal combustion engines are few and far between, due to the inherent difficulty in analysing a signal as complex as the ion current. For fuels such as petrol and diesel, the reaction mechanisms can involve hundreds of species and thousands of reactions [15]. When such a mechanism is used as a component of an engine model which may have many sub-models, simplicity is necessary in the reaction mechanism in order to keep computational costs low. The aim of this paper is to present the validation of a simple mechanism that allows easy testing of the effects of changing parameters on the ion current. Whilst it is difficult to completely describe the chemistry of hydrocarbon combustion with such a simple mechanism, an accurate representation of the trends followed by the ion current will make it possible to gain insight into ion formation in engines and the effects engine load, speed and intake charge have on the ion current generated. The purpose of this mechanism is its incorporation into internal combustion engine models in order to explain experimental measurements of the ion current signal in engines [5,7,12,13]. This may also aid in the prediction of engine emissions and performance.

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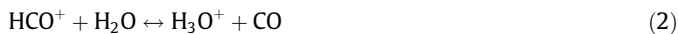
## 2. Simplified mechanism

In order to keep the reaction mechanism simple enough to be computationally efficient, methane was chosen as the fuel of interest. There exist a number of chemical reaction mechanisms for methane oxidation that are able to give very detailed results of species concentrations, heat release rates and temperature distributions in the flame. One such mechanism, GRI-Mech 3.0 [16], contains 325 reactions and 53 species, none of which are charged. Pedersen and Brown [17] devised an ionic mechanism which contained several positive ions but neglected the negative ion chemistry. In 2002, an ionic mechanism containing 392 reactions and 59 species was proposed by Starik and Titova [18] and used to predict the ion concentrations in a perfectly stirred reactor. More recently, Aithal et al. proposed a reduced ionic mechanism [19] which included 65 reactions and 29 species. This mechanism was used to predict the ion current observed in a two-zone model of methane oxidation in a constant volume chamber. Later, a two-zone equilibrium model was used by the same author [20] for the same purpose. The same equilibrium model was used to predict the ion current in an HCCI engine [21]. Prager et al. [22] developed a reaction mechanism for lean to stoichiometric methane–air flames. The mechanism for the neutral species consisted of 208 reactions with 38 species. An add-on ionic mechanism was also developed with 67 reactions and 11 charged species. All of the above mentioned mechanisms contain a large number of reactions and species. An application in internal combustion engine models requires a simpler mechanism.

The mechanisms for the generation of ions from neutral particles are well established [23–25]. Green and Sugden [23] found the primary source of ions in flames to be:



This reaction is then followed by:



Reaction (2) is inherently faster than (1), leading to the rapid conversion of  $\text{HCO}^+$  to  $\text{H}_3\text{O}^+$ . Hence, the concentration of  $\text{H}_3\text{O}^+$  is much higher than that of  $\text{HCO}^+$ .

Additionally,  $\text{O}_2^-$  ions are formed from free electrons and oxygen molecules via reaction (3).



The  $\text{H}_3\text{O}^+$  ion has been experimentally determined to constitute around 80% of the total positive ion concentration in a typical atmospheric pressure, stoichiometric methane–oxygen flame [17]. The same study determined that the  $\text{C}_2\text{H}_3\text{O}^+$  ion constituted approximately 16% of the positive ion concentration, with  $\text{CH}_3^+$  and  $\text{CHO}^+$  making up the remainder.  $\text{H}_3\text{O}^+$  was found to be the dominant positive ion in low-pressure lean flames as well. Goodings et al. [26] also report a peak concentration of  $\text{H}_3\text{O}^+$  approximately five times that of  $\text{C}_2\text{H}_3\text{O}^+$  in lean methane–oxygen flames, and an integral concentration 26 times greater. Another study has determined that the  $\text{H}_3\text{O}^+$  ion represents 70–90% of the total positive ion concentration [27]. Considering the mass of the  $\text{H}_3\text{O}^+$  ion is less than those of other ionic species likely to be formed, it will be responsible for a large fraction of the ion current due to positive species. Thus,  $\text{H}_3\text{O}^+$  and  $\text{HCO}^+$  (as a precursor species) are the only positive ions modelled in this mechanism.

$\text{O}_2^-$  is the first negative ion formed in appreciable concentration [28]. From  $\text{O}_2^-$ , many ions can form via charge transfer or proton transfer, most notably  $\text{CHO}_2^-$  and  $\text{OH}^-$  in lean flames, and  $\text{C}_2\text{H}^-$  in rich flames. The masses and ionic radii of these species, however, are many orders of magnitude higher than that of electrons,

leading to an increased collision frequency and a mobility that is smaller by orders of magnitude. For this reason, the only negatively charged species considered here are electrons and  $\text{O}_2^-$ . These simplifications should enable the developed mechanism to capture the dominant portion of the ion current signal in and near the flame front.

It must be noted that the mass spectrometric technique used to measure the ion concentrations in flames is subject to some inaccuracies. The sample gas is cooled upon entry to the mass spectrometer, leading to a shift in the equilibria present between ions [29]. Additionally, a plasma sheath is formed around either electrode [30] making detection of ions difficult. When negative ions are present in a flame, the Debye length increases leading to an increase in the thickness of the plasma sheath, further decreasing the accuracy of this technique [30].

The general reaction scheme and reaction rates of this mechanism is based on Turns [31] and is shown in Fig. 1.  $\text{CH}$  in the left side branch is involved in reaction (1), the primary source of ions in the flame.  $\text{C}_2$  chemistry has not been included in this mechanism in order to keep computational time low when it is used in internal combustion engine models. Even without the inclusion of  $\text{C}_2$  chemistry, the performance of the model was found to be accurate over the desired range of equivalence ratios, as seen in Section 3.

In addition to this, four ionic reactions and three H–O system reactions are included in the mechanism. The rates of these reactions have been obtained from various sources [32–34]. Thermodynamic data for all species was obtained from Burcat and Ruscic [35]. Transport data for most species was obtained from the Chemkin transport database [36]. Data was not available for some species; their coefficients were estimated from similar species. The full mechanism along with thermodynamic and transport data is included in the supplementary material of this paper.

## 3. Laminar flame validation

The reaction mechanism described in Section 2 was used with the Premix code from Chemkin II to model a laminar flame. These results were compared to experimental measurements. The mechanism is required to be accurate at values of equivalence ratio, pressure and temperature commonly seen in spark-ignition engines. While these engines can operate at equivalence ratios between 0.82 and 1.22 [37], closed-loop lambda control on modern engines is able to maintain equivalence ratios very close to 1.0 [38,39]. Peak pressure in naturally-aspirated SI engines is typically

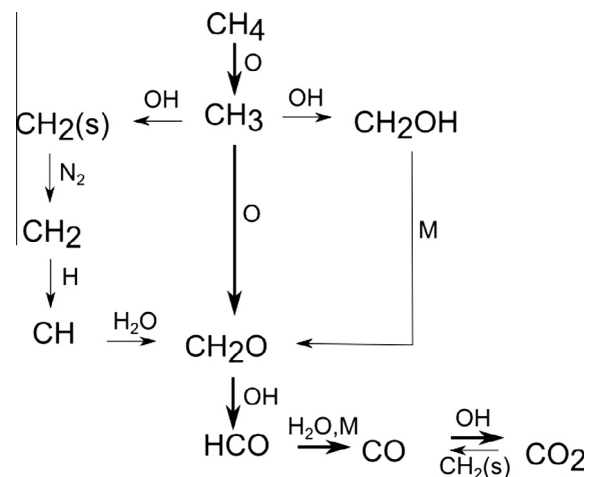


Fig. 1. Methane reaction mechanism.

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