Ion Current Simulation During the Post Flame Period in SI Engines

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ABSTRACT: *The application of ion current signals is one of the most recent approaches in engine management systems. By applying a small constant DC voltage across the electrodes of the spark plug and measuring the current through the electrode gap, the state of gas may be measured and investigated. In this paper a computer code is developed in order to analyze the state of gas during the combustion period. It is shown that there is a strong correlation between the peak pressure and the maximum current position. It is also shown that among all combustion products, the NO has the most contribution in generating electrical current. The two zones model is used for calculating the cylinder pressure and temperature.*

KEY WORDS: *Combustion species, Ion current, Modeling, Peak pressure position, SI engines.*

INTRODUCTION

The technique of measuring ion currents of flames has been well known for a long time. It is almost two centuries, since Volta in the year (1801) discovered the electrical conductivity of free flame propagation. Tufts (1906) was the first scientist arguing for an ionization process that had something to do with the chemistry in the flame front. In the early 1950's, this process was thoroughly investigated as one of the explanations for the high flame speed of burning hydrocarbons [1-4]. Recently, this area is the subject of a new born interest. The spark plug of SI engines is used as ion current sensors. The measured ion current, is related to the physical and chemical properties of the combustion products inside cylinder [5-15].

In this paper a computer code is developed in order to simulate the state of gas and the ion current during the post flame period. The relation of ion current with temperature and pressure are investigated. It is shown that there is a strong correlation between the ion current magnitude and the instantaneous temperature and pressure of the cylinder. Also, the contribution of different species in ion current generation is determined.

THEORY AND FORMULATION

The ion generating process

The ionization process may briefly be described as follows; the heat in the flame front ionizes the gas in the combustion chamber and the gas becomes conductive. An electrical field is then generated in the combustion chamber and the current is measured. The ionization

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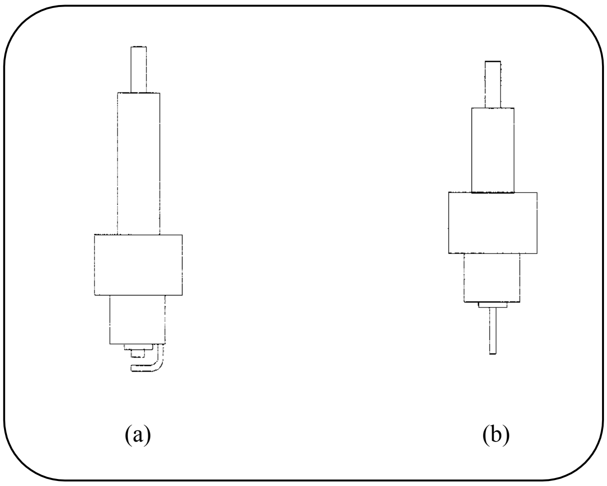

Fig. 1: Two different probes (a) the spark plug (b) A separate probe similar to the spark plug.

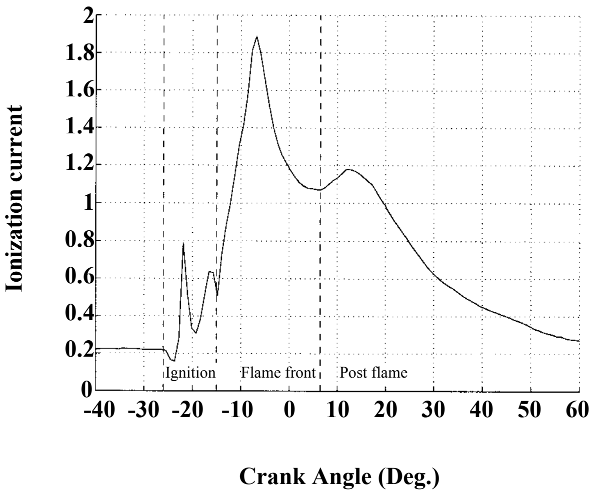

Fig. 2: Ionization current signal characteristic in three phases: Ignition, Flame front and Post flame.

current contains information about the combustion process and pressure. Equation (1) is an example of an ideal reaction in an internal combustion engine.

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \quad (1)$$

However, the actual combustion process has several stages. The high temperature inside the cylinder ionizes the molecules. The ionized molecules are recombined and more stable molecules are generated. Equation (2) includes some preliminary reactions in ion creation:

$$CH + O \rightarrow CHO^+ + e^- \quad (2)$$

$$CHO^+ + H_2O \rightarrow H_3O^+ + CO$$

$$CH + C_2H_2 \rightarrow C_3H_3^+ + e^-$$

The generated ions are not limited to those mentioned in Equation (2) Other ions such as $C_3H_3O^+$, OH^- and O^{2-} and a considerable amount of H_3O^+ and $C_3H_3^+$ are also generated. These positive ions and electrons become carriers of ionic currents [4].

To measure the degree of ionization, a probe is inserted into the combustion chamber. The probe is biased in order to create an electrical field that attracts and rejects ions in the vicinity of the probe. It is a well-known and confirmed fact that a positively biased probe generates a higher level signal [9, 16].

Measuring principles

The ionization current in the combustion chamber is measured either by a modified version of spark plug or with a separate pin inserted into the combustion chamber. These two different types of ion current sensors are shown in Fig. 1. Using a modified spark plug to measure the ion current, eliminates the extra cost of an additional measuring device. However, no ionization signal may be measured during ignition pulses. When the ignition is completed, the spark plug is available for measuring the ion current during the remaining part of the combustion [17].

Characterization of the ionization current

Many engine parameters such as temperature, air to fuel ratio, fuel type, E.G.R., by blow gases, engine load and humidity in air affect the ionization current [9,10,16,18,19].

In Fig. 2 the ionization signal is displayed as a function of crank angle. It has three phases: ignition, flame front and post flame. If we use of spark plug as ionization sensor in the ignition phase, the ionization signal is disturbed by the ignition pulse. Therefore, the measured ion current is disturbed and becomes noisy. At the next phase, the ion current signal increases rapidly. The high level signal at the beginning of this phase is due to the high ionization degree of the flame. Some of the generated ions in the flame are recombined quickly, to produce more stable molecules. Other ions have longer residential. The flame stays close to the spark plug for a short time, and then it propagates through the combustion chamber. This explains why the flame front has a steeply peak which decreases quickly. When this phase is over only the more stable ions remain.

The post flame ionization is mostly constituted of H_3O^+, CO^- and their hydrates [14].

Ionization Current Modeling

In order to derive appropriate relations between temperature, pressure and ion current, two major factors have to be evaluated. The ionization ratio and electron drift velocity are used for ion current analyzing.

Ionization ratio and Saha's equation

The ionization ratio η is given by the following relation:

$$\eta = \frac{\rho_e}{\rho_0 + \rho_i} \quad (3)$$

Assuming local thermodynamic equilibrium, the relation between the number densities of two ionized states with the electron number density is given by Saha's equation [20, 21]:

$$\frac{\rho_i \rho_e}{\rho_{i-1}} = 2\left(\frac{2\pi m_e \sigma T}{h^2}\right)^{3/2} \frac{B_i}{B_{i-1}} \exp\left[-\frac{E_i}{\sigma T}\right] \quad (4)$$

This equation, in our case, may be viewed as a balance between the two processes of ionization and recombination. The weakness of this equation is that it does not, take into consideration, except for the ionization energy, any species factor.

Taking only the dominating factor into account, we get the following solution.

$$\eta = \sqrt{\frac{\rho_H}{\rho_0 + \rho_i}} \quad (5)$$

Where

$$\rho_H = 2\left(\frac{2\pi\ m_e \sigma T}{h^2}\right)^{3/2} \frac{B_i}{B_{i-1}} \exp\left[-\frac{E_i}{\sigma T}\right]$$

Notice that $\rho_0+\rho_i$ is equal to the number of heavy particles. It is also assumed that each molecule or atom losses at most only one electron (one ionization degree).

Electron drift velocity

The electron drift velocity is a function of the mobility of the electrons, μ, and the electrical field X:

$$\upsilon_d = \mu X \quad (6)$$

There are a lot of interactions between electrons, ions and neutrals. We have elastic collision, in elastic interaction like excitation, ionization recombination, etc. The possibility of interaction between particles is given by their cross sections S, which is defined in classical physics, as the surface a particle sees as it passes through a volume, divided by density. Introducing λ as the mean free path length, we have:

$$\lambda = \frac{1}{\rho_{tot} S} \quad (7)$$

where

$$\rho_{tot} = \sum_i x_i \rho_i \quad (8)$$

We also introduce the species fraction x_i, and ρ_i as the number density of species, i.

If we assume that the gas temperature is the major factor and consequently the contribution of the electrical field is relatively small, we get the following expression:

$$\mu = \frac{e\lambda}{m_e \upsilon_T} \quad (9)$$

where

$$\upsilon_T = \sqrt{\frac{8\sigma T}{\pi\ m_e}}$$

Electrical current

Assuming that the geometry of the gas volume is cylindrical, we may formulate the current as:

$$I = e\eta\,\rho_i \upsilon_d \pi r^2 \quad (10)$$

Substituting Eqs.(5), (6) and (9) in Equation (10), we obtain;

$$I = U\frac{\pi\ r^2 e^2}{Sd}\left(\frac{\pi^3 x_i}{8 m_e \sigma\ T}\right)^{\frac{1}{2}}(AA) \quad (11)$$

where

$$AA = \sqrt{\frac{\frac{2(2\pi m_e \sigma T)^{3/2}}{h^3}\frac{B_i}{B_o}\exp\left[-\frac{E_i}{\sigma T}\right]}{\rho_{tot}}}$$

In this relation the current I, is a function of three parameters; temperature T, number density of total species ρ_{tot} and species fraction x_i. This is derived assuming only one ionization degree. Let,

$$\rho_{tot} = \frac{P}{\sigma T} \tag{12}$$

Then;

$$I = C x_i^{1/2} P^{-1/2} T^{3/4} \exp\left[-\frac{E_i}{2\sigma T}\right] \tag{13}$$

Where C is the product of all physical constants in Equation (11).

The relative current may be written as:

$$\frac{I}{I_{max}} = \left(\frac{x_i}{x_{i\,max}}\right)^{1/2} \left(\frac{P_i}{P_{max}}\right)^{-1/2} \left(\frac{T}{T_{max}}\right)^{3/4} \exp BB \tag{14}$$

where

$$BB = \left[-\frac{E_i}{2\sigma T_{max}}\left(\left(\frac{T_{max}}{T}\right) - 1\right)\right]$$

Variables, T_{max}, P_{max} and x_{max} are temperature, pressure and total number density at I_{max}, respectively.

Ionization model description

The ion current model is derived based on the Saha-Boltzmann's equation. It is assumed that the geometry of gas volume in the combustion chamber is cylindrical. We are also considering a one ionization degree for this model. This model, as given by equation (13) explains the relation between ion current and temperature, pressure and fraction species during the post flame period. The model also represents the contribution of each species in the generated ion current. It should be noted that the presented model is only valid for the post flame period. Therefore, it is not valid in the ignition and flame front phases.

Two Zones Model

In order to evaluate variables such as temperature, pressure and mole fraction of species, the two zone model is implemented [22, 23]. The major assumptions are:

a) The original charge is homogenous.
b) The pressure at any time is uniform throughout the cylinder.
c) The volume occupied by the flame reaction zone is negligible.
d) The burned gas is at full thermodynamic equilibrium.
e) The unburned gas is frozen at its original composition.
f) Both burned and unburned gases are uniform in local specific heat.
g) There is no heat transfer between burned and unburned zones.

The governing equations in combustion process are:

$$E_b + W_b = Q_b \tag{15}$$

$$E + W = Q \tag{16}$$

$$PV_u = m_u R_u T_u \tag{17}$$

$$PV_b = m_b R_b T_b \tag{18}$$

$$m_b + m_u = m \tag{19}$$

$$V_u + V_b = V \tag{20}$$

$$P\dot{V} + \dot{m}_u e_u + \dot{m}_b e_b + m_u \dot{e}_u + m_b \dot{e}_b = \dot{Q} \tag{21}$$

$$[e_b(t) - e_u(t)]\dot{m}_b + m_b \dot{e}_b(t) + P\dot{V}_b - \frac{1}{\rho_u} P\dot{m}_b = \dot{Q}_b \tag{22}$$

Equations (15) to (22) are used for two zone combustion model calculation. Since there are only 6 equations with 7 unknowns, we need another equation. In this paper Wiebe function is used for mass burn rate as the last equation.

$$\dot{m} = \dot{m}_u + \dot{m}_b \tag{23}$$

Wiebe function is defined as follows:

$$x_n = 1 - \exp\left[a\left(\frac{\theta - \theta_s}{\Delta\theta_b}\right)^{(n+1)}\right] \tag{24}$$

Parameters "a" and "n" are constants [24].

SIMULATION RESULTS

In this section the ion current is evaluated based on the related equations with parameters given in Table 1. Also the contribution of each species in current generation is calculated.

Table 1: Parameters in Eq. (11).

$U = 80V$
$B_0 = B_i$
$r = 1mm$
$d = 1.5mm$
$e = 1.6022\times10^{-19}C$
$m_e = 9.1095\times10^{-31}kg$
$h = 6.620755\times10^{-34}$ (J.s / molecule)
$\sigma = 1.38065812\times10^{-23}$ (J / K.molecule)

Table 2: Ionization energy of species and the maximum generated currents.

Species	Ionization Energy (eV)[10]	Current (μ A) (Calculated)
N_2	15.5	0.001105
N	14.53	6.91e-6
NO	9.25	46.8366
CO	14.05	0.004329
CO_2	13.84	0.013246
O	13.614	0.001926
O_2	12.2	0.117968
H	13.595	0.001961
H_2	15.427	9.6e-5
H_2O	12.6	0.170119
OH	13.18	0.01272

The two zones model is applied in this paper and it is assumed that the combustion products are 11 species as shown in Table 2. In this table the ionization energy and generated current are shown for all species. It is very interesting to see that NO is the only major source for the ion current generation and the contribution of other species is negligible. A chart based on the proposed results is shown in Fig. 3.

In Figs. 4 and 5 the cylinder pressure and temperature are shown verses the crank angle, while Fig. 6 shows the burned gas temperature variation. The maximum burned gas and mean cylinder temperatures are 2710 K and 2516 K, respectively.

The difference between the burned gas and the mean cylinder temperature variation verses crank angle is shown in Fig. 7.

Fig. 8 shows the variation of ion current in post flame period. The ion current has its peak value at the crank angle equal to 372°.

Fig. 9 shows the simulation results of normalized pressure and ion current verses crank angle. Fig. 10 shows the experimental results for the same variables [16]. As it is shown in these figures, the maximum ion current coincide with the peak pressure position. According to the state equation, when volume is constant, the maximum pressure and temperature are coincided to each other. Also, maximum NO concentration occurs at the maximum temperature. Therefore, the maximum ion current occurs at the peak pressure position.

CONCLUSION

In this paper the following results are obtained:

1- The generated ion current during the post flame period in SI engine is simulated. The simulation has been analyzed with a thermodynamic ionization equilibrium approach.

2- A computer code is developed to investigate the simulation results.

3- The simulation results indicate that the ionization of NO is the major source of free electrons in a fully combusted hot gas.

4- The correlation between peak pressure and maximum current position is clearly shown.

5- The simulation results are validated by comparing with the experimental test data.

Nomenclature

B_i	Internal partition function
d	Spark plug gap (mm)
E	Internal energy (J)
E_i	Ionization energy of state i (eV)
e	Electric charge (C)
e_b	Burned gas specific internal energy (J/kg)

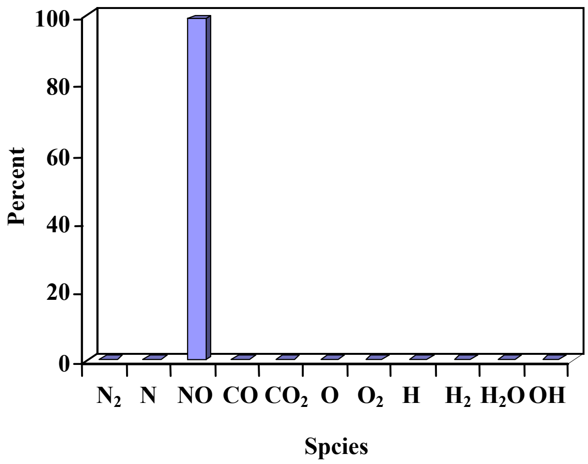

Fig. 3: Contribution of all species in ion current generation (Calculated).

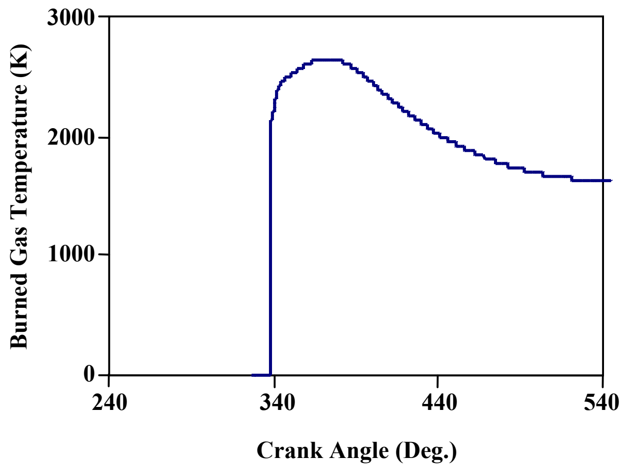

Fig. 6: Burned gas temperature variation verses crank angle (Simulated).

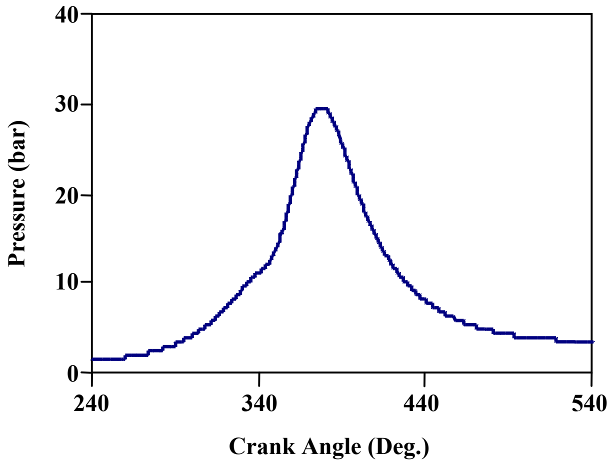

Fig. 4: Cylinder pressure variation (Simulated).

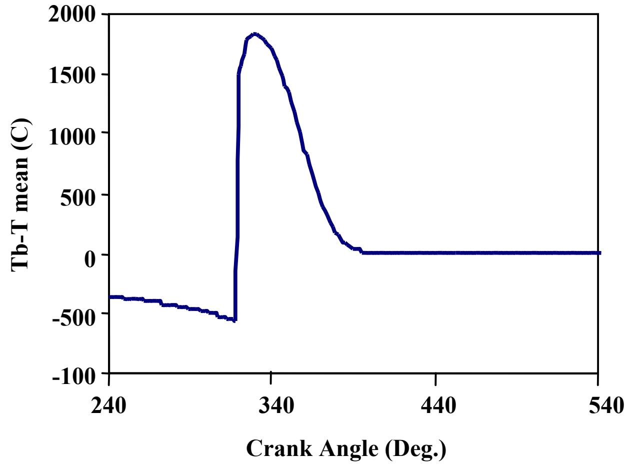

Fig. 7: Burned gas and cylinder mean temperature difference variation verses crank angle (Simulated).

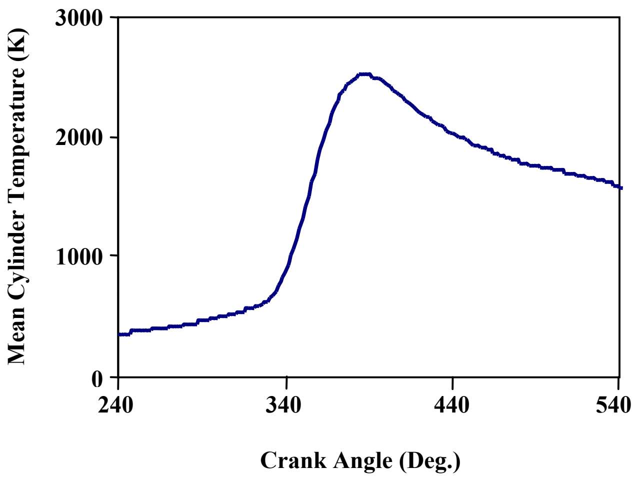

Fig. 5: Mean cylinder temperature verses crank angle (Simulated).

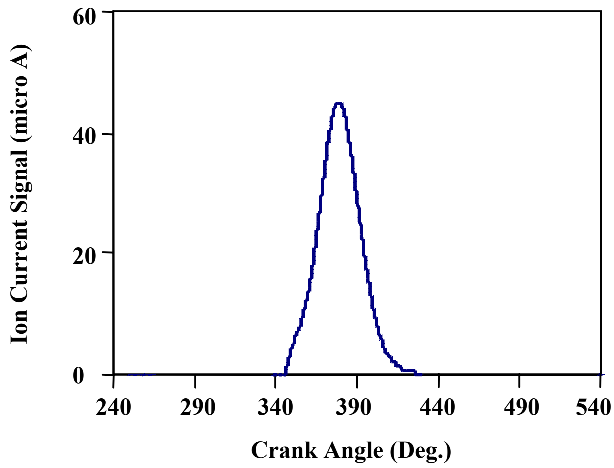

Fig. 8: Ion current variation in post flame period (Simulated).

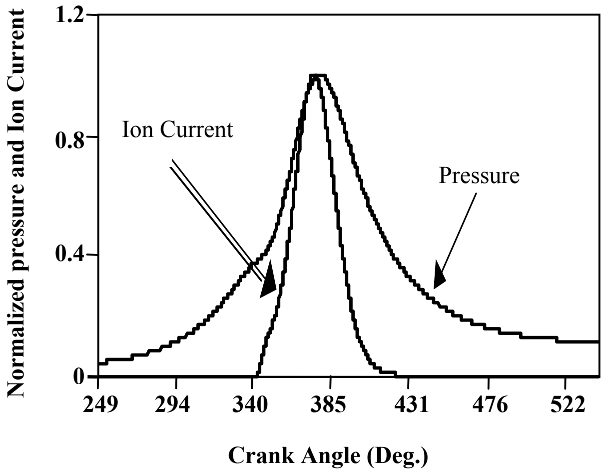

Fig. 9: Normalized ion current and pressure variation via crank angle (Simulated).

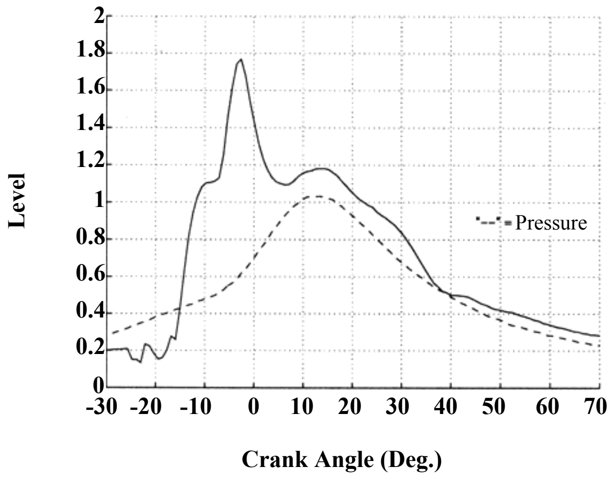

Fig. 10: Normalized ion current and pressure variation via crank angle (Experimental).

e_u	Unburned gas specific internal energy (J/kg)
h	Plank's constant (J.sec/molecule)
I	Electric current (A)
i	Electric current density
m	Mass of in cylinder gas (kg)
m_e	Electron mass(kg)
P	Combustion chamber pressure (Pa)
Q	Heat transfer (J)
R	Gas constant (J / kg.K)
r	Radius (mm)
S	Particles cross sections
T	Absolute temperature(K)
U	Voltage (V)
V	Cylinder volume(m^3)
W	Work done (J)
X	Electrical field (N / C)
x_b	Mass fraction burned
x_i	Species fraction

Greek Letters

ρ	Density (kg / m^3)
ρ_e	Electron number density
ρ_i	Number density of species, i
ρ_0	Neutrals number density
ρ_{tot}	Number density of all species
λ	Mean free path (m)
η	Ionization ratio
σ	Boltzmann's constant (J/K.molecule)
μ	Mobility (C.sec / kg)
θ	Crank angle (rad)
θ_s	Start of combustion angle (rad)
$\Delta\theta_b$	Combustion duration (rad)
υ_d	Drift velocity (m/sec)
υ_T	Mean random velocity (m/sec)

Subscripts

b	Burned
i	Number density of ionized states i
u	Unburned

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