Numerical study of combustion-wave propagation initiated by non-equilibrium discharge

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Abstract. In the work, we present the results of a numerical study of the combustion initiation of the lean propane–air mixture under the conditions of an homogeneous-charge-compression-ignition engine. We show that preliminary discharge treatment could accelerate the ignition and study how the size of discharge area, specific input energy and other parameters influence upon the delay time. The role of chemical reactions occurring during the compression cycle (before discharge treatment) is also discussed.

1. Introduction
Modern requirements on the fuel consumption, the content of automotive exhaust gas and the power efficiency make demands for the research of the ignition of the lean air–fuel mixtures (fuel–air equivalence ratio $\phi < 1$) in homogeneous-charge-compression-ignition (HCCI) engines. In this type of engines the air–fuel mixture auto-ignites as a consequence of piston compression and a lot of experimental and theoretical research is focused on finding new effective regimes (general overview of the progress in this area could be found elsewhere [1]). It was shown in the experiments that preliminary discharge treatment of the fuel–oxidizer mixture may significantly reduce the induction time of the ignition (see, for example, [2]), but in the simulation of this kind of system one usually encounters a problem: the time scales are very different for the discharge (ns) and for the evolution of the combustion wave (ms–s). This difference makes almost impossible complete hydrodynamic simulations with discharge evolution and combustion chemical kinetics due to the unreasonable amount of computational time. Nevertheless, the effect of discharge on fuel–oxidizer mixture could be estimated.

In this work, to examine the discharge effect on the ignition of fuel–air mixture, we carried out 1D (one-dimensional) numerical simulation by means of computational fluid dynamics (CFD) under the conditions of HCCI engine. The calculations were performed in the axisymmetric formulation (cross-section of the cylinder parallel to the plane of the piston). Activation of the ignition was conditioned due to the non-equilibrium effects of the electrical discharge of the pulsed corona type, which creates the region in the combustion chamber with a high chemical reactivity near the axis of the cylinder. Estimated concentrations of active species and temperature after discharge stage are taken as initial parameters for CFD-modeling of combustion wave.
2. Numerical simulation

In this work the combustion process (the formation and evolution of combustion wave and auto-ignition) is simulated using Navier–Stokes compressible solver from [3]. The set of conservation laws (for mass, momentum and total energy) for the entire gas mixture is coupled with the multicomponent diffusion equations for every component with chemical kinetic source terms:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (\rho U r) = 0,$$

$$\rho \frac{\partial U}{\partial t} + \rho U \frac{\partial U}{\partial r} = -\frac{\partial P}{\partial r} + \frac{\partial}{\partial r} \left[ \eta \left( \frac{4}{3} \frac{\partial U}{\partial r} - \frac{2}{3} U r \right) \right] + \frac{2\eta}{r} \left( \frac{\partial U}{\partial r} - \frac{U}{r} \right),$$

$$\frac{\partial \rho e^0}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \left( \rho e^0 + P \right) U - \lambda \frac{\partial T}{\partial r} - \eta \left( \frac{4}{3} \frac{\partial U}{\partial r} - \frac{2}{3} U r \right) U \right) = 0,$$

$$\frac{\partial \rho_i}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (\rho_i U r) - \frac{1}{r} \frac{\partial}{\partial r} \left( D_i r \frac{\partial \rho_i}{\partial r} \right) = \dot{\omega}_i,$$

where $\rho$ is the overall mixture density, $U$ is the flow velocity, $P$ is the gas pressure, $T$ is the temperature, $\eta$ is molecular viscosity coefficient (depending on temperature and composition of mixture), $e^0 = e + U^2 / 2$ is the specific total energy, $e$ is the specific internal energy, $\lambda$ is the thermal conductivity, $\rho_i$ is the density of the $i$-th component, $D_i$ is the diffusive coefficient of $i$-th component, $\dot{\omega}_i$ is the chemical kinetic source term for $i$-th component. Transport properties of multicomponent fluid are estimated on the bases of temperature approximations of collision integrals of viscous and diffusion type. Thermodynamic properties of species are determined by specifying the formation enthalpies and polynomial dependencies of constant-pressure heat capacities on temperature. Ideal gas equation-of-state is assumed to hold for every species, and Dalton’s law is used to determine the gas pressure.

Detailed chemical kinetic scheme was developed earlier for modeling of combustion of the air–propane mixture including 103 components and 700 reactions [4]. This scheme was validated by comparison of the measured experimental results with calculated velocity of laminar flame propagation [5]. Laminar flame propagation velocity is a unique characteristic for specified fuel–air equivalence ratio for certain mixture and this comparison is an established way to validate different chemical schemes.

The calculation domain is a cylinder with radius 5 cm, where 1D numerical simulations (along radius) are performed. The boundary conditions are established as follows: on the left border ($r = 0$) there is symmetry boundary condition and on the right ($r = 5$ cm) there is no-slip non catalytic adiabatic wall. The discharge area occupies cylindrical region near the axis of symmetry ($r = 0$). In this area initial concentrations of the active radicals and temperature are different from non-activated part of the simulation domain.

Initial stage of ignition (when discharge is on) is characterized by a fast formation of active radicals. It was shown earlier that O atoms play the main role in the ignition acceleration which affects the reduction of induction time [6]. Initial stage could be effectively described with simplified kinetic scheme resulting in production of active particles and then the obtained concentrations of active particles and temperature rise could be an input for the modeling by means of CFD:

$$e + O_2 \rightarrow O + O + e,$$

$$e + N_2 \rightarrow e + N_2^*,$$

$$e + C_3H_8 \rightarrow e + C_3H_7 + H.$$  

In reaction (6), $N_2^*$ is the total sum of the exited states of $N_2$ molecule with excitation energy $E \geq 6.17$ eV. The concentrations of primary active particles are estimated via the rate constants of reactions (5)–(7) and specific input energy (per one molecule) using G-values method [7]. G-values represent the number of the particles produced per 100 eV of the discharge energy.
Figure 1. The evolution of temperature at $W = 0.05$ eV/molecule, $d = 5$ mm, $P_0 = 42.2$ atm and $T_0 = 925$ K.

3. Results and discussion

All simulations below was carried out for the lean air–propane mixture with equivalence ratio $\phi = 0.7$ (0.0286C$_3$H$_8$ + 0.2043O$_2$ + 0.7671N$_2$). Initial conditions (temperature and pressure) were corresponding to the HCCI engine cycle (table 1). We start our simulations not from the beginning of the compression cycle and so we need to take into account that the volume is filled not only with fuel and oxidizer (and with active radicals in the discharge area) but with some intermediate products of low temperature oxidation reactions. In the discharge area for specific input energy $W = 0.05$ eV/molecule corresponding temperature rise and concentration of active species (using G-values method) are 91 K, $[O] = 4570$ ppm, $[H] = 180$ ppm, $[C_3H_7] = 180$ ppm. For specific energy 0.1 eV/molecule the temperature rise and concentration of active species are twice as large as for $W = 0.05$ eV/molecule. It would be optimal for the ignition to occur straight after point of maximal compression (top dead center or TDC, 360 crank angle degree, CAD), so there is no need to run simulation over 8, 6 and 2 ms for simulation with initial conditions (IC) 1, 2 and 3 correspondingly (see table 1).

At the simulation with IC 3 for input energy $W = 0.05$ eV/molecule and discharge activation area $d = 1$ cm, there is formation of combustion wave with following auto-ignition (simultaneous ignition of end-gas), and there is no combustion wave formation during 10 ms run for IC 1 and 2. In previous work, we also performed a simulation for $P = 30$ atm and $T = 800$ K and there was combustion-wave propagation without auto-ignition during 9 ms of simulation. In sum, the closer to the point of maximal compression we turn on the discharge, the faster ignition occurs. In figure 1, the evolution of temperature during combustion is demonstrated (for $W = 0.05$ eV/molecule, $d = 5$ mm, IC 3). Spatial distribution of temperature is shown...
Figure 2. The evolution of temperature and pressure at $W = 0.1$ eV/molecule, $P_0 = 12$ atm, $T_0 = 700$ K. Lines $T^*$ correspond to the simulation with initial composition of the mixture equal to one before compression.

Table 1. Initial conditions.

| IC number | CAD | Time before TDC (ms) | $P$ (atm) | $T$ (K) |
|-----------|-----|----------------------|-----------|---------|
| 1         | $310^\circ$ | 5.5 | 6.76 | 600 |
| 2         | $325^\circ$ | 3.8 | 12.36 | 694 |
| 3         | $355^\circ$ | 0.5 | 42.2 | 925 |

in figure 1(a); at first, there is formation and propagation of a combustion wave, and then the combustion wave is slowing down, and then auto-ignition is occurring. In figure 1(b), there is time dependency of temperature in several points of the computational domain. At the moment of auto-ignition there is simultaneous temperature rise in the area before the combustion wave (see lines corresponding to 2, 3, 4 cm in figure 1(b)). Temperature pulsations in figure 1(b) are caused by propagation of cylindrical compression waves. Estimated time, which is needed for the compression wave to travel to the wall and back, is corresponding to the periods of the temperature and pressure pulsation in different points. Compression waves propagates with speed of sound, for example, the pulsation frequency at the position 1 cm after auto-ignition (see figure 1(b) after 1.8 ms) is equal to 10.7 kHz and corresponding speed of sound is 1000 m/s (approximately). Magnitude of the pulsations is decreasing with time.

At that point let us examine what parameters are effecting combustion process and how. Firstly, we change the discharge parameters $W$ (specific input energy) and $d$ (radius of activated area). At first we vary $d$ with fixed $W = 0.05$ eV/molecule in simulation with IC 3 and look at the time of auto-ignition. Auto-ignition time for non-activated mixture is about 3 ms, and it is occurring later then TDC point. With discharge activation the new auto-ignition times
Figure 3. Concentrations of fuel (C\textsubscript{3}H\textsubscript{8}), products (CO\textsubscript{2} and H\textsubscript{2}O), active radicals (H and O) and some intermediate oxidation products, \(t = 3\) ms, \(W = 0.1\) eV/molecule, \(P_0 = 12\) atm, \(T_0 = 700\) K.

for \(d = 2.5\), 5 and 10 mm are, correspondingly, 2.31, 1.74 and 0.81 ms. Thus the enlarging of activated area facilitate the combustion process. We would like to underline here that we are working in cylindrical coordinate system and activated area with \(d = 1\) cm is not 0.2 part of whole volume but only 0.04 part of the whole volume.

Next we increase the specific energy input \(W\). For this we repeat simulation with IC 2 (where no ignition occurs for \(W = 0.05\) eV/molecule) with \(W = 0.1\) eV/molecule. There is formation of combustion wave after 2.5 ms (figure 2), so the increasing of the specific energy input results in faster combustion (figure 3, for concentration profiles during combustion-wave propagation). At first sight this is rather obvious result, but let us examine more closely discharge activation mechanism. There is widespread view that discharge effect is mostly caused by temperature rise. Of course, if one heats mixture high enough, the combustion will initiate without any additional active radicals. Nevertheless, in our opinion, the role of active radicals is crucial in the situations where temperature rise is rather low. To illustrate this we repeated the simulation with \(\Delta T = 182\) K (heating of the activated area), \(d = 10\) mm, \(P_0 = 12\) atm, \(T_0 = 700\) K, but without active radicals, and in the result there was no formation of combustion wave after 8 ms despite heating of the activated area. So, heating indeed facilitates combustion initiation but for low specific energy input the role of active O atoms is more important, especially for lower \(T\) and \(P\), and it is easier to start the discharge at lower pressures.

It is generally thought that low-temperature reactions (700–900 K) does not play significant role during initiation of high temperature combustion in HCCI engine. To prove the opposite we exclude preliminary zero-dimensional simulation of chemical kinetics and repeat simulations with initial concentrations of air and fuel only (0.0286 C\textsubscript{3}H\textsubscript{8} + 0.2043 O\textsubscript{2} + 0.7671 N\textsubscript{2}) without any other intermediate oxidation products. For \(W = 0.05\) eV/molecule, IC 3 the time of auto-ignition is increasing, and the difference for \(d = 2.5\) and 5 mm is 1.3 and 0.8 ms correspondingly. For \(W = 0.1\) eV/molecule, \(d = 10\) mm, IC 2 the formation and propagation of combustion
wave is occurring later (see figure 2) and time delay is 0.6 ms. Time delay is larger for smaller activated area and for simulation with less initial $T$ and $P$, and delay of several milliseconds could be significant in HCCI engine cycle. Thus one need to take into account that initial composition of the mixture is not the same as before compression.

4. Conclusions
In this work, we show that preliminary discharge treatment could accelerate the ignition of lean air fuel mixture and even small energy input could result in significant decrease of induction time. The closer to the point of maximal compression activation of mixture is occurring, the faster the ignition. Increasing of discharge specific energy input or discharge area (or both) results in decreasing of induction time and in combustion for initial conditions where ignition does not occur for lower $W$. Active radicals in discharge area play significant role in combustion acceleration, even more significant than temperature rise for the simulations far away from TDC. There was also shown that in the calculations of ignition and propagation of the combustion wave it is very important to consider changes in the composition of the mixture at the moment of switching on the discharge. If the composition of the mixture is the same as before the beginning of compression, the ignition delay time may increase significantly. All these factors could vary induction time for several ms and for the conditions of HCCI engine this could be crucial.

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