Role of pressure waves in the heating of the end-gas in HCCI engine with activation by pulsed corona discharge

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Abstract. In this paper we present numerical research of pressure waves influence on the end-gas in HCCI engine with discharge activation. It is shown that there is certain promotion of exothermic chemical reactions by pressure waves. That leads to the slight heating of the end-gas, but mainly the end-gas is heated due to the compression in the process of combustion wave propagation.

1. Introduction
Main trends in engine research nowadays are energy efficiency and “green operation” which prompt scientists and engineers to explore combustion strategies other than ones realized in conventional spark-assisted or compression engines. Low temperature combustion strategy in homogeneous charge compression ignition (HCCI) engines is one of the possible alternatives. In this type of engines an air-fuel mixture is heated under compression and then autoignites, this process is governed by chemical kinetics, and HCCI engines work stable under low loads but need some activator of combustion to achieve stable ignition and combustion control under high loads [1]. Possible way to stabilize combustion under high loads is to use non-equilibrium discharge which increases the reactivity of the mixture in the part of combustion chamber due to plasma-chemical reactions and heating (for example, [2]). Thus, energy release in the combustion chamber is prolonged in time while combustion wave (CW) propagates from discharge region to the walls, which is better for the engine construction than simultaneous autoignition in the whole volume. Controlling combustion process in this type of engine is important research issue and so, understanding detailed physical mechanisms of the events in combustion chamber is needed.

In this paper we continue our previous [3] numerical investigation of the processes, occurring in the combustion chamber of HCCI engine with high frequency corona discharge as a combustion initiator. The noticeable volume of initial ignition is one of the main features of combustion initiation by nanosecond corona discharge (several cm³, whereas for a spark discharge it is several mm³). That ignition happens not far before top dead center (TDC) and generates pressure waves in the chemically active medium.

2. Model and results
In our study, the hybrid engine (HCCI engine with combustion initiation by pulsed corona discharge) is presented in a simplified form. Our simulation domain is a cylinder filled with lean homogeneous propane-air mixture (fuel-air equivalence ratio is equal to 0.7) with area around the axis activated by the
discharge, for details see [3]. Such formulation justifies one-dimensional simulation along radius and allow us to solve full Navier-Stokes system with detailed kinetic scheme (103 substances, 710 reactions [4]). We also introduce special source terms to mimic compression by piston along axis in the 1D simulation. Intake temperature is 380 K, pressure is 1.28 bar, compression ratio is 15 and engine speed is 1500 rpm, cylinder radius R is 5 cm, activated area in the form of a cylinder has radius 0.5 cm. A misfire regime of engine operation is observed under the same conditions but without discharge. In the simulations a pulsed nanosecond corona is switched on at 310 crank angle degree (CAD, top dead center is 360 CAD) and treated a mixture during 555 μs (5 CAD), then discharge is switched off, and our CFD calculations are started. Temperature and chemical composition in the activated area are estimated based on the dynamics of a propagation of the streamer.

In the typical combustion process in such system a simultaneous ignition of activated area occurs, then combustion wave (flame) is formed and propagates, causing the formation of autoignition waves in the end-gas. Autognition of the end-gas is registered when flame reaches the point \( r = 2.5 \) cm, in the Figure 1 one can see temperature and pressure in the activated area and in the end-gas at \( r = 4.5 \) cm. The ignition in the activated area proceeds in three stages: low, intermediate, and high temperature heat release stages as discussed in [3]. Fast heat release in the volume of several cm³ generates pressure wave which propagates to the wall and then reflects and propagates through end-gas several times before autoignition (peaks (2) in the Figure 1). It is known that pressure waves influence development of flame and transition from deflagration to detonation [5] in closed volume. They also play an important role in the transition from deflagration to autoignition via the heating of the end-gas and corresponding chemical reactivity enhancement [6]. Under considered conditions there are three main sources of mixture heating: (I) upward movement of the piston, (II) end-gas compression due to the combustion products expansion, (III) positive feedback from chemical reactions to the pressure wave (the same mechanism as in thermoacoustic instability). Rayleigh criterion [7] says that if pressure rise and heat release are in phase, the compression wave is fed by this heat.

Temperature and pressure range under consideration corresponds to studies of intermediate and high temperature energy release. The kinetic scheme includes, among other reactions, exothermic reactions, the rate of which increases with increasing pressure and temperature. For example, the reaction

\[
\text{H}_2\text{O}_2 + \text{M} \leftrightarrow \text{OH} + \text{OH} + \text{M} + \Delta E
\]  

Figure 1. Typical combustion process in HCCI with discharge activation. (1) discharge ignition, (2) oscillations due to pressure waves propagation, (3) autoignition.
at intermediate temperature heat release stage and

$$\text{O} + \text{CO} + \text{M} \leftrightarrow \text{CO}_2 + \text{M} + \Delta E$$  \hspace{1cm} (2)

at high temperature heat release stage are both exothermic and strongly dependent on pressure with corresponding rate constants $k_1$ in cm$^3$ mol$^{-1}$ s$^{-1}$ and $k_2$ in cm$^6$ mol$^{-2}$ s$^{-1}$. Reaction rates are:

$$W_1 = k_1\left[\text{H}_2\text{O}_2\right](\rho M)^2, \quad W_2 = k_2[\text{CO}][\text{O}](\rho M)^3,$$

where $M$ is molar mass of mixture in g/mol, $\rho$ – density in g/cm$^3$, [H$_2$O$_2$], [CO] and [O] are corresponding molar fractions of H$_2$O$_2$, CO and O. It is easy to see (Figure 2) that rate $W_1$ increase by 2-3 times in the pressure wave, heat capacity ratio reflects change of composition. Rate $W_2$ follows pressure as well, but its input is much smaller. We would like to estimate input of this mechanism in the integral heating of the end-gas in the system under consideration. It is possible if we calculate processes taking place in the end-gas under influence of compression by piston and by flame front but without pressure waves.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Pressure, heat capacity ratio and reaction rates oscillations in the end-gas ($r = 4.5$ cm); $W_1$ is rate of reaction (1), $W_2$ is rate of reaction (2).}
\end{figure}

In our previous work [3] we introduced additional terms for compression along z-axis in one-dimensional Navier-Stokes equations along $r$, which depend on parameters of gas and volume change: $-\rho \frac{dv}{dt} \frac{1}{v}$ in the continuity equation and $-h\rho \frac{dv}{dt} \frac{1}{v}$ in the energy equation, where $\rho$ is density, $V(t) = l(t)\pi R^2$ is volume of cylinder ($R$ is radius, $l(t)$ is the distance from piston to cylinder head), $h$ is specific enthalpy. To clarify role of the pressure waves we can carry out zero-dimensional simulation of autoignition of the end-gas in the cylinder with piston compression and compression by flame front. To estimate compression with flame front we use mass coordinate: $X = \int_0^{RX} \rho \pi r^2 dr / \int_0^R \rho \pi r^2 dr$. Using results of one-dimensional simulation, we chose some $X_1$ in the end-gas and use its changing position $r_1(t)$ to evaluate change of $V(t)$ for the end-gas due to flame front propagation. Compression by piston is defined by

$$\left( \frac{dv}{dt} \frac{1}{v} \right)_{\text{piston}} = \frac{dl(t)}{dt} \frac{1}{l(t)} \tag{3}$$

Volume change during compression by piston and combustion wave for the $m_1$ is (see Figure 3):
\[
\frac{dV}{dt} = \frac{\partial}{\partial t} \left[ \frac{1}{\ell(t)} \pi (R^2 - r_X(t)^2) \right] = \left( \frac{dV}{dt} \right)_{\text{piston}} - \frac{2r_X(t)}{(R^2 - r_X(t)^2)} \frac{dV}{dt}
\]

and thus, there is no need to calculate exact enthalpy changes during combustion and corresponding pressure rise in the combustion chamber.

Figure 3. Scheme of the model of compression with the combustion wave.

To compare autoignition with and without pressure waves we use simulation where discharge was turned on at 310 CAD (50 CAD before TDC), when pressure and temperature of end-gas was 6 bar and 600 K. In the full one-dimensional simulation, the ignition of the mixture activated by discharge occurs at 4.75 ms after beginning of the simulation and then combustion wave propagates leading to the formation of autoignition waves. In the zero-dimensional simulation there is no combustion wave, compression before 4.75 ms is (3) by piston only and after 4.75 ms compression term is (4) by piston and combustion wave. The results are shown in the Figure 4 where blue line is pressure near the wall in the one-dimensional area, dashed line is pressure without discharge and red line is pressure in zero-dimensional simulation. The difference in the time of autoignition is about 0.15 ms (~1.5 CAD), it is noticeable but not crucial for the combustion process. So, in both cases compression by flame front plays major role in the heating of the end-gas in comparison by the pressure waves.

Figure 4. Time dependence of pressure near the wall. 1D is taking into account the pressure waves in the formation of auto-ignition, 0D is without taking into account the pressure waves arising after the ignition of the discharge activated zone.
3. Conclusion
The compression effects from three sources on the occurrence of autoignition are considered. In the cylinder of the HCCI engine, (I) compression of the mixture by the piston, (II) compression by the front of the combustion wave, and (III) compression by the pressure waves resulting from the ignition of the mixture activated by the discharge are taken into account. As a result of the activation of pressure-dependent chemical reactions, the composition and heating of the mixture ahead of the flame front change, that leads to the appearance of autoignition waves. It is shown that the source (III) plays an insignificant role in the generation of autoignition waves under the conditions considered.

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