A kinetic model for the electrostatic spark discharge in atmospheric-pressure air

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Abstract. This paper presents a 0-D kinetic model of electrostatic spark discharges consisting of the time-dependent Boltzmann equation of electrons, a discharge-circuit equation, and heavy particles’ kinetic equations to investigate the energy-transfer mechanisms from the electrostatic energy given to the energy of gases by the spark discharge. In this report, the model is applied to the discharges in atmospheric-pressure air under optimum conditions corresponding for the minimum ignition energies of the typical flammable gases, hydrogen, ethylene and propane, in three types of explosion groups for gases.

1. Introduction
Spark discharges are the most likely electrostatic hazards of an ignition source, where they have led to more than 70% of incidents involving fires and explosions attributable to static electricity in the chemical industry [1]. Therefore, we developed a zero-dimensional (0-D) kinetic model for electrostatic spark discharges to understand the initiation processes of such an ignition in flammable atmospheres—how the electrostatic energy transfers to the ignition energy through electron energy during discharge. The model consists of the time-dependent Boltzmann equation of electrons, an electrical-circuit equation for the discharge, and chemical kinetic equations for heavy particles. In addition, von Pidoll et al. [2] have suggested a method to determine the incendivity of electrostatic discharges (spark and brush discharges) using the charge transferred by a discharge without flammable gases in air, and this has been adopted to the test method in the international standard for electrostatic hazards [3]. In this paper, the model is applied to the electrostatic spark discharges in air at atmospheric pressure to investigate the mechanism of the energy transfer, and the results are compared with experimental data collected in [2].

2. Model
Since the 0-D kinetic model is applied to electrostatic discharges in air at atmospheric pressure, species considered in the discharges are then as follows: electron; N\(_2\) and O\(_2\) molecules involving rotational, vibrational and electronically excited states; N and O atoms involving electronically excited states; positive ions of N\(_2\), O\(_2\), N and O; and negative ions of O\(_2\) and O. The electron collisions considered are elastic momentum-transfer collisions; rotational, vibrational and electronically excitations; ionisation; attachment; recombination including dissociative one; dissociation collisions; in addition, Coulomb collisions (electron–electron/ion), and momentum-transfer collisions with excited species including super-elastic collisions due to the high densities
of them. Corresponding cross sections of these collisions were mainly taken from [4]. The time-dependent Boltzmann equation of electrons is then expressed as

\[
e^{1/2} \frac{\partial F_0}{\partial t} = \frac{\gamma E^2}{3} \frac{\partial}{\partial e} \left( \sum_s N_s q_{m,s}(e) \frac{\partial F_0}{\partial e} \right) + 2m_e \frac{\partial}{\partial e} \left[ e^2 \sum_s N_s q_{m,s}(e) \left( F_0 + \frac{k_BT_g}{e} \frac{\partial F_0}{\partial e} \right) \right] + \sum_s \left( \tilde{C}_{0,ex,s} + \tilde{C}_{0,ion,s} + \tilde{C}_{0,att,s} + \tilde{C}_{0,sup,s} + \tilde{C}_{0,rec,s} + \tilde{C}_{0,dis,s} + \tilde{C}_{0,ei,s} \right)
\]

where \( e \) is electron energy, \( \gamma = \left( \frac{2e}{m} \right)^{1/2} \), \( E \) is the electric field, \( m \) is the electron mass, \( N_s \) is the density of species \( s \) except for the electron, \( q_{m,s} \) is the effective (total) momentum-transfer collision cross section of species \( s \), \( q_{m,s} \) is the elastic momentum-transfer collision cross section of species \( s \), \( k_B \) is the Boltzmann constant, \( T_g \) is the gas temperature, \( e \) is the electron charge, \( \tilde{C}_0 \) represents corresponding collision terms, and the electron energy distribution function \( F_0 \) is normalised as \( \int_0^\infty e^{1/2} F_0(e) \, de = 1 \).

The electrostatic spark discharge is modelled as a capacitive discharge between a charged conductive sphere (2.54 cm in diameter) and an earthed plane, where the sphere–plane separation is set to the onset gap length, \( L_g \), obtained from the onset criterion [5] for modelling electrostatic discharges. Thus, the circuit equation of this discharge is represented by

\[
-C \frac{dV_d}{dt} = \frac{V_d}{R_d} = I_d,
\]

where \( C \) is the capacitance of the gap involving a stray capacitance of the sphere itself which can be calculated from [6]. The values of the capacitance, including an external capacitance, must then be those not lower than the stray one. \( V_d \) is the discharge voltage (the voltage between the sphere and plane), \( R_d \) is the resistance of the discharge, and \( I_d \) is the discharge current. The electric field in the gap assumed to be uniform is then obtained from \( E = \frac{V_d}{L_g} \). The resistance is obtained from the electron mobility, \( \mu_e = -\frac{3}{2} \int_0^\infty \frac{E}{N_e q_{m,s}} \frac{\partial F_0}{\partial e} \, de \), as

\[
R_d = \frac{L_g}{N_e e \mu_e \pi r_e^2},
\]

where \( N_e \) is the electron density, \( N_e \mu_e \) is the conductivity of the channel, and \( r_e \) is the channel radius of the discharge, which is obtained from the energy conservation in the channel,

\[
\frac{\partial}{\partial t} [(h_c - h_0) V] = (Q_J - Q_L) V,
\]

where \( h_c \) is the enthalpy in the channel, which is obtained from \( h_c = \frac{5}{2} N_e k_BT_e + \frac{7}{2} N_\text{e} k_BT_g + \sum_s (\epsilon_{ex,s} N_{ex,s} + \epsilon_{ion,s} N_{ion,s}) \), where \( N_e, N_a \) and \( N_m \) are the densities of electrons, atomic and molecular species, respectively; \( T_e \) is the electron temperature; \( \epsilon_{ex,s} \) and \( \epsilon_{ion,s} \) are the potential energies of rotational, vibrational, and electronically excited and ionised species \( s \); and \( N_{ex,s} \) and \( N_{ion,s} \) are the densities of the corresponding species; \( h_0 \) is the background enthalpy, i.e., \( h_0 = h_c |_{t=0} \); \( V = \pi r_e^2 L_g \) is the volume of the discharge channel; and \( Q_J \) and \( Q_L \) are the rates of Joule heating and radiative loss resulting in light emissions. Here, the gas temperature, \( T_g \), is obtained from the energy conservation of gases in the discharge as

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} \frac{N_a k_BT_g}{2} + \frac{5}{2} N_m k_BT_g \right) = Q_{el} + Q_{rt} + Q_{et} + Q_{vv} + Q_{et} + Q_{rec} + Q_{dis},
\]
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Table 1. Conditions [2] of the voltage, $V_{\text{opt}}$, capacitance, $C_{\text{opt}}$, and gap length, $L_{\text{opt}}$, optimum for the minimum ignition energy, $W_{\text{min}}$, with the discharge energy by the model in parentheses, and the comparison of the transferred charge, $q_{\text{min}}$, with the residual one in parentheses, between the model and experiments [2] for the typical flammable atmospheres of the explosion groups, where in the model, the optimum conditions with the values of $L_{\text{opt}}$ in parentheses obtained from the onset criterion [5] are used.

| Flammable gas | $V_{\text{opt}}$ (kV) | $C_{\text{opt}}$ (pF) | $L_{\text{opt}}$ (mm) | $W_{\text{min}}$ (mJ) | $q_{\text{min}}$ (nC) | Experiment | Model |
|---------------|------------------------|------------------------|-----------------------|-----------------------|----------------------|-----------|-------|
| Hydrogen (IIC) | 2.9 | 3.8 | 0.5 | (0.56) | 0.016 | (0.016) | 12 | 11.0 ($\approx 0$) |
| Ethylene (IIB) | 5.4 | 5.6 | 1.0 | (1.27) | 0.082 | (0.082) | 32 | 29.7 (0.7) |
| Propane (IIA) | 7.2 | 9.6 | — | (1.82) | 0.25 | (0.249) | 70 | 64.0 (5.4) |

where $Q_{el}$, $Q_{et}$, $Q_{vt}$, $Q_{vv}$, $Q_{et}$, $Q_{rec}$ and $Q_{dis}$ are the heat rates due to elastic momentum transfer with electrons; rotational–translational, vibrational–translational, and vibrational–vibrational relaxations; de-excitation; ion recombination; and dissociation, respectively.

The densities of all species are obtained from density-balance equations consisting of productions and losses by processes considered, where rate coefficients involving electron collisions are obtained from $F_0$ with the corresponding collision cross sections, and those regarding neutral and ion species are mainly taken from [7].

Initial conditions at time $t = 0$ are as follows: dry air (N$_2$–O$_2$, 4:1) at 0.1 MPa and $T_g = 298.15$ K, including positive ions (N$_2^+$ and O$_2^+$, 4:1) with their densities, $N_{N_2^+} + N_{O_2^+} = N_e = 3 \times 10^9$ m$^{-3}$; $T_e = T_g$ with the Maxwell energy distribution of electrons; and $r_e = 10 \mu$m [8].

Calculation was made until the electron density became half the initial value after discharge.

3. Results and discussion

In this paper, the model investigates the electrostatic spark discharges in air at atmospheric pressure under the conditions [2] of the voltage, $V_{\text{opt}}$, capacitance, $C_{\text{opt}}$, and gap length, $L_{\text{opt}}$, optimum for giving the minimum energies necessary for ignition of the typical flammable gases, hydrogen (IIC), ethylene (IIB), and propane (IIA), of the explosion groups, where the groups are defined according to the international standard [9]. The optimum conditions [2] are shown in table 1. For the gap length, calculated values from the onset criterion [5], denoted in parentheses in table 1, are used for modelling electrostatic discharges, as described in section 2.

The results from the calculations by the model are shown in figure 1. The charges transferred by the spark discharges obtained from the time integration of their discharge currents and residual charges are shown in table 1. Since the breakdown field is typically higher at a shorter gap length [10] (5.21 MV/m for hydrogen optimum conditions, IIC$_{\text{opt}}$; 4.26 MV/m for IIB$_{\text{opt}}$; and 3.95 MV/m for IIA$_{\text{opt}}$), their electron energies before breakdown are higher, leading to earlier breakdown at lower breakdown voltage with a shorter gap length, as shown in figure 1a. On the other hand, during discharge, a high electric field remains slightly longer at a higher $C_{\text{opt}}$; thus, the period during which the electrostatic energy stored in the capacitance can be transferred to electrons to gain sufficient energy for inelastic collisions from the electric field becomes slightly longer at higher capacitance, resulting in higher conductivity and leading to a higher discharge current, as shown in figure 1a, as well as the higher particle densities, as shown in figure 1c–e. With regard to the mechanism of the energy transfer to gases, it was found that the main process of gas heating is the de-excitation of electronically excited species. The gas temperatures obtained then reach 378 K (IIA$_{\text{opt}}$), 722 K (IIB$_{\text{opt}}$), and 1453 K (IIA$_{\text{opt}}$), as shown in figure 1b, where their auto-ignition temperatures are 400 °C for hydrogen, 515 °C for ethylene, and 450 °C for propane [11]. Although the gas temperature for IIC$_{\text{opt}}$ is considerably lower than its auto-ignition temperature, excited molecules and atoms, including vibrationally excited ones, remaining after the discharge can increase it much more.

In future work, this model will be applied to the electrostatic spark discharges in flammable
atmospheres of hydrogen/air mixtures with chemical kinetic calculation for a much longer period after discharge in order to detail the mechanism of the energy transfer for ignition, where the ignition energy of the mixtures can be changed by the concentration of hydrogen. Losses by diffusion and thermal conduction, which may not be negligible in modelling for such a longer period, will also be taken into account.

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