Simulations of Vacuum Arcs and Gas Discharges with Liquid Cathodes

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Background and Motivation

- Simulations of vacuum arcs and gas discharges with liquid electrodes require coupling plasma physics with multi-phase flow science
- Specifics of gas breakdown and vacuum breakdown (volume processes vs surface processes)
- **Computational challenges:**
  - Different time scales for liquid dynamics and plasma dynamics (ms and ns, respectively)
  - Disparity of electron and ion time scales
  - Explosive Electron Emission: continuous phase transition (solid $\rightarrow$ liquid $\rightarrow$ gas $\rightarrow$ plasma)
  - Plasma expansion into vacuum or into a background gas vs ionization wave development
Negative Corona on Liquid Water Cathode

Experimental setup for corona discharge using Taylor cone

Principle of Taylor cone formation. (a) Initial state, (b) Taylor cone formation, and (c) Corona discharge at the tip of Taylor cone

Atmospheric-pressure air
Cathode-anode gap is 5-20 mm

Corona discharge using Taylor cone and shape of the liquid surface

N. Shirai, R. Sekine, S. Uchida, and F. Tochikubo, Atmospheric negative corona discharge using Taylor cone as a liquid cathode, JJAP 53, 026001 (2014)
Computational Model for Liquid Dynamics

Navier-Stokes equation for two-phase flows:

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \left( -p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right) + \frac{\rho}{l} \mathbf{n} \]


Two competitive forces at interface: surface tension and electrostatic

Laplace equation for electrostatic potential

\[ \Delta \varphi = 0 \]

\[ \varphi_{\text{top}} = 0, \quad \varphi_{\text{bottom}} = \varphi_0 \]

Time scale is milliseconds \( \rightarrow \Delta t \sim 10^{-7} - 10^{-6} \text{ s} \)
Dynamics of Taylor Cone Formation in Electric Field

- 3 kV
  - $t = 0.0$ ms
  - $t = 2.0$ ms
  - $t = 5.5$ ms

- 4 kV
  - $t = 0.0$ ms
  - $t = 1.5$ ms
  - $t = 2.5$ ms

- 6 kV
  - $t = 0.0$ ms
  - $t = 0.5$ ms
  - $t = 1.5$ ms

- Interplay between surface tension and electrostatic forces leads to Taylor cone formation
- The cone development terminates with droplet ejection from the tip (electrospray)
- Voltage influences the cone shape and height, and the droplet ejection rate
Gas Breakdown: Electron Kinetics

\[ \frac{\partial f_e}{\partial t} + v \frac{\partial f_e}{\partial x} - \frac{eE - F(v)}{m_e} \frac{\partial f_e}{\partial v} = S_{\text{ion}}(v) \]

\[ n_e = \int_{-\infty}^{+\infty} f_e dv \]

\[ \frac{dn_i}{dt} = S_{\text{ion}} \quad \frac{d^2 \varphi}{dx^2} = \frac{e}{\varepsilon_0} (n_e - n_i) \]

\[ S_{\text{ion}}(v) = S(v) \int_{-\infty}^{+\infty} n_g \sigma_{\text{ion}}(v') f_e(x, v', t) dv' \]

\[ F(\varepsilon_e) = \frac{e^4 Z_n g}{8\pi \varepsilon_0^2 \varepsilon_e} \ln \left( \frac{\varepsilon_e}{I} \right), \text{ where } \varepsilon_e = \frac{m_e v^2}{2} \]

400 Torr, initial plasma density $2 \times 10^{11}$ m$^{-3}$, gap $d = 6$ mm, $dU/dt = 8.4 \times 10^{10}$ V/s, $\sigma_{\text{ion}} = 2 \times 10^{-20}$ m$^{-2}$

Kolobov et al, Boltzmann-Fokker-Planck Kinetic Solver with Adaptive Mesh in Phase Space, AIP Conf. Proc. 2132, 060011 (2019); https://doi.org/10.1063/1.5119551
Fluid Model: Gas Breakdown and Plasma Formation

Drift-diffusion approximation for both electrons and ions:

\[ \frac{\partial n_k}{\partial t} + \nabla \cdot \Gamma_k = S_k \]

\[ \Gamma_k = -\mu_k n_k \nabla \varphi - D_k \nabla n_k \]

Electron energy balance:

\[ \frac{\partial \varepsilon_e}{\partial t} + \nabla \cdot \Gamma_{\varepsilon} = S_{\varepsilon} \]

Poisson equation for the electrostatic potential:

\[ \Delta \varphi = \frac{q_e}{\varepsilon_0} (n_e - n_i) \]

Time scale is nanoseconds → \( \Delta t \sim 10^{-14} - 10^{-12} \) s

Dynamics of Gas Breakdown

Mesh is adapted on \((n_e-n_i)\)

Mesh is adapted on field

Quasi-neutral plasma near the anode
Paschen Curves for Pulsed Gas Breakdown

- Voltage rise time $\tau$ affects the Paschen curves for planar gaps.
- Both kinetic and fluid models predict the experimentally observed shift of the curves toward higher voltages and the shift of Paschen minima toward higher $pd$ with decreasing $\tau$.
- On the right branch, the agreement between both models is obtained for all $\tau$.
- The fluid model could not describe the left branch of the Paschen curves.

Dynamics of Corona Discharge Development

Negative corona discharge is ignited at low voltages; ionization wave propagates toward the anode.

Plasma density does not exceed $10^{15}$ m$^{-3}$; Electric field remains undistorted; Highest $T_e$ is obtained at the cone tip.

Primary avalanche leaves behind uncompensated positive space charge; ions propagate to the cathode on much longer time scale.
The anode-directed ionization wave stops and follows the fast-axial wave propagating towards the cathode: the cathode sheath is formed. Further development of the discharge occurs at the (slow) ion time scale.
Discharge formation between cone tip and droplet

The cone growth stops once droplets are ejected from the tip; they shield the electric field.

Electric field sufficient for gas breakdown is obtained between the cone tip and the droplet.

Plasma density in the vicinity of the cathode is $\sim10^{21}$ m$^{-3}$ and keeps growing; sheath thickness is $<0.1$ µm.
A distinctive feature of electric discharges in a vacuum is rapid phase transitions of the cathode material from a solid state to liquid, gaseous, and plasma states.

The plasma state changes from a dense non-ideal to a moderately rarefied, and to a collisionless.

The cathode material is emitted from micro-explosions (ectons) and progressively accelerated to velocities of about $10^6$ cm/s, the particle density decreases from $10^{23}$ to $10^{10} \text{ cm}^{-3}$.
Vacuum Discharge Ignition from Liquid-Metal Cathodes

Types of liquid metal cathodes

Shadow photographs showing (a) growth and (b) decay of a protrusion on the liquid metal cathode with diameter 4 mm

InGa is liquid at room temperature

Taylor cone formation on Liquid Metal Cathode

Conditions:
InGa liquid cathode
Cathode potential -40 kV
Cathode-anode gap is 2 mm

Electric field distribution (10^8 V/m)

- Electric field at the cathode tip increases with time
- Unstable Taylor cone is formed during 0.2 ms
- Liquid droplets are ejected from the cone tip
- Droplet ejection precedes the field emission onset
Liquid Metal Protrusion Heating

Axisymmetric model of micro-protrusion heating:
\[ \rho C_p \frac{\partial T(r, t)}{\partial t} = \nabla (\lambda(T) \nabla T(r, t)) + F(r, t) \]

Heating is due to electric current and Thomson effect:
\[ F(r, t) = j(r, t)E(r, t) + g(T)(j(r, t)\nabla T(r, t)) \]

Solve the Poisson’s equation to define the current density:
\[ \nabla [\sigma(T)\nabla \phi(r, t)] = 0 \quad \rightarrow j(r, t) = \sigma(T)\nabla \phi(r, t) \]

Boundary conditions:
\[ \lambda(T) \frac{\partial T(r, t)}{\partial n} = \frac{j_{FE}(E_{surf}, T_{surf})}{e} \Delta E(E_{surf}, T_{surf}) - \sigma_{SB} T_{surf}^4 \]
\[ \sigma(T) \frac{\partial \phi(r, t)}{\partial n} = j_{FE}(E_{surf}, T_{surf}) \]

\( g(T) \) is the Thomson constant, \( \sigma(T) \) is the conductivity, \( \Delta E \) energy carried out by emitted electrons; takes into account the Nottingham effect, \( \sigma_{SB} \) is the Stefan-Boltzmann constant, and \( j_{FE}(E_{surf}, T_{surf}) \) is the known function of the emitter shape from Glazanov, Baskin and Fursey, Journal of Technical Physics 59, 60 (1989)
Liquid Metal Protrusion Heating

- Thermal instability develops only when the current density at the tip exceed $10^8$ A/cm$^2$ in agreement with the Mesyats’ theory
- Then, the micro-protrusion temperature at the tip starts exceeding the boiling temperature on the ns time scale
- This clearly indicates that the field-to-explosive electron emission occurs after 1 ns
- Now we know the metal mass which experiences phase transition from solid to non-ideal plasma: can use it for plasma expansion modeling;
Plasma Expansion: Gas-Dynamic LTE Model

LTE model is widely used for pulsed laser ablation (Saha equation)

Adaptive Computation Domain

- Implemented 2D planar and axisymmetric solvers with ACD
- Generic EOS to describe continuous phase transition

Dynamically Adaptive Cartesian Mesh
Fluid Model for Plasma Expansion into Vacuum

Collisionless, cold ions, Boltzmann-electron model:

\[ \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \vec{u}_i) = 0, \]
\[ m_i \frac{\partial \vec{u}_i}{\partial t} + m_i (\vec{u}_i \cdot \nabla) \vec{u}_i = -e \nabla \varphi, \]
\[ \nabla^2 \varphi = \frac{e}{\varepsilon_0} (n_e - n_i) \]
\[ n_e = n_0 \exp \left( \frac{e \varphi}{k_B T_e} \right) \]

Very sharp ion density peaks predicted (peak widths a few \( \lambda_D \))

- Good agreement with other 1D computations using both Eulerian and Lagrangian approaches. Both spatial and temporal profiles are well reproduced
- The code can be used to study collisionless plasma expansion dynamics in multi-dimensions

J. E. Allen and M. Perego, On the ion front of a plasma expanding into a vacuum, Physics of Plasmas 21, 034504 (2014);
Applied voltage starts influencing the plasma front propagation only when it is far from the “core” dense plasma: the plasma density decreases → Debye length decreases → external electric field starts penetrating the plasma.

Front velocity increases with time because the electric field between the front and the right boundary increases with time.
Two Types of Positive Ions

\[
\frac{Z_1}{Z_2} = \frac{1}{2}
\]

\[
\frac{n_1}{n_2} = \frac{8}{2}
\]

- Ions with larger charge propagate faster
- Density of Ion \#2 has multi-peak structure: the 1st peak coincides with the position of the Ion \#1 peak, and the 3rd peak is the ion front
- All the peaks are formed at different stages: the 3rd peak is formed at the earliest stage of the front formation
- Velocity of the Ion \#1 only slightly depends on the applied voltage
- Velocity of the Ion \#2 increases with time
- Ion \#1 moves slower than in the case of one ion species plasma
Conclusions

• We have developed computational models for multi-phase plasmas with adaptive Cartesian mesh
• Simulated dynamics of Taylor cone formation on liquid cathodes using Volume-of-Fluid model
• Illustrated development of Corona and Glow Discharges with liquid cathodes
• Plasma expansion into vacuum has been simulated with fluid models
• Adaptive Computation Domain methodology has been introduced
• The differences between gas breakdown and vacuum breakdown have been identified and illustrated
Outlook

• Combine fluid and kinetic models for expanding plasma
• Simulate dynamics of vacuum breakdown and clarify effects of anode processes
• Quantify effects of background gas pressure on electron emission and volume ionization processes during breakdown and plasma formation
• Identify mechanisms of nano-particle production during adiabatic expansion of dense plasma into vacuum and background gas
• Identify similarities and differences between pulsed laser ablation (from fs to ns scales) and dynamics of spark and arc discharges
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