Supporting Information

Low-Cost Heat Assisted Ambient Ionization Source for Mass Spectrometry in Food and Pharmaceutical Screening

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Abstract: This supplementary material details the numerical model of computational fluid dynamics, heat transfer, and the tracing of caffeine protonated molecules for heat-assisted dielectric barrier discharge ionization (HA-DBDI). For the model, COMSOL Multiphysics 4.4 was used according to the description below.

Geometry

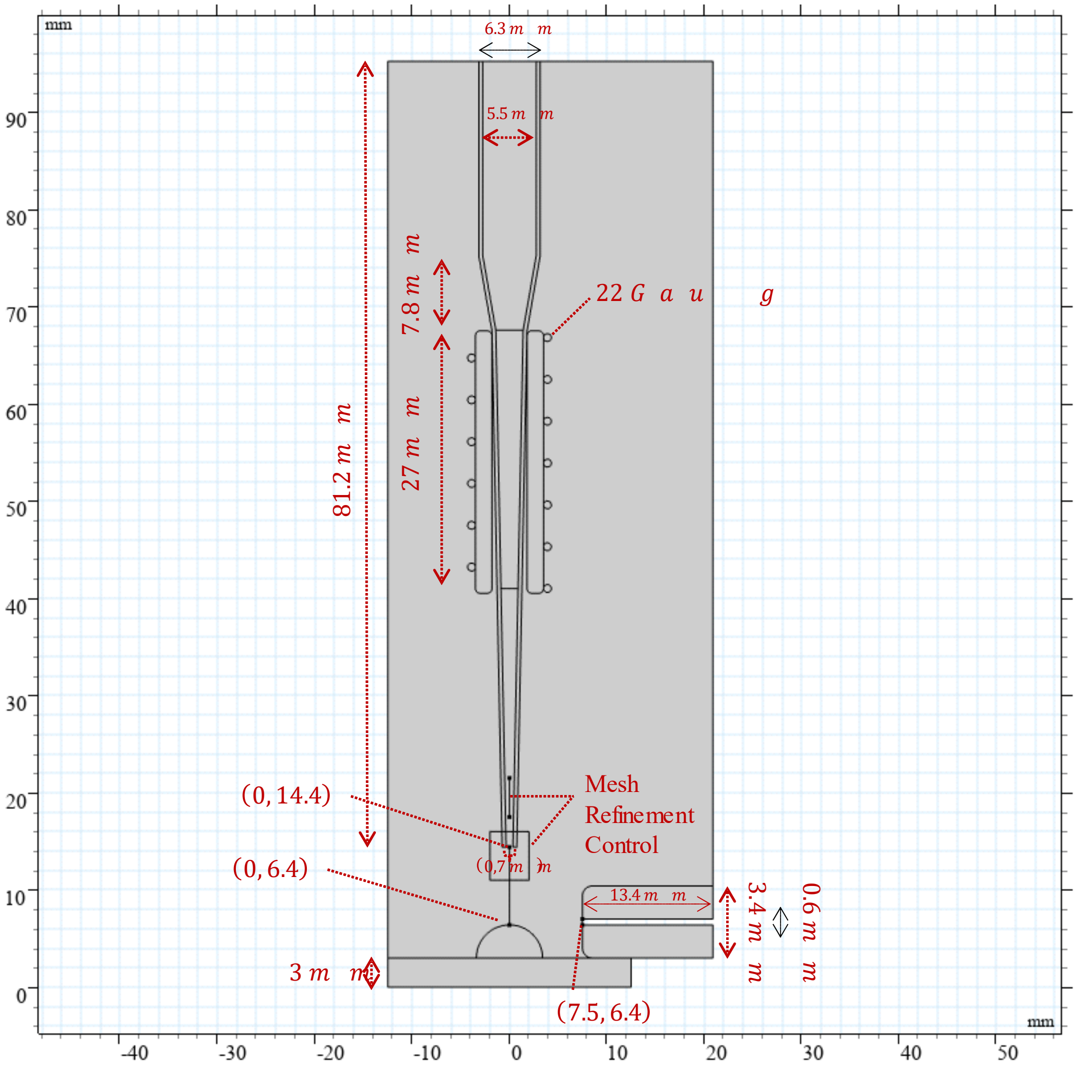

Figure S1: Description of the computational domain of the simulation.

Materials

In order to define the parameters for the different materials, we used the internal library of COMSOL. These materials are summarized in **Table S1**

Table S1: Actual materials vs materials as named by COMSOL library.

Part	COMSOL Material Name
Main domain	Helium [gas]
Pipette body	Quartz
Nichrome wire	Nichrome [solid, steady-state]
Fuse	Alumina
MS inlet	High-strength alloy steel
Coffee bean	Wood (pine)

Physics Models

In order to capture the physics behind the phenomena under interest 3, different modules of COMSOL have been used: the Heat Transfer, the Turbulent Flow, k-ε and the Particle Tracing for Fluid Flow.

The equation that describes the heat transfer module was:

$$\rho C_p u \cdot \nabla T + \nabla \cdot (-k \nabla T) = Q$$

where C_p denotes the specific heat capacity (J/(kg·K)), T is the temperature (K), k is the thermal conductivity (W/(m·K)), ρ is the density (kg/m^3), **u** is the velocity vector (m/s), and Q is a sink or source term. In the solid parts, the velocity vector, **u** = (u, v, w), is set to zero in all directions.

The boundary conditions are set as open boundaries for all outer edges except for the inlet of the pipette and the outlet of the MS inlet. At the inlets, we specified constant temperatures that are known from the experimental parameters, while for the heat source and the temperature of the nichrome wire, we did trials and errors until we reached a temperature at the exit of the pipette that was close to the actual experimental conditions. At the outlets, convection dominates heat transport, so we applied the convective flux boundary condition:

$$-k\nabla T\cdot n=0$$

The boundaries are presented in **Figure S2**.

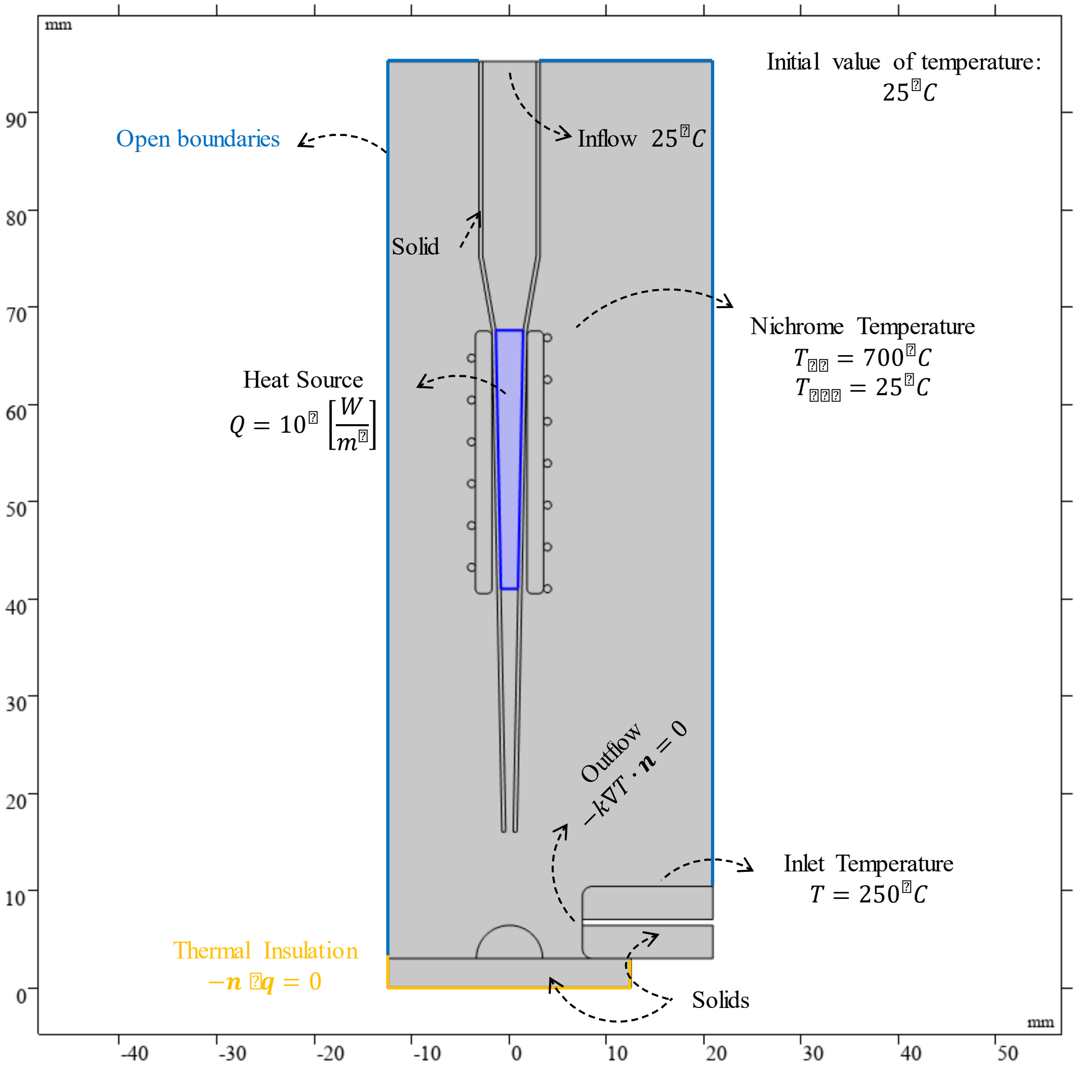

Figure S2: Boundaries of heat transfer model of HA-DBDI.

The basic equations that describe the turbulent flow module are the Navier-Stokes equation and the continuity equation:

$$\rho(u \cdot \nabla)u = \nabla \cdot [-pI + K]$$

$$\nabla \cdot (\rho \cdot u) = 0$$

where **u** is the velocity vector (m/s) and I the identity matrix. Factor **K** describes the turbulence, and the details about it can be found in CFD Module User's Guide of COMSOL. The boundaries of this module are given in **Figure S3.**

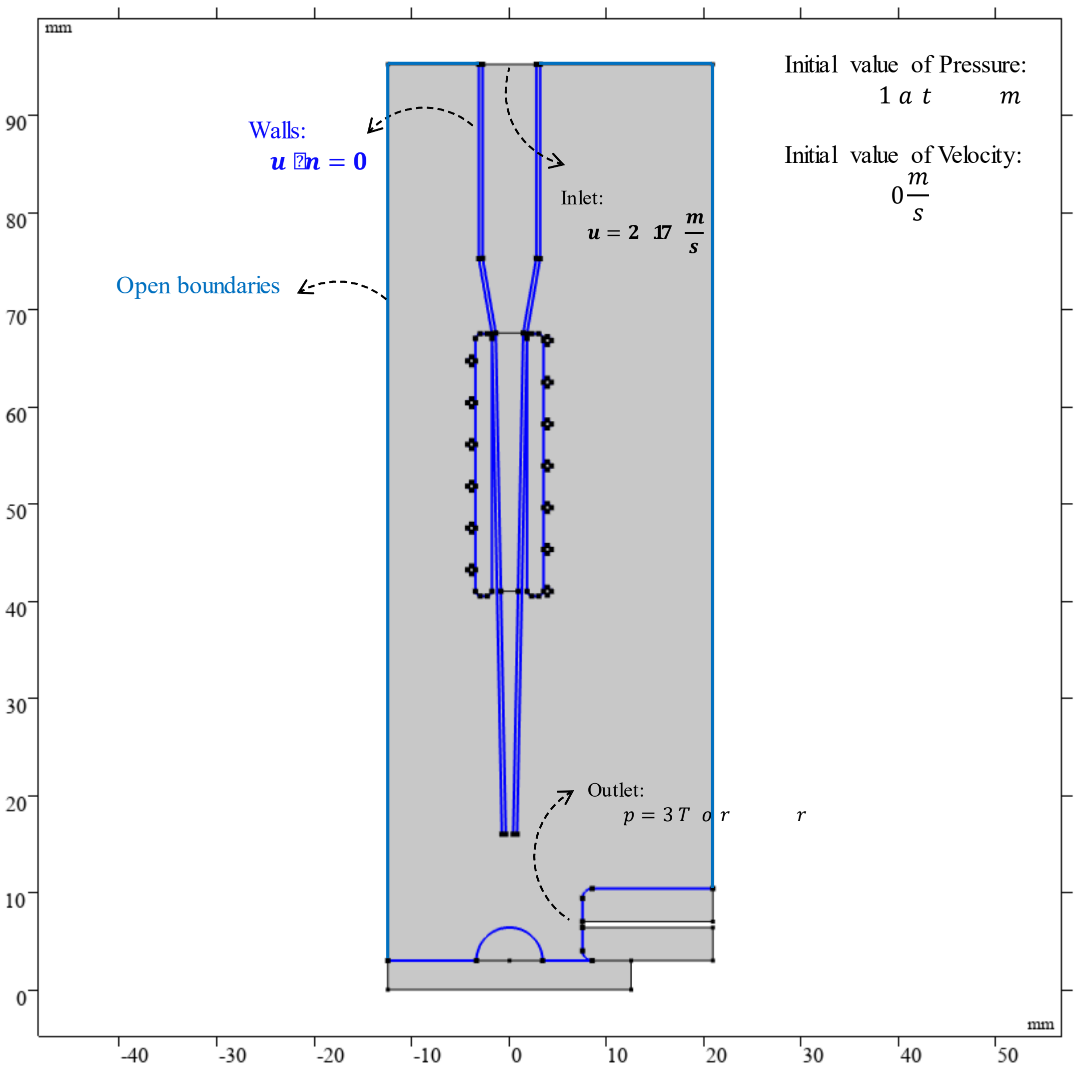

Figure S3. Boundaries of turbulent flow model of HA-DBDI.

The equation that describes the particle tracing for fluid flow are as follows:

$$\frac{d(m_p u)}{dt} = F_t$$

where m_p (kg) is the mass of the protonated caffeine, u **(m/s)** the velocity and F_t the driving force caused by the pressure created from the previous models. The boundaries are given in **Figure S4.**

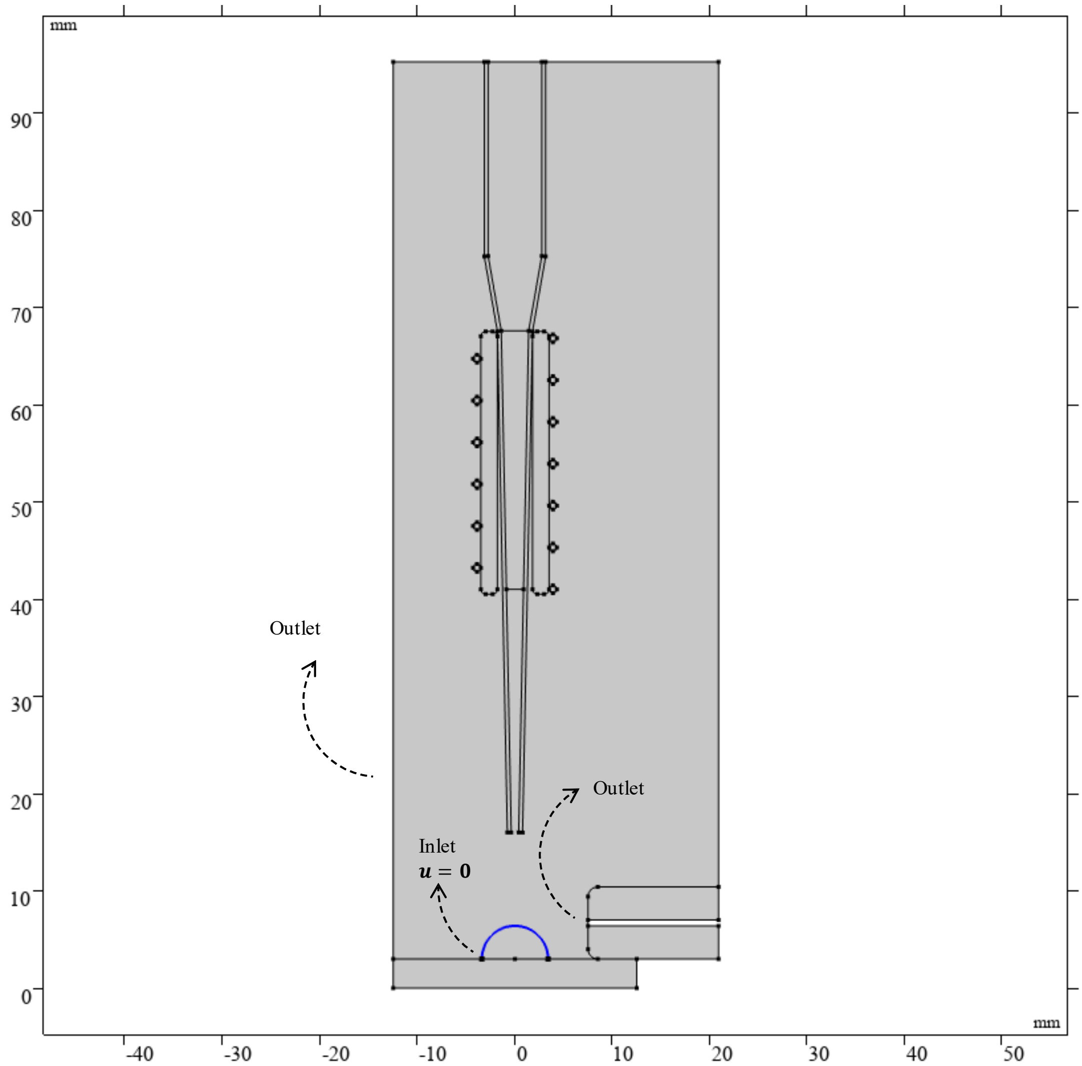

Figure S4. Boundaries of fpf model of HA-DBDI.

Mesh

The mesh that was used for this model is given in **Figure S5.** In the exit of the pipette as well as in the regions of nichrome wire, it was necessary to dense the mesh for convergence reasons. In the dense regions, we used triangular elements of maximum size of 0.1 mm and minimum size of 0.05 mm. For the rest of the domain, we used triangular elements with a maximum size of 1.17 mm and a minimum size of 0.0334 mm.

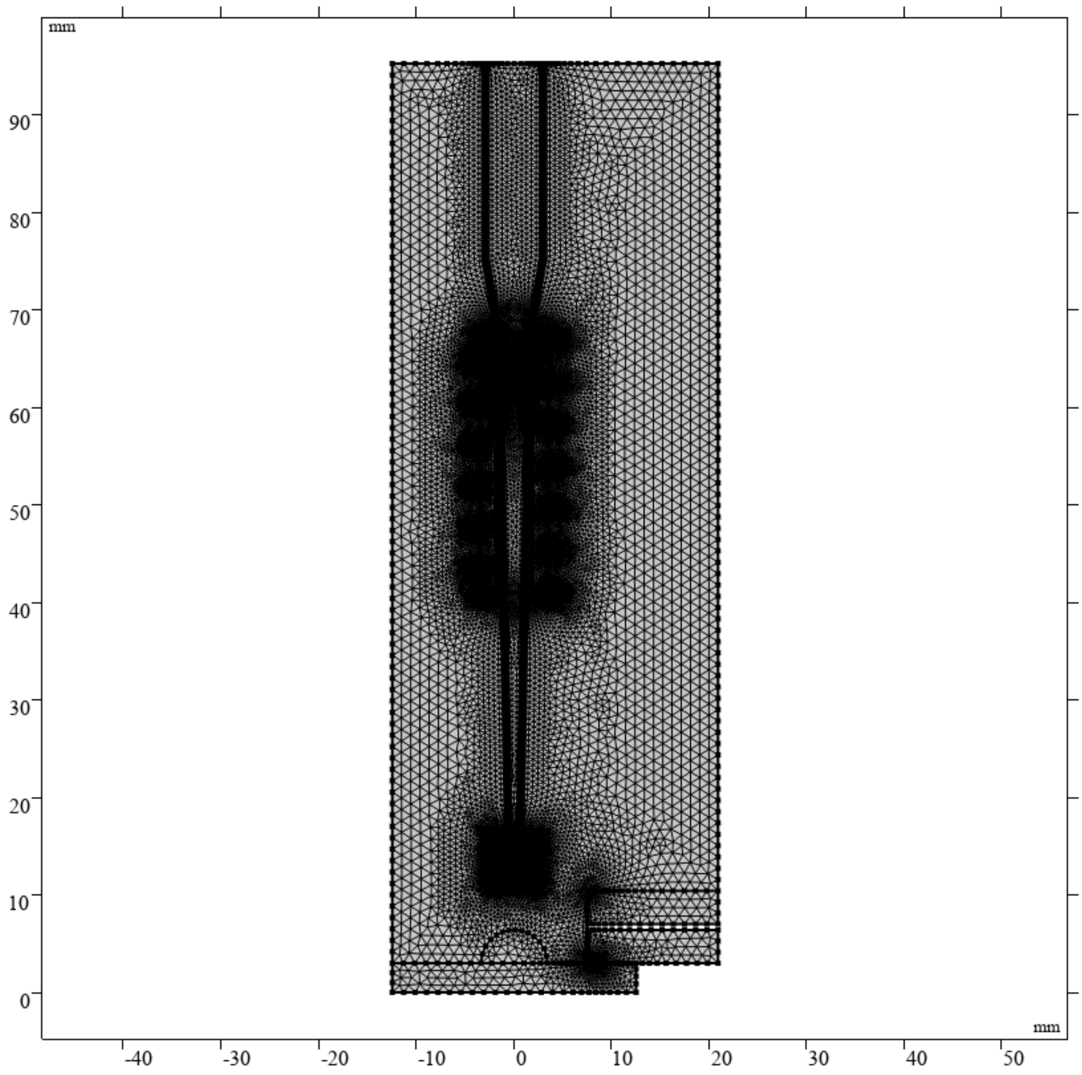

Figure S5: Mesh of HA-DBDI computational model.

Study for the Heat Transfer, the Turbulent Flow, k-ε and the Particle Tracing for Fluid Flow models

All models are coupled together by the Multiphysics interface of no isothermal fluid and are solved for steady-state conditions. For the tracing for fluid flow model, a time-dependent solver was used for 10 ms in steps of 0.1 ms. The total computational time was 30 min for each case and solved on a server with 16 core processors (Intel Xenon E5–2667 V4 3.2 kHz), 252.2 Gb RAM and 5.5 Tb hard drive.