SIMULATION OF COMBUSTION AND CHARGED PARTICLE TRANSPORT UNDER DC ELECTRIC FIELD

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Applying electric field to flame is regarded as a promising technique to enhancing combustion characteristics. A flame applied electric field having better stability[1] and a sooting diffusion flame subject to electric field emitting less amount of soot[2] have been reported.

Ions and electrons generated in hydrocarbon flames are usually not considered in combustion simulations since they are very small in numbers and have little effect unless external electric field is applied. Therefore, eReactingFoam is written based on reactingFoam, one of OpenFOAM's basic solvers for reacting flows, to simulate flames under DC electric field. Models implemented in eReactingFoam and required data are briefly introduced here.

Drift-diffusion approximation is adopted to calculate charged species' drift flux in species transport equation (eq. 1, the last term of its left hand side).

$$\rho\partial_t Y_i + \nabla\cdot\left(\rho\vec{U}Y_i\right) + \nabla\cdot\left(\rho\mu_i\vec{E}Y_i\right) = \nabla\cdot\left(\rho D_i\nabla Y_i\right) + \dot{\omega_i} \tag{1}$$

Electric drift of charged species induces net space charge ρ_q. Space charge in applied electric field create momentum source by Lorentz force (See eq. 2, the last term of its right hand side).

$$\rho\partial_t\vec{U} + \nabla\cdot\left(\rho\vec{U}\vec{U}\right) = \nabla\cdot\left(\mu\nabla\vec{U}\right) + \nabla\cdot\left(\mu\left(\nabla\vec{U}^T - \frac{2}{3}\mathrm{tr}\left(\nabla\vec{U}\right)I\right)\right) + \nabla p + \rho_q\vec{E} \tag{2}$$

Electric field $\vec{E}$ is calculated from electro-static potential Φ (eq. 3) and Φ is obtained by solving Poisson's equation (eq. 4). ϵ_0, e, n_i and z_i are repspectively vacuum permittivity, elementary charge, number density of ith species and charge number of ith species.

$$\vec{E} = -\nabla\Phi \tag{3}$$

$$\nabla^2\Phi = -\frac{\rho_q}{\epsilon_0} = -\frac{e}{\epsilon_0}\sum_{i=1}^{N} n_i z_i \tag{4}$$

Hydrocarbon flames generate ions via chemi-ionization reactions [3, 4]. Those reactions should be included in the reaction mechanism to be used. The reaction mechanism consists of GRI-Mech 3.0[5] gas combustion mechanism and 3 chemi-ionization reactions [4] were used for the following results.

Diffusivity and mobility of electrons are calculated using electron scattering cross section data. [6]

Diffusivities of ions are calculated assuming they have the same diffusivity of their parent neutral species. Cantera[7] is coupled with the solver to calculate species diffusivities. Binary diffusivities are calculated using Stockmayer interaction potential and mixture-average formula is used to caculate diffusion coefficients of species transport equations. Mobilities of ions are calculated from their diffusivities using Einstein relation (eq. 5).

$$\frac{D_i}{\mu_i} = \frac{k_B T_i}{q_i} \tag{5}$$

A counterflow diffusion flame under DC electric field [8] was simulated. Figure 1 shows that two perforated metal plates are placed at the ends of two nozzles (for fuel and oxidizer streams) to provide uniform electric field parallel to nozzle axis.

2D-axisymmetric simulation was conducted using wedge type mesh. Dimensions and boudary conditions of the computational domain are described in Figure 2 and Table 1 .

Figure 3 shows overlays of streamlines and CH mass fraction image for simulation cases with and without externally applied electric field. Streamlines show flow modification by ionic wind and CH images imply blue flame position. The figure clearly shows flame position displacement toward the lower nozzle, which agrees with the experiment. However, the model should be impoved to obtain quantitative prediction.

Currently implementation of $(n, 6, 4)$ potential which models ion-neutral interaction and screened Coulomb potential which models interaction between charged particles [9] is in progress to calculate transport properties more accurately.

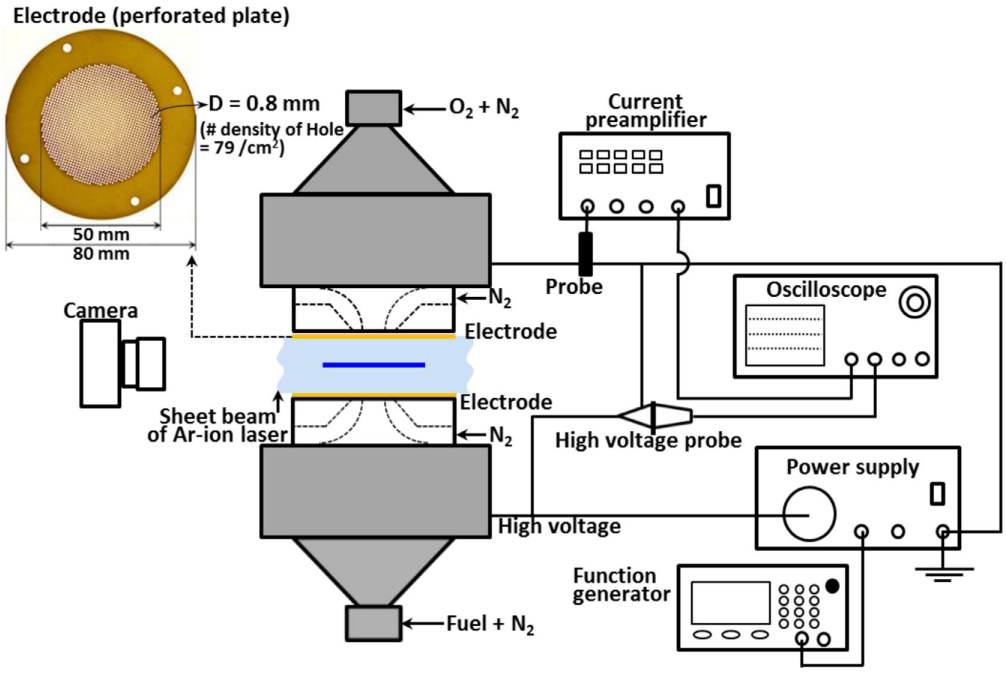

Figure 1: Schematic of experimental setup, taken from [8]

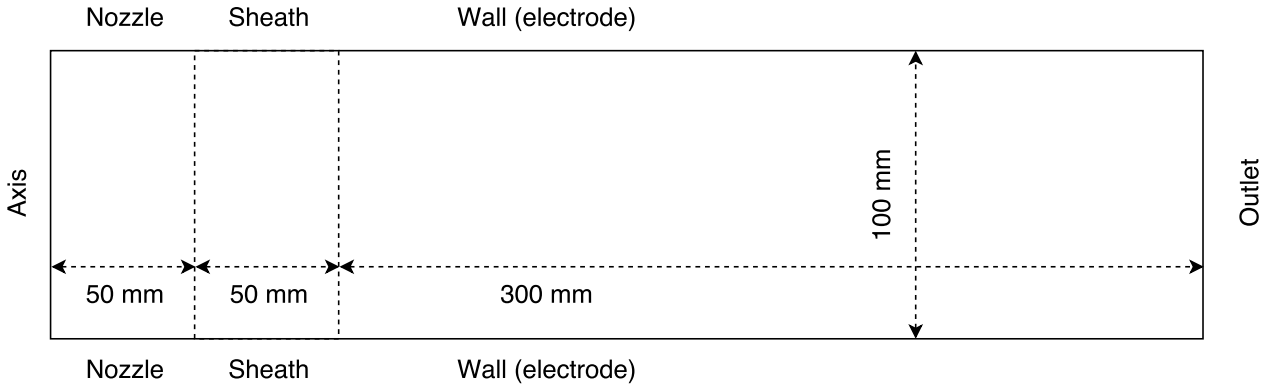

Figure 2: 2D-Axisymmetric simulation domain

Table 1: Boundary conditions

	Upper			Lower		
	Nozzle	**Sheath**	**Wall**	**Nozzle**	**Sheath**	**Wall**
U	20 cm/s	20 cm/s	Slip	20 cm/s	20 cm/s	Slip
T	300 K	300 K	$\frac{\partial}{\partial \vec{n}} = 0$	300 K	300 K	$\frac{\partial}{\partial \vec{n}} = 0$
Y_{CH_4}	0	0	$\frac{\partial}{\partial \vec{n}} = 0$	0.14046	0	$\frac{\partial}{\partial \vec{n}} = 0$
Y_{O2}	0.559989	0	$\frac{\partial}{\partial \vec{n}} = 0$	0	0	$\frac{\partial}{\partial \vec{n}} = 0$
Y_{N_2}	0.440011	1	$\frac{\partial}{\partial \vec{n}} = 0$	0.85954	1	$\frac{\partial}{\partial \vec{n}} = 0$
Y_i (neutral)	0	0	$\frac{\partial}{\partial \vec{n}} = 0$	0	0	$\frac{\partial}{\partial \vec{n}} = 0$
Y_i (charged, +)	0	0	$\frac{\partial}{\partial \vec{n}} = 0$	$\frac{\partial}{\partial \vec{n}} = 0$	$\frac{\partial}{\partial \vec{n}} = 0$	$\frac{\partial}{\partial \vec{n}} = 0$
Y_i (charged, -)	$\frac{\partial}{\partial \vec{n}} = 0$	$\frac{\partial}{\partial \vec{n}} = 0$	$\frac{\partial}{\partial \vec{n}} = 0$	0	0	$\frac{\partial}{\partial \vec{n}} = 0$
Φ	0	0	0	-2400	-2400	-2400

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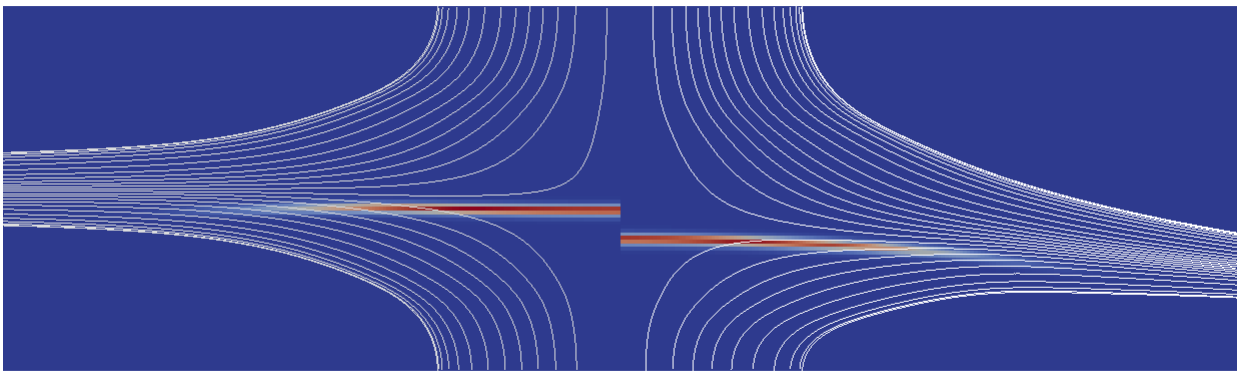

Figure 3: Flow modification due to ionic wind induced by DC electric field. Upper electode at 0 kV in all cases. Left: Lower electrode at 0 kV; Right: Lower electrode at -2.4 kV

References

[1] M. Belhi, P. Domingo, and P. Vervisch, "Direct numerical simulation of the effect of an electric field on flame stability," *Combustion and Flame*, vol. 157, no. 12, pp. 2286–2297, dec 2010. [Online]. Available: http://dx.doi.org/10.1016/j.combustflame.2010.07.007http://linkinghub.elsevier.com/retrieve/pii/S0010218010001951

[2] D. G. Park, B. C. Choi, M. S. Cha, and S. H. Chung, "Soot Reduction Under DC Electric Fields in Counterflow Non-Premixed Laminar Ethylene Flames," *Combustion Science and Technology*, vol. 186, no. 4-5, pp. 644–656, 2014. [Online]. Available: http://www.tandfonline.com/doi/abs/10.1080/00102202.2014.883794

[3] J. Prager, H. Najm, M. Valorani, and D. Goussis, "Structure of n-heptane/air triple flames in partially-premixed mixing layers," *Combustion and Flame*, vol. 158, no. 11, pp. 2128–2144, nov 2011. [Online]. Available: http://linkinghub.elsevier.com/retrieve/pii/S0010218011001039

[4] N. Speelman, M. Kiefer, D. Markus, U. Maas, L. de Goey, and J. van Oijen, "Validation of a novel numerical model for the electric currents in burner-stabilized methaneair flames," *Proceedings of the Combustion Institute*, vol. 35, no. 1, pp. 847–854, 2015. [Online]. Available: http://dx.doi.org/10.1016/j.proci.2014.05.067http://linkinghub.elsevier.com/retrieve/pii/S1540748914000704

[5] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer, M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, J. Gardiner, William C., V. V. Lissianski, and Z. Qin, "GRI-Mech 3.0." [Online]. Available: http://www.me.berkeley.edu/gri{_}mech/

[6] F. Bisetti and M. El Morsli, "Calculation and analysis of the mobility and diffusion coefficient of thermal electrons in methane/air premixed flames," *Combustion and Flame*, vol. 159, no. 12, pp. 3518–3521, dec 2012. [Online]. Available: http://linkinghub.elsevier.com/retrieve/pii/S0010218012002295

[7] D. G. Goodwin, H. K. Moffat, and R. L. Speth, "Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes," http://www.cantera.org, 2017, version 2.3.0.

[8] D. G. Park, S. H. Chung, and M. S. Cha, "Bidirectional ionic wind in nonpremixed counterflow flames with DC electric fields," *Combustion and Flame*, vol. 168, pp. 138–146, jun 2016. [Online]. Available: http://linkinghub.elsevier.com/retrieve/pii/S0010218016300426

[9] J. Han, M. Belhi, and F. Bisetti, "Numerical modeling of ion transport in flames," *Combustion Theory and Modelling*, vol. 19, no. 6, pp. 744–772, 2015. [Online]. Available: http://www.tandfonline.com/doi/abs/10.1080/13647830.2015.1090018?journalCode=tctm20{&}instName=Cranfield+University