Simulation of combustion and charged particle transport under DC electric field

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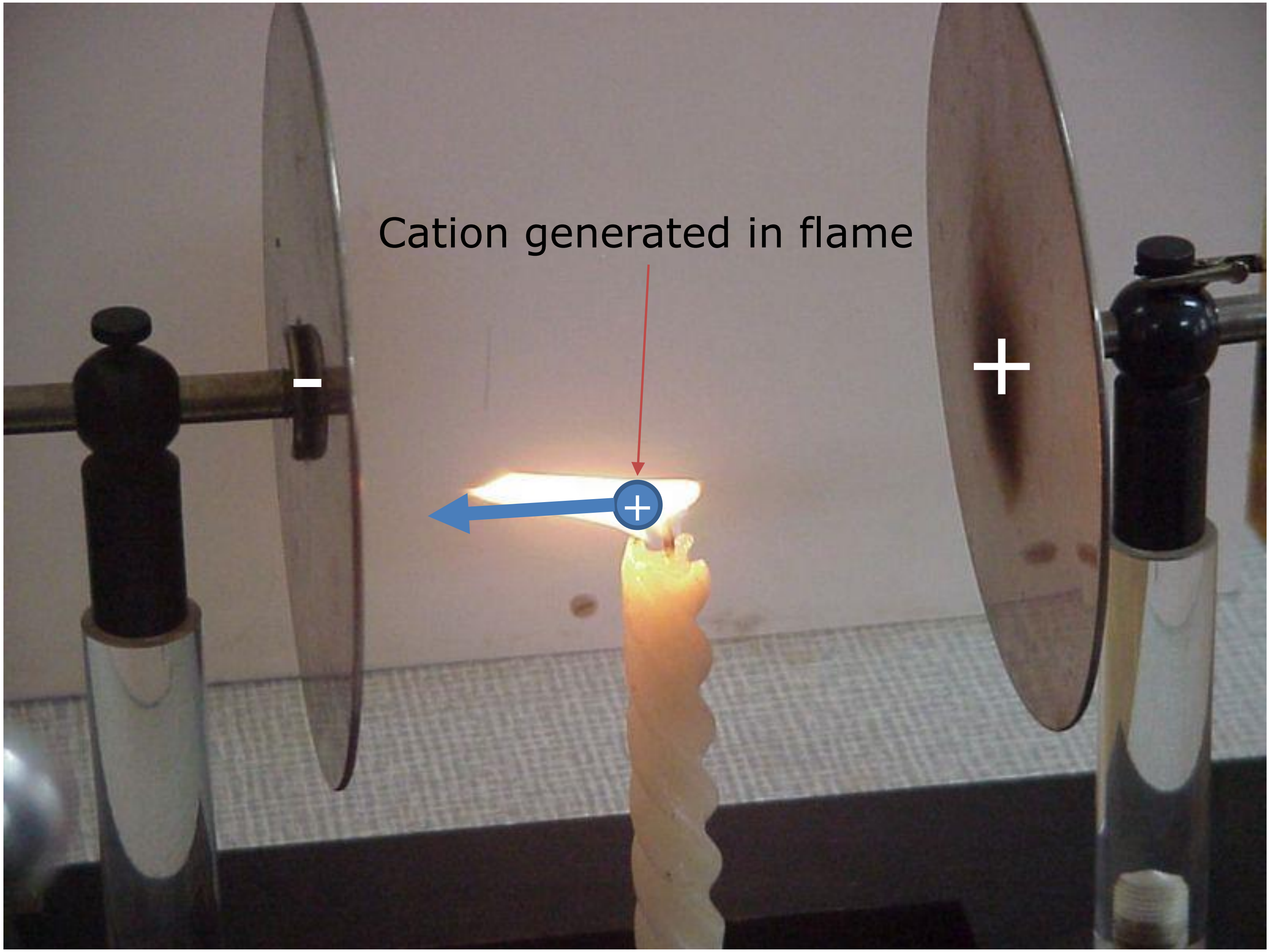
Introduction

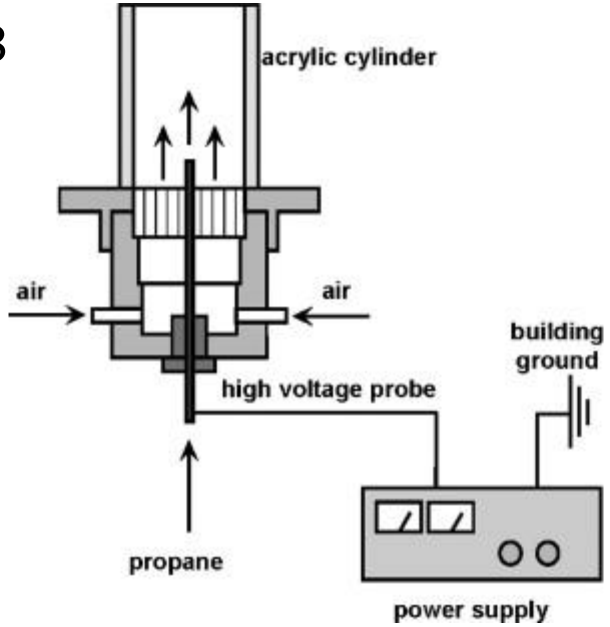
Candle subject to electric field

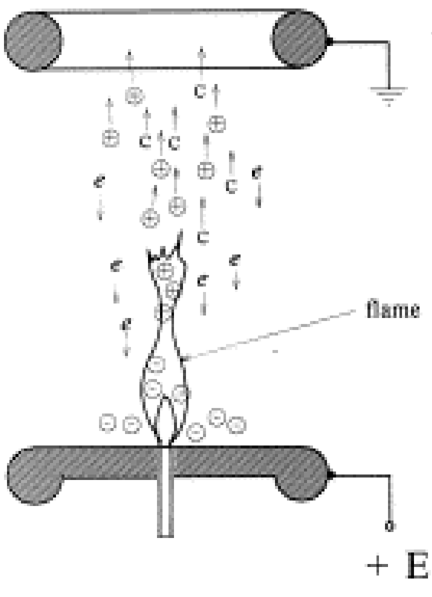


Introduction

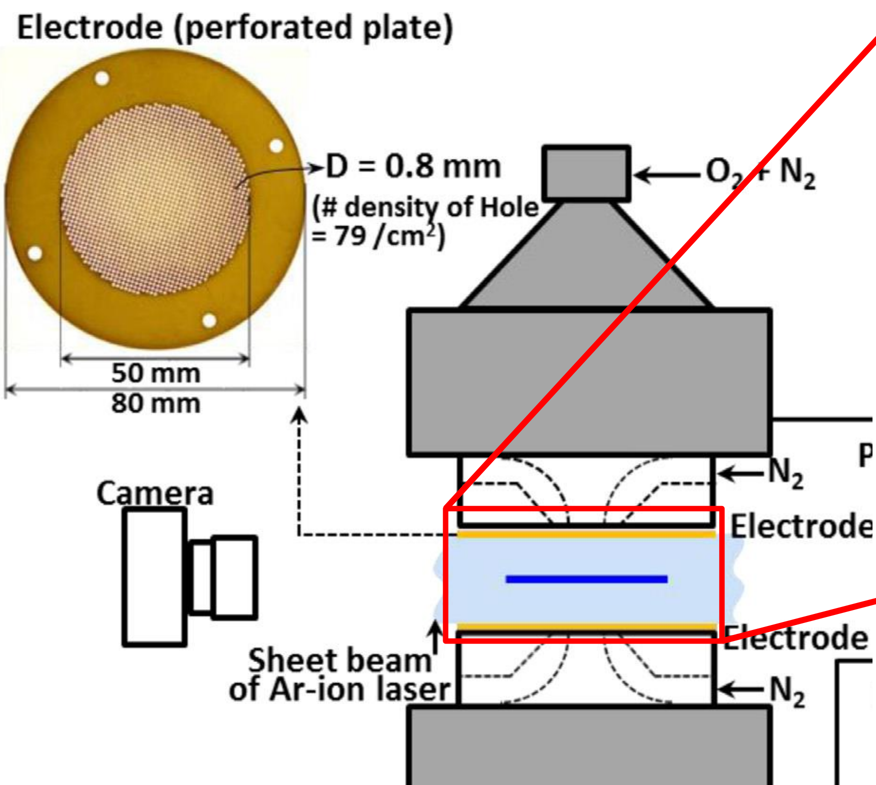
Combustion improvement by electric field

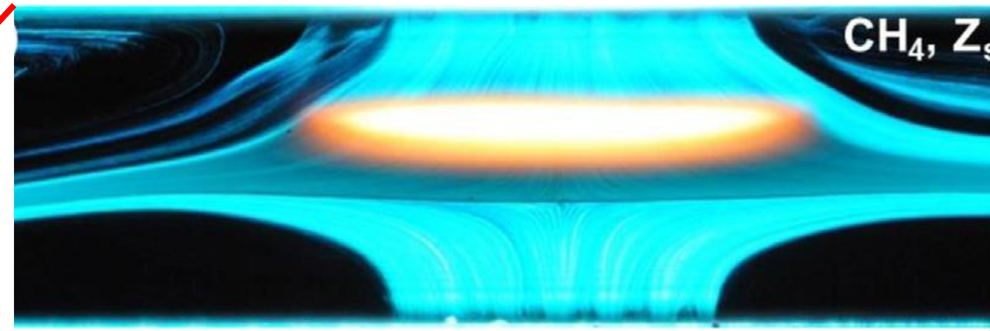
- Flame stabilization
  - Kim et al. 2010, 2011, 2012
  - Lee et al. 2005
- Flame speed enhancement
  - Cha & Lee 2012
  - Won et al. 2007, 2008
- Soot suppression
  - Xie et al. 1992
  - Saito et al. 1992
  - Ohisa et al. 1999
  - Cha et al. 2005





CH4/O2/N2 counterflow diffusion flame





Nozzle diameter	10 mm
Nozzle distance	10 mm
Nozzle exit velocity	20 cm/s
CH4 mole fraction	1.0
Oxygen mole fraction	0.274

Flow modification is observed

(Shift of flame and stagnation plane)

when high negative voltage applied to lower (fuel side) electrode

Park, D. G., Chung, S. H., & Cha, M. S. (2016). Bidirectional ionic wind in nonpremixed counterflow flames with DC electric fields. *Combustion and Flame*, *168*, 138–146. https://doi.org/10.1016/j.combustflame.2016.03.025

Governing equations

- Species transport

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

Drift of charged species by electric field

Reaction source

- Momentum

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

Lorentz force

- Electric field (Poisson's equation)

$$\nabla^2\Phi = -\frac{\rho_q}{\epsilon_0} \qquad \vec{E} = -\nabla\Phi$$

Transport properties (1)

- Mixture averaged species mass diffusivity

$$\frac{1}{D_{km}} = \sum_{j\neq k}^{K} \frac{X_j}{\mathcal{D}_{kj}} + \frac{X_k}{1-Y_k}\sum_{j\neq k}^{K} \frac{Y_j}{\mathcal{D}_{kj}}$$

- Binary diffusivity

$$D_{ij} = \frac{3}{16}\frac{\sqrt{2\pi N_A (kT)^3/M_{ij}}}{p\pi\sigma_{ij}^2\Omega_{ij}^{(1,1)*}(kT/\epsilon_{ij})}$$

- Collision integral

$$\pi\sigma^2\Omega^{(1,1)*} = \frac{1}{2!}\int_0^\infty \exp(-\frac{E}{kT})(\frac{E}{kT})^2 Q^{(1)}(E) d\frac{E}{kT}$$

  - Precalculated tables are available from literature

- Cross section $Q^{(1)}(E)$
  - Calculated from interaction potential of collision pair

Transport properties (2)

- Neutral Species
  - L-J / Stockmayer interaction potential

- Ion Species Mobility/Diffusivity
  - Ions are treated as neutrals when calculating their diffusivities
    - $HCO^+ \sim CHO$
    - $C_2H_3O^+ \sim CH_2CHO$

  - Ion mobility is calculated from diffusivity using Einstein relation

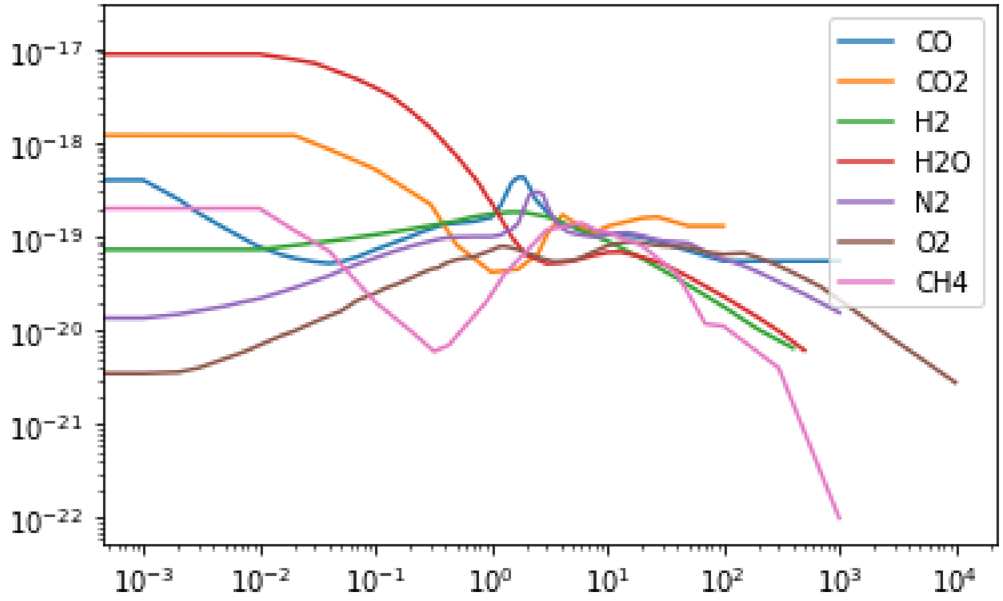
$$\mu_k = \frac{q_k D_k}{k_B T_k}$$

Transport properties (3)

- Electron Mobility/Diffusivity
  - Since interaction potential is not available for electron-neutral pairs, collision integral is computed using scattering cross section data for each major combustion species.

$$\pi\sigma^2\Omega^{(1,1)*} = \frac{1}{2!}\int_0^\infty \exp\left(-\frac{E}{kT}\right)\left(\frac{E}{kT}\right)^2 Q^{(1)}(E)\,d\frac{E}{kT}$$

  - Cross section data are available at LXcat Database (https://fr.lxcat.net/)



Implementation

❖ Added new ThermoType in OpenFOAM

```
typedef
sutherlandTransport        <-- canteraTransport
<
    species::thermo
    <
        janafThermo
        <
            perfectGas<specie>
        >,
        sensibleEnthalpy
    >
> gasHThermoPhysics;
```

Implementation

- canteraTransport uses Cantera to calculate diffusivity

- It stores mole fraction vector X

Illustration of Cantera C++ API usage

```
// Initialization
gas  = Cantera::IdealGasMix("canteraInputFileName", "phaseName")
tr = Cantera::newTransportMgr("Mix", gas)

// Calculate diffusivity
gas->setStateTPX(T, p, X) // scalar T, scalar p, scalar* X
tr->getMixDiffCoeffsMass(buf) // scalar* buf
```

Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes.
David G. Goodwin and Harry K. Moffat and Raymond L. Speth, http://www.cantera.org

Implementation

- Modified basicMultiComponentMixture
  - It contains mass fraction Y fields

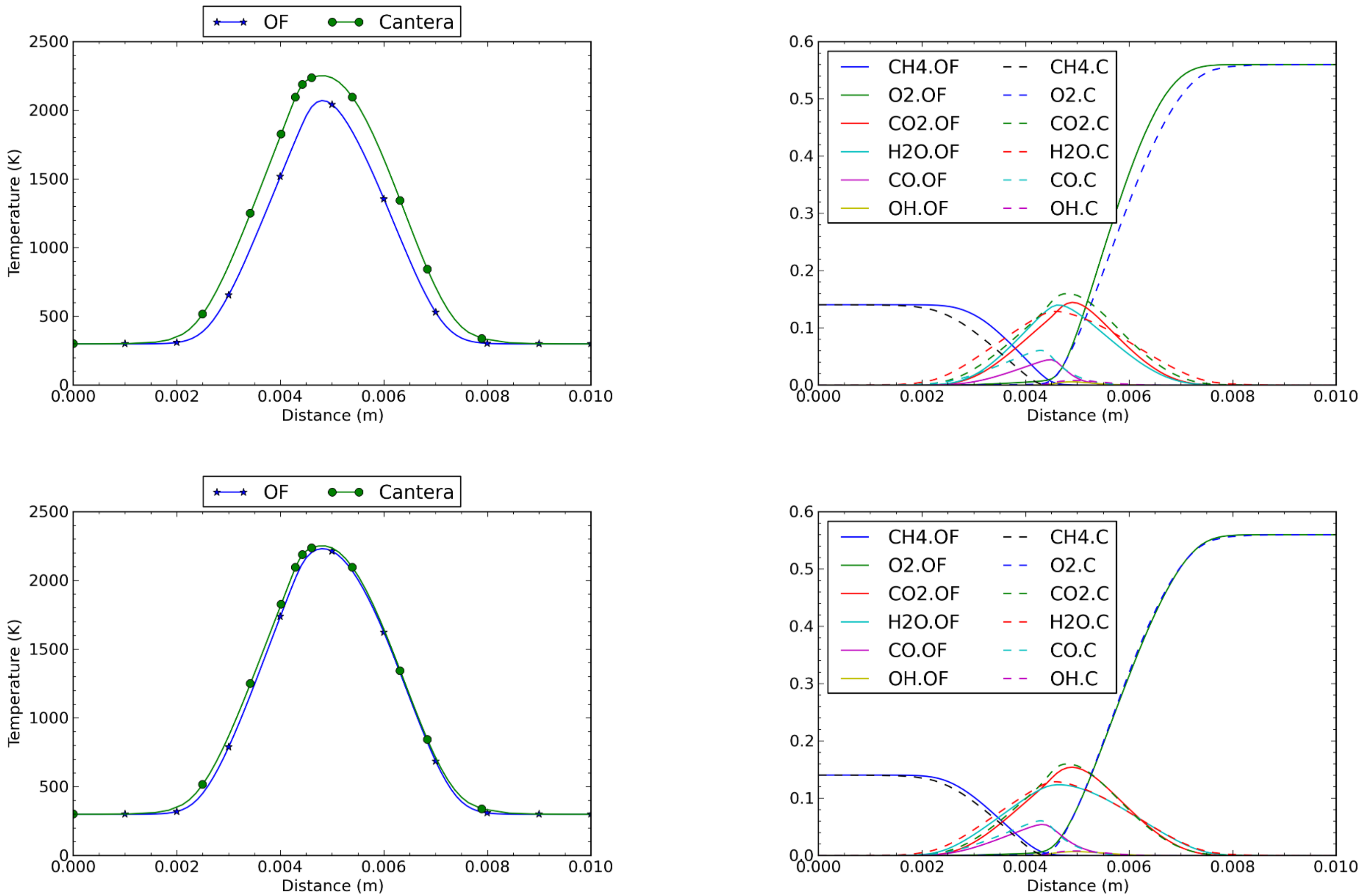
    PtrList<volScalarField> Y_;

  - Mass diffusivity D fields for all species are added to its attribute set

    PtrList<volScalarField> D_;

  - New method "calculateDiffusivities(p, T)" is added to calculate D fields when called explicitly in top-level solvers.

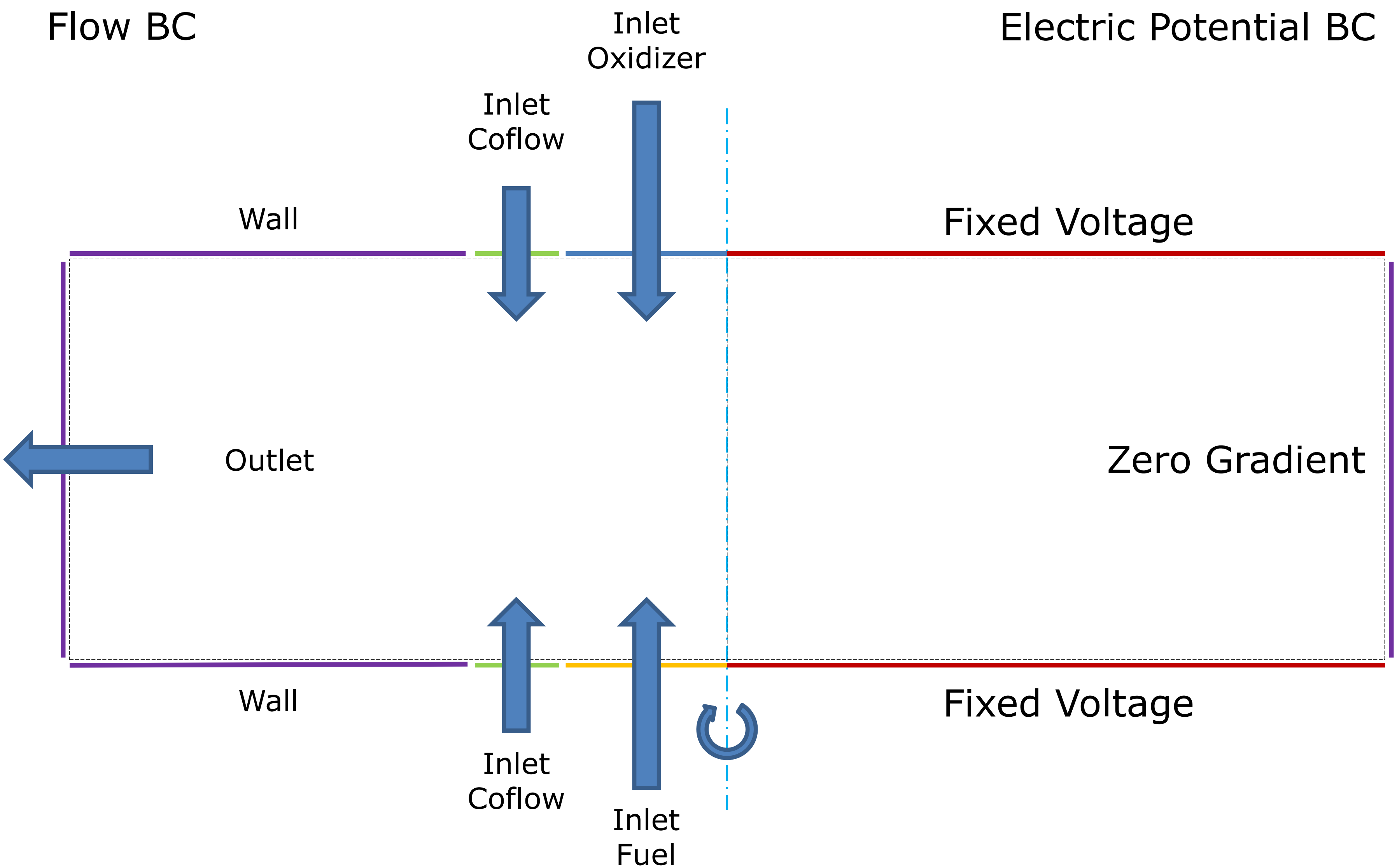
Verification



The same laminar counterflow diffusion flame simulated using reactingFoam(suthelandTransport, upper row), eReactingFoam(canteraTransport, lower row) and Cantera

Simulation condition

- 2D axisymmetric domain



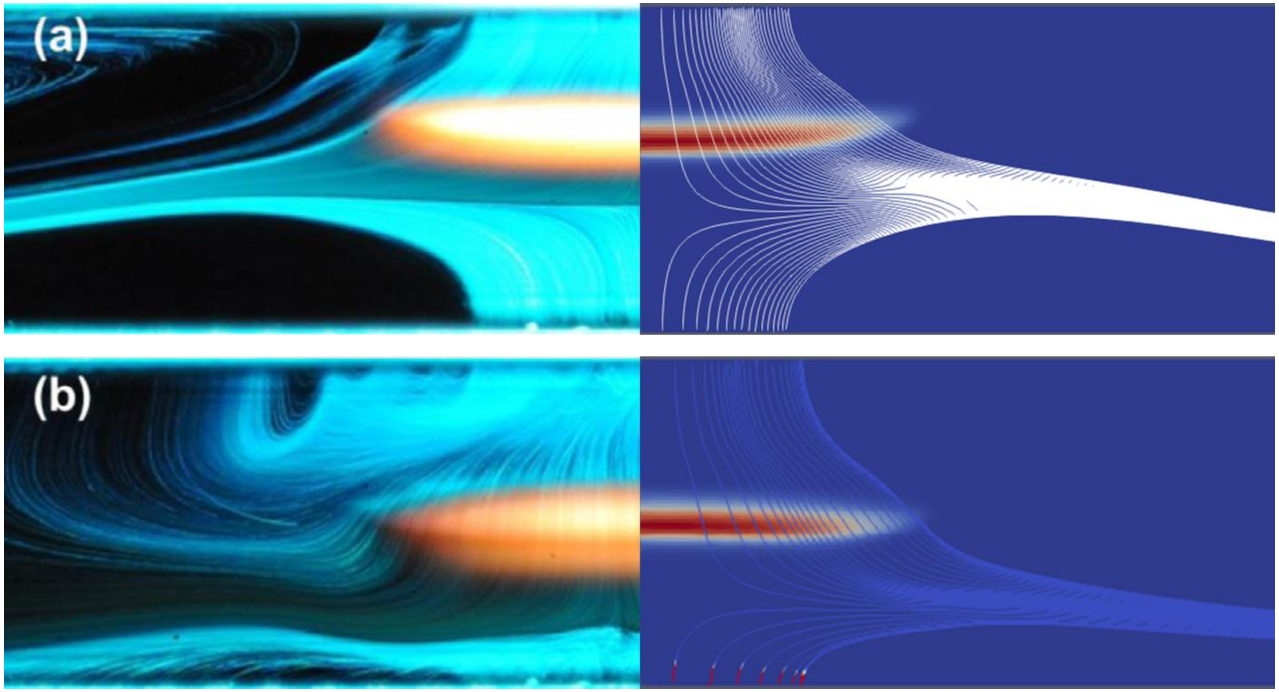
Reaction mechanisms

- Methane combustion
  - GRI 3.0 Mech
  - 52 species / 325 reactions

- Chemi-ionization
  - Mechanism from Prager’s Ph.D. thesis
  - 11 charged species (4 cations, 6 anions and electron) / 65 reactions

RESULTS

Results



No electric field

Lower electrode at -2.4 kV

Flame images from experiment

OH mass fraction and streamlines from simulation

Flame and stagnation plane moved toward cathode in simulation as well as the experiment

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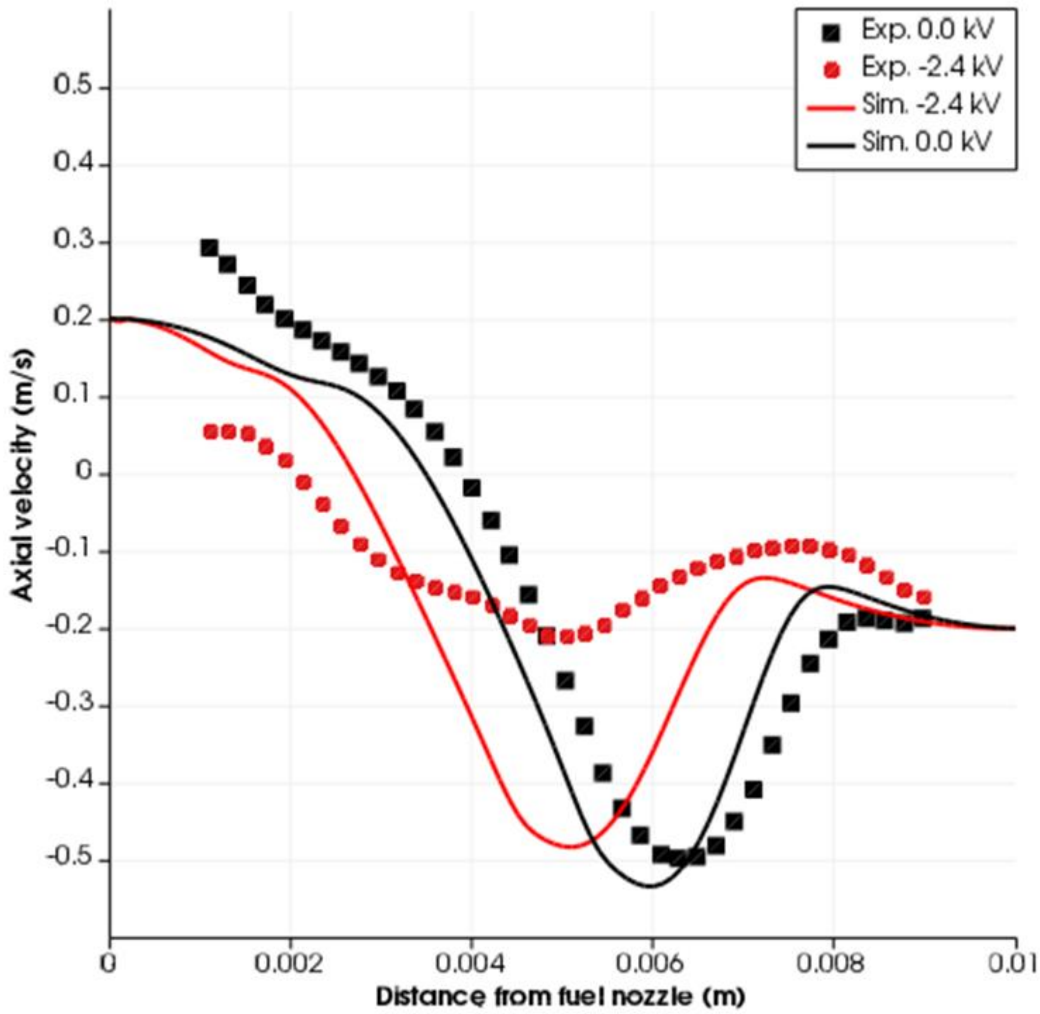
Result



Axial velocity curves along nozzle axis

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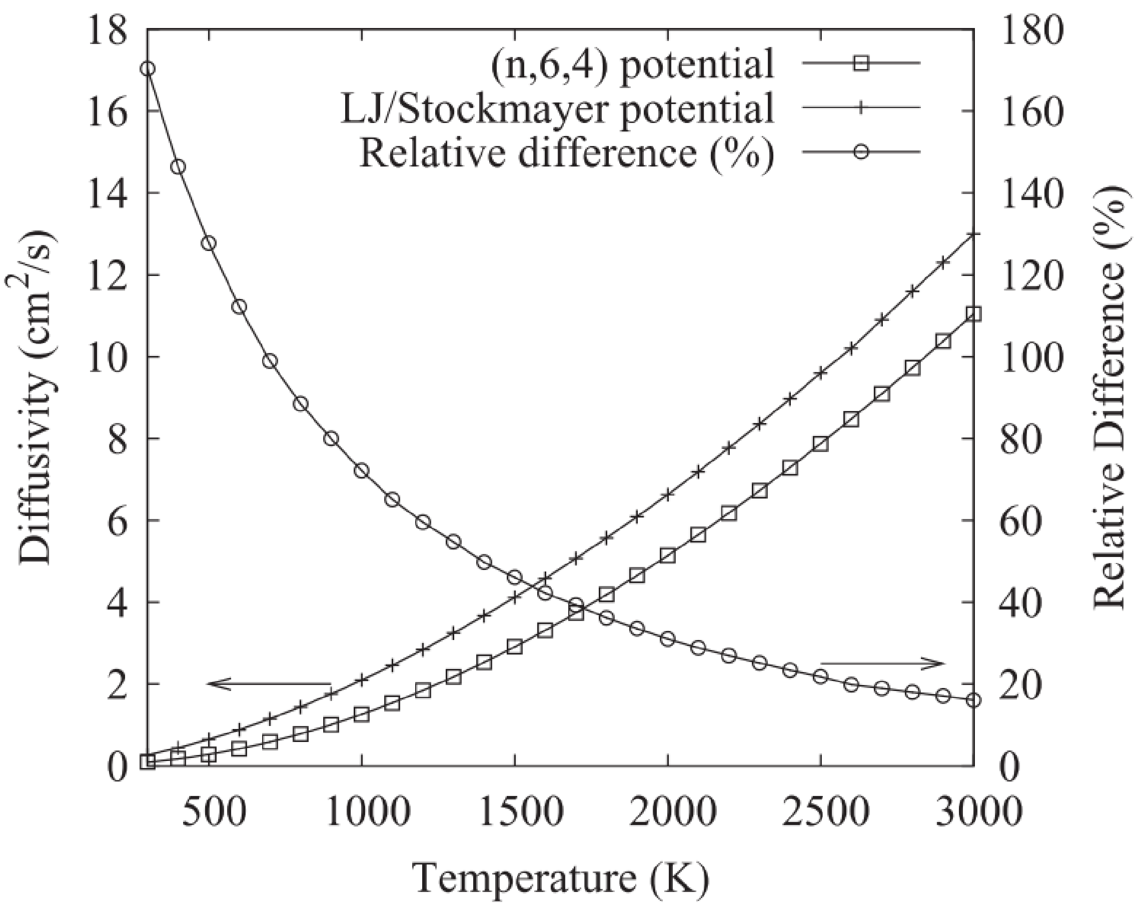
Why?



Treating H3O+ ion as neutral (L-J/Stockmayer) result in its higher binary diffusivity into O2

Han, J., Belhi, M., & Bisetti, F. (2015). Numerical modeling of ion transport in flames. *Combustion Theory and Modelling*, *19*(6), 744–772. https://doi.org/10.1080/13647830.2015.1090018

Work in progress

Implementing diffusivity model consist of following 4 different interactions.

Ion-Ion and Ion-Neutral interactions are introduced.

	Electron	Ion	Neutral
Electron	Coulomb	Coulomb	Cross section
Ion		Coulomb	(n,6,4)
Neutral			L-J/Stockmayer

Han, J., Belhi, M., & Bisetti, F. (2015). Numerical modeling of ion transport in flames. *Combustion Theory and Modelling*, *19*(6), 744–772. https://doi.org/10.1080/13647830.2015.1090018

Summary

- Implemented combustion code with charged particle transport
- Computed CH4/O2/N2 counterflow flame
- Flow modification in CH4 flame reproduced in simulation
- Work in progress to implement more accurate diffusivity model to improve quantitative prediction

QUESTIONS

THE END