Simulations of Low Mach Number Reactive Flows Coupled with Electric Fields

Preprint

Lucas Esclapez,[1] Marc Day,[1] and John Bell[2]

1 National Renewable Energy Laboratory
2 Lawrence Berkeley National Laboratory

Presented at the 2022 Spring Meeting of the Western State Session of the Combustion Institute
March 21-22, 2022

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

Contract No. DE-AC36-08GO28308

Conference Paper
NREL/CP-2C00-82382
July 2022

Simulations of Low Mach Number Reactive Flows Coupled with Electric Fields

Preprint

Lucas Esclapez,[1] Marc Day,[1] and John Bell[2]

1 National Renewable Energy Laboratory
2 Lawrence Berkeley National Laboratory

Suggested Citation
Lucas Esclapez, Marc Day, and John Bell. 2022. *Simulations of Low Mach Number Reactive Flows Coupled with Electric Fields: Preprint*. Golden, CO: National Renewable Energy Laboratory. NREL/CP-2C00-82382 https://www.nrel.gov/docs/fy22osti/82382.pdf.

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

Contract No. DE-AC36-08GO28308

Conference Paper
NREL/CP-2C00-82382
July 2022

National Renewable Energy Laboratory
15013 Denver West Parkway
Golden, CO 80401
303-275-3000 • www.nrel.gov

NOTICE

This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. This work was supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Applied Mathematics Program (under Award Number DESC0008271 and under contract No. DE-AC02-05CH11231). The views expressed herein do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

Simulations of low Mach number reactive flows coupled with electric fields

Lucas Esclapez[1*], *Marc Day*[1], *and John Bell*[2]

[1]*HPACF, National Renewable Energy Laboratory, 15013 Denver W Pkwy, Golden, CO 80401, USA*

[2]*CCSE, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA*
[*]*Corresponding author:* lucas.esclapez@nrel.gov

Abstract: Applying electric fields to flames can provide an effective, non-invasive control of the combustion process. In this work, an algorithm recently introduced to handle the interactions between reactive flows and an electric field is extended to handle multiple dimensions and adaptive mesh refinement (AMR), and applied to a series of laminar flames. Experimental data allows to validate the ability of the algorithm to capture the mechanisms driving the flame response to electric fields.
Keywords: AMR, Electric field, Ionic wind

1. Introduction

Experiments have shown that applying electric fields to flames can provide an effective control of the combustion process by enhancing flame propagation speed, improving flame stabilization and reducing pollutant emissions [1, 2]. The development of predictive numerical tools to analyze the flames/electric field interactions is however challenging due to the large disparity in time scales between the bulk fluid transport and the fast motion of the charged chemical species. In particular, because the electrons are light, they exhibit a tight coupling with the electric fields and introduce a strong constraint on explicit time stepping. Most of the early work in this area focused on steady-state problems [3, 4] and multi-dimensional simulations have only recently been reported [5, 6], and only in a compressible Navier-Stokes context. In the framework of low Mach number simulations, one needs to alleviate the electron time stepping constraint, and an implicit approach requires careful numerical treatment to avoid numerical instabilities.

In this work, we introduce PeleLMeX [7] a low Mach number AMR solver which implements the numerical strategy proposed in Esclapez et al. [8] to tackle the implicit treatment of the electron/electro-static potential. The solver is then used to study two canonical laminar flame cases: a simple 2D triple flame and a premixed bunsen flame.

2. Numerical Methods

PeleLMeX [7] is based on the low Mach number reactive flow algorithm of PeleLM [9], and is built upon the block-structured AMR framework of AMReX [10], leveraging AMReX's intrinsic parallelism and broad portability (PeleLMeX uses a MPI+X approach, where X can be CUDA, HIP,

DPC++ or OpenMP). In contrast with PeleLM, PeleLMeX features a non-subcycling approach for time stepping the AMR hierarchy: all the AMR levels advance in time at the same time step size, whereas PeleLM allows each level to advance with a step size prescribed by the level's local constrain, using a recursive mechanism, with synchronization between two consecutive levels when the same physical time is reached. This algorithmic change converts linear systems driving the time-stepping from level solves operating across a single AM level, to composite solves operating over the entire AMR hierarchy. This modification is essential to provide an efficient AMR implementation of the implicit electron/electro-static potential solve described hereafter.

In order to include the effect of electric fields, the classical low Mach number multi-species Navier-Stokes equations are supplemented with a drift term for the charged chemical species, as well as an equation for the electron number density n_e, and a Poisson equation for the electrostatic potential ϕ:

$$\begin{cases} \dfrac{\partial (n_e)}{\partial t} = -\nabla \cdot n_e (U_{adv} - \kappa_e \nabla \phi) \\ \qquad\qquad + \nabla \cdot D_e \nabla n_e + I_{R,e} & \text{(1a)} \\ \varepsilon_0 \varepsilon_r \nabla^2 \phi = -\sum_m z_m \rho Y_m + e n_e, & \text{(1b)} \end{cases}$$

, where U_{adv} is the advection velocity, κ_e and D_e are respectively the electron mobility and diffusivity, $I_{R,e}$ is the reaction source term, z_m is the charge per unit mass of ion species m and Y_m is the mass fraction of species m. This system exhibits very fast time scales relative to the other charged species since the large electron mobility leads to a rapid response to changes in the electric fields. To overcome the corresponding stringent constraint on the time step, this non-linear system is solved implicitly using a Jacobian-free Newton-Krylov (JFNK) method for which a preconditioner based on the Schur complement of the system Jacobian matrix [8] is employed. The resulting block preconditioner is applied using a classical geometric multigrid. This approach is well suited to an AMR framework. The interactions of the charged particles with the neutral species give rise to a volumetric force in the momentum equation (the Lorentz forces) and generates a bulk flow motion called "ion wind". The work done by the forces also appears as a source term in the energy equation.

3. Results and Discussion

The algorithm accuracy is detailed in Esclapez et al. [8]. Pseudo one-dimensional simulations of premixed flames were performed and confirm that the PeleLMeX implementation reproduces the initial results obtained with the 1D code. In the following, we focus on two cases relevant for practical applications: the effect of an external electric field on a 2D freely propagating edge flame and a laminar premixed methane/air bunsen flame subjects to transverse electric field for which experimental data are available.

3.1 Freely-propagating edge flames

Edge flames are an essential feature of flame stabilization in many combustion devices. The complex flame structure couples with the flow hydrodynamics to allow edge flames to propagate faster than their planar, premixed counterpart. To better understand the interactions of electric fields with edge flames, it is important to first identify the mechanism coupling the flame motion and the

forces resulting from the application of an electric field in an idealized situation. With this goal in mind, we analyze the effect of applying external forcing of increasing strength on a freely propagating edge flame propagating in a 2D methane/air mixing layer in ambient conditions, where the electro-static field is aligned with the flame propagation direction. The inlet velocity is dynamically controlled to maintain the flame at a fixed position in the computational domain, allowing measurement of the displacement speed of the flame as it accelerates under the effect of the electric field.

Figure 1(a) shows the edge flame structure as well as the Lorentz force field induced by the interactions of charged chemical species with the surrounding neutral gas under the effect of the vertical electric field. Indeed, the positively charged species generated during the high temperature chemical decomposition of methane near the triple point (peak of heat release, highlighted by the black iso-contours) are driven towards the grounded electrode at the bottom of the domain, pushing on the incoming fresh gases.

Once this Lorentz force field is established, the edge flame accelerates. Figure 1(b) shows the integral of the Lorentz forces and the measured flame acceleration after applying the external forcing for 2 ms, both as functions of the external forcing intensity. Following, an initial quadratic increase, the Lorentz forces eventually plateau as the electric field fully penetrates the flame structure and charged species are driven away from the reaction zone as fast as they are produced by chemical kinetics. Comparing the flame speed increase to the edge flame speed in absence of ΔV shows that strong external forcing can lead to more than doubling of the flame speed within the span of 2 ms. Conversely, it provides an estimate of the flame response time scale as function of the forcing intensity, which is of interest in designing a control mechanism to mitigate, for instance, thermo-acoustic instabilities.

3.2 Premixed laminar bunsen methane/air flame

The second test case is the premixed methane/air Bunsen burner studied experimentally by Park et al. [11] and numerically by Belhi et al. [5]. A transverse electric field is applied on the burner and both qualitative visualization of the flame shape and quantitative measurement of the velocity field are available to visualize the effect of the ionic wind. In the following, we focus on the case of a strong DC electric field where the negative electrode potential is set to -16kV. The simulation is performed on a 5 cm cube computational domain, with the burner oriented in the z direction and the electric field oriented in the x direction. A 128^3 base grid is used, with three levels of refinement for a minimum grid spacing of 49 μm, clustered around the reaction zone and the charged species gradients. The simulation is currently ongoing, but an instantaneous visualization of the interaction between the electric field and the flame is provided in Fig. 2. The flame location is highlighted by a grey iso-contour of heat release rate and also visible on the temperature field extracted on a plane in the center of the domain. The back plane shows the local charge density, with charge separation resulting from the motion of negative charges towards x^- (mostly electrons) and positive ions moving toward the negatively charged electrode a x^+. This induces the development of a Lorentz force field, the x component of which is represented on the horizontal plane: positive and negative lobes develop on each side of the flame and will in time induce tilting of the flame tip towards the cathode.

Preliminary tests conducted on a 2D slot burner indicates that the flame response time is close to the one reported in Belhi et al. [5] and the flame is thus expected to bend towards x^+ within 5

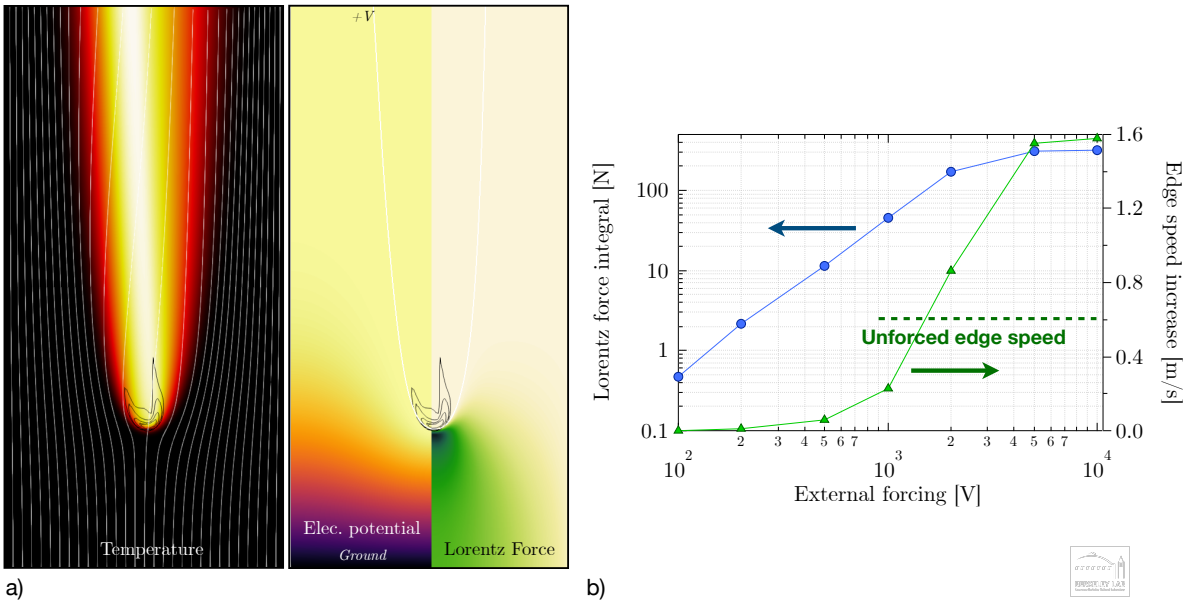

Figure 1: a) Temperature field showing the edge flame structure with superimposed velocity streamlines (white) and heat release rate iso-contours (black), electro-static potential and Lorentz forces. b) Lorentz forces integral and flame speed acceleration as function of the external electric field strength.

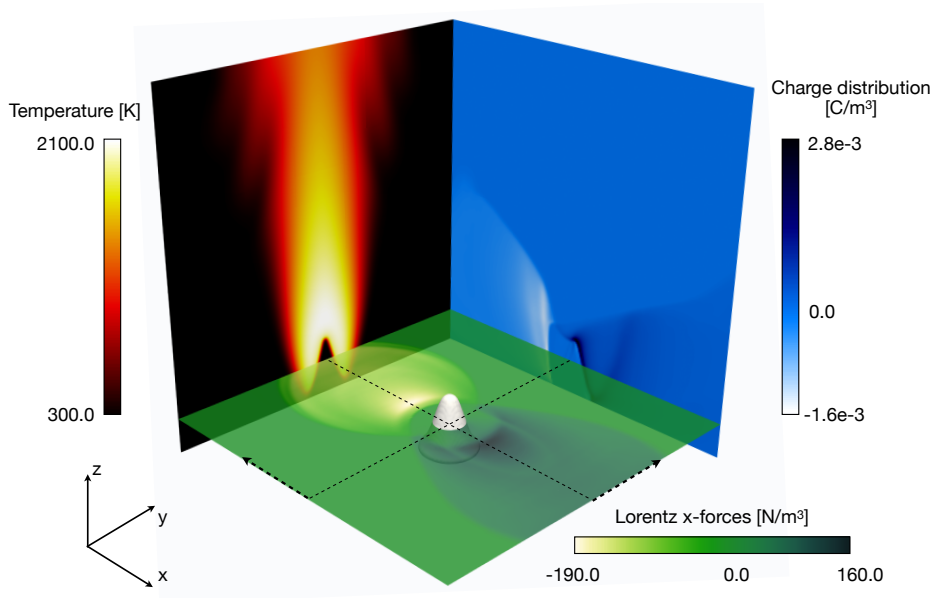

Figure 2: Instantaneous field of temperature, charge density and x-Lorentz forces on a x-normal, y-normal and z-normal planes, respectively. The grey iso-contour of heat release rate at 1e8 W/m^3 indicates the position of the flame.

ms.

4. Conclusions

In this work we extended the SDC-JFNK method for flame/electric field interactions previously developed in 1D to multiple dimensions, and implemented the algorithm in the low Mach number AMR solver PeleLMeX. Following a series of pseudo-1D tests to validate the ability of the solver to reproduce the results of the initial 1D implementation, two test cases relevant for realistic applications are conducted briefly analyzed. Further work will focus on extending the solver validation with multi-dimensional cases and will use this unique capability to investigate the processes leading to better flame stabilization and pollutant emission reduction in practical devices.

5. Acknowledgements

This work was supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Applied Mathematics Program (under Award Number DE-SC0008271 and under contract No. DE-AC02-05CH11231).

References

[1] A. B. Fialkov, Investigations on ions in flames, Progress in Energy and Combustion Science 23 (1997) 399–528.

[2] A. Starikovskiy and N. Aleksandrov, Plasma-assisted ignition and combustion, Progress in Energy and Combustion Science 39 (2013) 61–110.

[3] J. Prager, U. Riedel, and J. Warnatz, Modeling ion chemistry and charged species diffusion in lean methane-oxygen flames, Proceedings of the Combustion Institute 31 (2007) 1129–1137.

[4] N. Speelman, L. de Goey, and J. van Oijen, Development of a numerical model for the electric current in burner-stabilised methane–air flames, Combustion Theory and Modelling 19 (2015) 159–187.

[5] M. Belhi, B. J. Lee, M. S. Cha, and H. G. Im, Three-dimensional simulation of ionic wind in a laminar premixed Bunsen flame subjected to a transverse DC electric field, Combustion and Flame 202 (2019) 90–106.

[6] M. Di Renzo, HTR-1.3 solver: Predicting electrified combustion using the hypersonic task-based research solver, Computer Physics Communications 272 (2022) 108247.

[7] PeleLMeX, *An adaptive mesh hydrodynamics simulation code for low Mach number reacting flows without level sub-cycling: https://github.com/AMReX-Combustion/PeleLMeX*.

[8] L. Esclapez, V. Ricchiuti, J. B. Bell, and M. S. Day, A spectral deferred correction strategy for low Mach number reacting flows subject to electric fields, Combustion Theory and Modelling 24 (2020) 194–220.

[9] A. Nonaka, M. S. Day, and J. B. Bell, A conservative, thermodynamically consistent numerical approach for low Mach number combustion. Part I: Single-level integration, Combustion Theory and Modelling 22 (2018) 156–184.

[10] W. Zhang, A. Almgren, V. Beckner, J. Bell, J. Blaschke, C. Chan, M. Day, B. Friesen, K. Gott, D. Graves, et al., AMReX: a framework for block-structured adaptive mesh refinement, Journal of Open Source Software 4 (2019) 1370–1370.

[11] D. G. Park, S. H. Chung, and M. S. Cha, Visualization of ionic wind in laminar jet flames, Combustion and Flame 184 (2017) 246–248.