

A computational approach for the study of electromagnetic interactions in reacting flows

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Abstract

This document reports additional information in support of the discussion of the results presented in the main paper. The structure of the Supporting Information is as follows.

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S1. Methodology

S1.1. *Electrostatic/Magnetostatic fields solver (EMI-static)*

The developed code is called Electromagnetic Interactions (EMI). EMI is integrated into a modified version of the SENGAs [1, 2] Direct Numerical Simulation (DNS) code. The DNS modifications concern the electromagnetic field effects on the conservation equations, boundary conditions, and molecular transport properties. EMI takes as an input the properties of the reacting flow and solves for the propagation of the electromagnetic fields. EMI also computes the electromagnetic forces, which are then introduced into the conservation equations for the flow and the species. SENGAs then solves the conservation equations of the reacting flow using the Direct Numerical Simulation (DNS) method. Moreover, SENGAs advances the governing equations using a Runge-Kutta algorithm. The flow chart with the structure of EMI-SENGA for static fields is shown in Fig. S1. Both Eqs. (12) and (14) of the main paper are solved in a similar manner. The overall process is described below:

1. The 1st and 2nd order derivatives are discretized using the finite difference approach and keeping a 10th order accuracy in each x , y , and z direction.
2. The accuracy drops from 10th to 2nd as the x -direction boundaries are approached. This is explained schematically in Fig. 1 of the main paper. Moreover, Table S1 shows the coefficients of each term of the discretized equations. Note that it is assumed that the Dirichlet boundary conditions are applied in the x -direction. This means that in the y and z directions, the 10th-order accuracy holds everywhere.
3. The resulting system is of the form of $AX = \Omega$, where matrix A contains the left-hand side parameters of the discretized 1st and 2nd derivatives, X contains the discretized Φ or Ψ potential fields, and Ω contains the right-hand side parameters. For the study of one- or two-dimensional flows, the discretization in y and z directions is not included in the A matrix.
4. $A = A_1 + A_2$. A_1 matrix corresponds to the parameters of the second-order derivatives of Eq. (12) and Eq. (14). A_2 corresponds to the parameters of the first-order derivatives. Therefore, A_2 depends on the χ_e

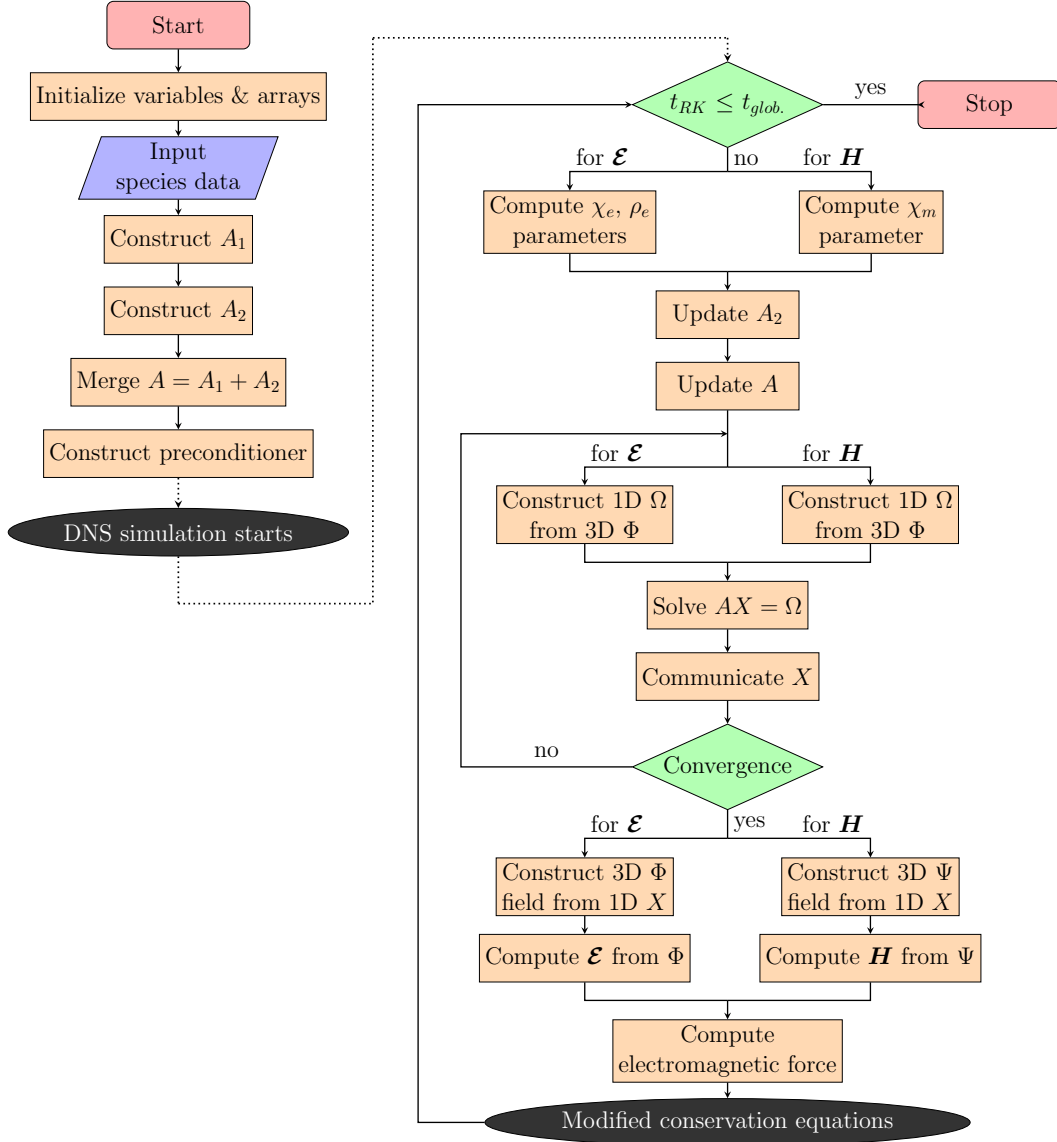


Figure S1: Flow chart of the EMI-SENGA implementation for static fields.

Table S1: 1st and 2nd order derivative coefficients using central finite difference.

1 st order derivative						
Accuracy	Grid points					
	$i - 5$	$i - 4$	$i - 3$	$i - 2$	$i - 1$	i
2					-1/2	0
4				1/12	-2/3	0
6			-1/60	3/20	-3/4	0
8		1/280	-4/105	1/5	-4/5	0
10	-1/1260	5/504	-5/84	5/21	-5/6	0
Accuracy	Grid points					
	$i + 1$	$i + 2$	$i + 3$	$i + 4$	$i + 5$	
2	1/2					
4	2/3	-1/12				
6	3/4	-3/20	1/60			
8	4/5	-1/5	4/105	-1/280		
10	-5/3	5/21	-5/126	5/1008	-1/3150	

2 nd order derivative						
Accuracy	Grid points					
	$i - 5$	$i - 4$	$i - 3$	$i - 2$	$i - 1$	i
2					1	-2
4				-1/12	4/3	-5/2
6			1/90	-3/20	3/2	-49/18
8		-1/560	8/315	-1/5	8/5	-205/72
10	1/3150	-5/1008	5/126	-5/21	5/3	-5269/1800
Accuracy	Grid points					
	$i + 1$	$i + 2$	$i + 3$	$i + 4$	$i + 5$	
2	1					
4	4/3	-1/12				
6	3/2	-3/20	1/90			
8	8/5	-1/5	8/315	-1/560		
10	5/3	-5/21	5/126	-5/1008	1/3150	

and χ_m fields. The population of the A matrix for 1D and 3D domains is shown in Fig. S2.

- For the Dirichlet boundary conditions, the values of matrix A are unity and the values of Ω are equal to the electric and magnetic boundaries defined by the user.

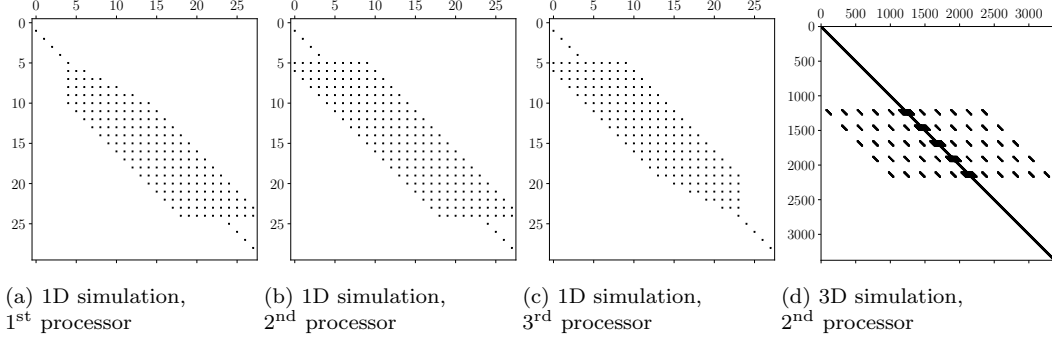


Figure S2: Population of matrix A for 1D and 3D simulations decomposed into 3 processors along the x -direction. For the 1D simulation $N_x = 60$, while for the 3D $N_x = 15$, $N_y = 5$, $N_z = 5$.

6. The system of equations $AX = \Omega$ is solved using either the direct LU decomposition method or the iterative Biconjugate gradient stabilized method (BiCGSTAB) of the LAPACK library [3]. Due to the exceedingly high computational cost of the former method, the simulations of this study are performed using the BiCGSTAB method.
7. The preconditioner matrix used for the BiCGSTAB solver is equal to A_1^{-1} . The inverse of the A_1 matrix is computed at the beginning of the simulation using routines of the LAPACK library [3]. As long as A_2 does not change significantly, i.e., as long as the gradients of electric and magnetic susceptibilities are low, it is expected that convergence can be achieved with this preconditioner.

The parallelization strategy of the EMI code for static fields is as follows:

1. To retain a fully parallel solver, each core holds and solves a separate $AX = \Omega$ system, using either direct or iterative methods.
2. If the core is an internal core, then its ghost cells hold the values from the adjacent cores. These ghost cells are treated as Dirichlet boundary conditions. In other words, for the ghost cells, the values of matrix A are unity and the values of Ω are equal to the X values from the adjacent cells of the neighbouring processor.
3. If the core is a boundary core, then it holds the Dirichlet boundary conditions. In this case, the residual ghost cells do not hold any information and they are not part of the solution.
4. After the $AX = \Omega$ system is solved, the ghost cells of each processor are updated with values from the other processors and the system is solved again until convergence is reached. The process is repeated until the specified absolute and relative tolerances are satisfied.

Note also that, as can be seen from Fig S1, the static fields are solved inside the Runge-Kutta solver of SENG. This coupling is expected to increase the stability and robustness of the code.

S1.2. Electromagnetic waves solver (EMI-FDTD)

A schematic diagram of the structure of the EMI-FDTD code is shown in Fig. S3. As discussed in Section 2.1.2 of the paper, the Finite-Difference Time-Domain (FDTD) solver of EMI code is formulated on a grid different from the SENG grid. The FDTD grid also holds the additional boundary cells. The structure of the code is as follows:

1. The medium properties (see Section 2.4) are interpolated on the Yee cell positions. Specifically, ϵ and σ^e are interpolated on the positions of the electric field components, while μ is interpolated on the positions of the magnetic field components.
2. Inside the main loop of each SENG timestep, the nested loop of the EMI-FDTD code propagates the electromagnetic waves with a timestep of Δt_{FDTD} . The electric field components are updated first. Then, the electric field sources and boundary conditions are superimposed on the new electric field solution. At this point, the final solution of the electric field is transferred to the other processors. The parallelization strategy is discussed below in this section.
3. Afterwards, the magnetic field components are updated using a procedure similar to that used for the electric field components. The boundary conditions are applied and the ghost cells between processors are communicated.
4. At the end of electromagnetic field propagation, the fields are interpolated in space and time to be consistent with the SENG code. Next, the electromagnetic forces are computed.

The parallelization of the EMI-FDTD solver follows the domain decomposition method of SENG. Therefore, the computational domain is decomposed into subdomains which are solved by each processor. Ghost cells are necessary to communicate information between processors. Since SENG uses a 10th-order accuracy, at least 5 ghost cells in each direction are required. However, in the EMI-FDTD method, each processor needs to communicate only one row of ghost cells, since the FDTD method is of 2nd-order accuracy. The CPML regions are assigned to the boundary CPU processors. It should be noted here that, since SENG requires at least 5 ghost cells in each direction, if the thickness of the CPML regions is equal to or less than 5 cells, there will not be any additional memory load to the processors.

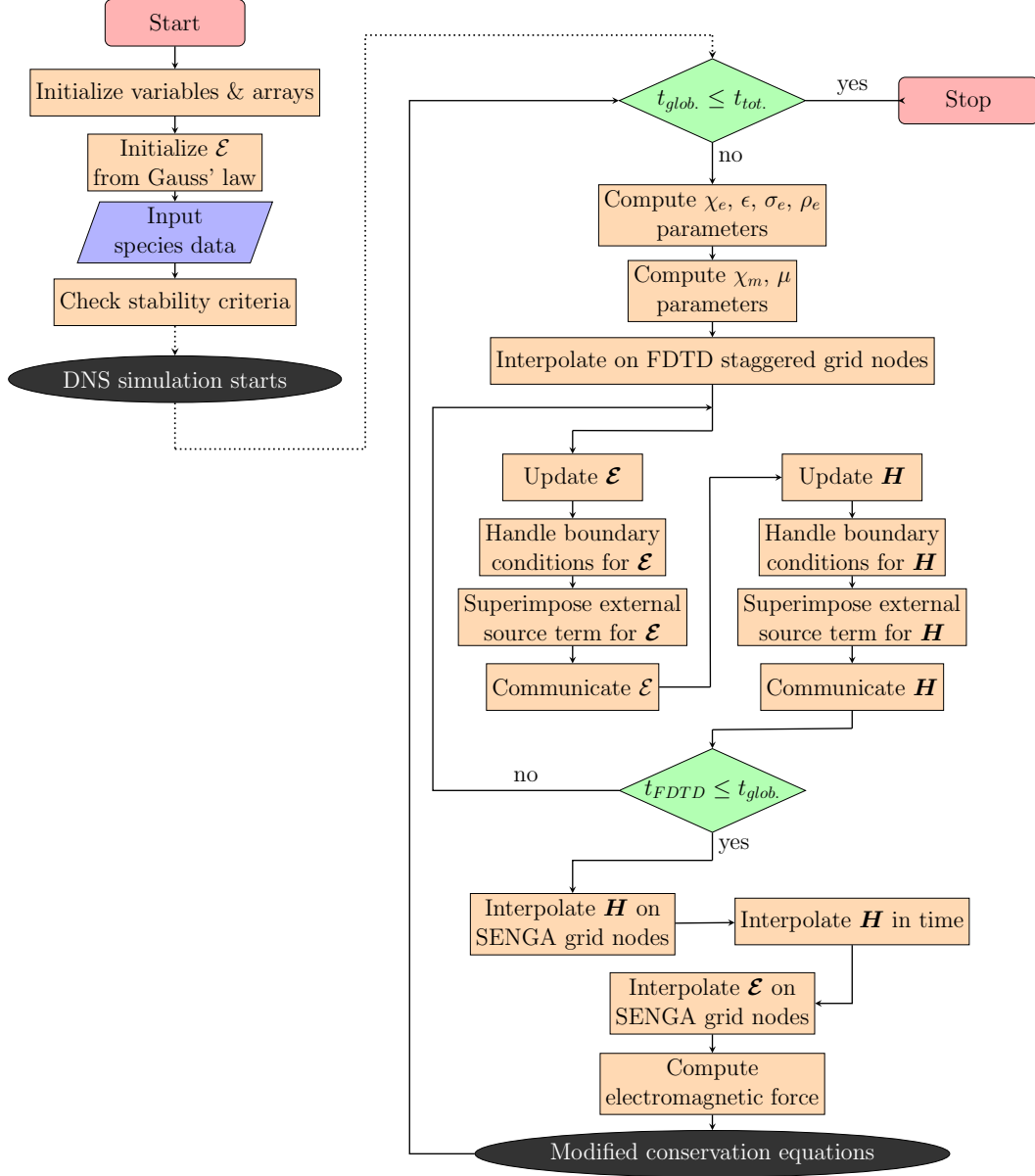


Figure S3: Flow chart of the FDTD method implemented in EMI-SENGA.

S1.3. CPML formulation

The parameters needed for the CPML formulation, namely σ , α , and κ as detailed in Ref. [4] and computed in the EMI-FDTD code, are described here. Two widely used approaches for the computation of these parameters are the polynomial grading and geometric grading approaches [5]. A polynomial grading approach is selected in this study for the CPML regions, as commonly found in the literature [5, 6, 7]. Therefore,

- The σ_w term, where $w \in [x, y, z]$, is computed in the x -direction by

$$\sigma_x(x) = \left(\frac{x}{l_x}\right)^m \sigma_{x,\max}, \quad (\text{S1})$$

where x is the distance of the electric or magnetic field component node under consideration from the interface between the main computational domain and the CPML region. In addition, m is the order of the polynomial and l_x is the thickness of the CPML layer. In a similar manner, the $\sigma_y(y)$ and $\sigma_z(z)$ are computed in the y and z directions, respectively. It should be noted that the values that x can take are different for the electric and magnetic field components since they are located at different positions (see Fig. 2 of the main paper). According to Ref. [7], and references therein

$$\sigma_{x,\max} = \sigma_{\text{factor}} \sigma_{x,\text{opt}}, \quad (\text{S2})$$

where for the electric field

$$\sigma_{x,\text{opt}}^e(x) = \frac{m+1}{150\pi\sqrt{\epsilon_r}\Delta x}, \quad (\text{S3})$$

and for the magnetic field

$$\sigma_{x,\text{opt}}^m(x) = \frac{\mu_0}{\epsilon_0} \frac{m+1}{150\pi\sqrt{\epsilon_r}\Delta x}. \quad (\text{S4})$$

In Eqs. (S3) and (S4), ϵ_r is the relative permittivity of the background material. For this implementation, it is assumed that the background material is a vacuum. Therefore, $\epsilon_r = 1$.

- The κ_w term is computed in the x -direction using

$$\kappa_x(x) = 1 + (\kappa_{\max} - 1) \left(\frac{x}{l_x}\right)^m, \quad (\text{S5})$$

for both the electric and magnetic fields. In the above equation, $\kappa_{\max}$ is an input parameter. The parameter κ_w is equal to unity at the interface between the CPML region and the main computational domain, while it becomes maximum, i.e., $\kappa_{\max}$, at the outer side of the CMPML region.

- The parameter α_w in the x -direction is computed for the electric field using

$$\alpha_x(x) = \alpha_{\min} + (\alpha_{\max} - \alpha_{\min}) \left(1 - \frac{x}{l_x}\right) \quad (\text{S6})$$

and for the magnetic field using

$$\alpha_x(x) = \frac{\mu_0}{\epsilon_0} \left[\alpha_{\min} + (\alpha_{\max} - \alpha_{\min}) \left(1 - \frac{x}{l_x}\right) \right]. \quad (\text{S7})$$

At the CMPL region and computational domain interface, the α_w parameter becomes maximum, i.e., $\alpha_{\max}$, while it reaches a minimum value, i.e., $\alpha_{\min}$, at the outer CMPL side.

It should be noted that the parameters σ_w , κ_w , and α_w mentioned above are assumed to have an offset in their x distance from the main computational domain interface [7]. Specifically, when the parameters are computed on the electric field components' nodes, then a $0.25\Delta x$ offset is subtracted from the x distance. Moreover, when the nodes of the magnetic field components are considered, then a $0.75\Delta x$ offset is subtracted from the x distance. The reason for this offset is to make sure that the CPML algorithm updates the same number of electric and magnetic field components [7]. The values subtracted correspond to the distance of the components from the CPML interface, due to the fact that the fields are staggered in the FDTD formulation (see Fig. 2 of the main paper).

S1.4. Properties of species

Table S2: Electrical properties of species.

Species	q [e]	α [$\text{\AA}^3$ (cgs units)]	Species	q [e]	α [$\text{\AA}^3$ (cgs units)]
N ₂	0	1.710 [8]	CH ₂	0	2.143 [12]
H ₂	0	0.787 [8]	CH ₂ (S)	0	2.143 [†] [12]
H	0	0.667 [9]	C	0	1.760 [9]
O ₂	0	1.562 [8]	CH	0	1.883 [10]
O	0	0.802 [9]	CH ₃ OH	0	3.210 [13]
H ₂ O	0	1.501 [8]	CH ₃ O	0	3.450 [12]
OH	0	1.121 [10]	CH ₂ OH	0	3.450 [†] [12]
H ₂ O ₂	0	2.300 [11]	CH ₂ O	0	2.800 [14]
HO ₂	0	1.972 [12]	HCO	0	2.485 [12]
CO	0	1.953 [8]	CHO ⁺	1	—
CO ₂	0	2.507 [8]	H ₃ O ⁺	1	—
CH ₄	0	2.448 [8]	O ₂ [−]	-1	—
CH ₃	0	2.341 [12]	e [−]	-1	—

[†] The polarizabilities of ionic species can be neglected since, due to their low concentration, they do not significantly contribute to the overall mixture properties (cf. Eq. (29) of the main paper).

Table S3: Properties of (a) paramagnetic and (b) diamagnetic species.

(a) Paramagnetic species		(b) Diamagnetic species	
Species	$\mathcal{S}$	Species	$\chi_m^{\text{molar}}/10^{-6} [\text{cm}^3/\text{mol}]^\dagger$ [14]
H	1/2	N ₂	-12.0
O ₂	1	H ₂	-3.99
O	1	H ₂ O	-13.1
OH	1/2	H ₂ O ₂	-17.3
HO ₂	1/2	CO	-11.8
CH ₃	1/2	CO ₂	-21.0
CH ₂	1	CH ₄	-17.4
CH ₂ (S)	1	CH ₃ OH	-21.4
C	1	CH ₂ O	-18.6
CH	1/2	CHO ⁺	NF
CH ₃ O	1/2		
CH ₂ OH	1/2		
HCO	1/2		
H ₃ O ⁺	1/2		
O ₂ ⁻	1/2		

[†] Values are given in the CGS system. Note that to obtain the volume magnetic susceptibility, the reported values should be multiplied by $\rho Y_s/M_s$.

S1.5. Polynomial fitting method

SENGA implementation follows the CHEMKIN [15] formulation for the computation of the transport properties. Thus, the computation of viscosity, η_α , thermal conductivity, λ_α , and binary diffusion coefficients, $D_{\alpha\beta}$, is based on a polynomial formulation [16]

$$\begin{aligned}
 \ln \eta_\alpha &= \sum_{j=1}^J a_{\alpha,j} (\ln T)^{j-1}, \\
 \ln \lambda_\alpha &= \sum_{j=1}^J b_{\alpha,j} (\ln T)^{j-1}, \\
 \ln D_{\alpha\beta}^{(P_0)} &= \sum_{j=1}^J d_{\alpha\beta,j} (\ln T)^{j-1},
 \end{aligned} \tag{S8}$$

where a , b , and d are polynomial coefficients. The polynomials are fitted with respect to a reference temperature T_0 . Note that the binary diffusion coefficients are also given with respect to a reference pressure P_0 . For pressures other

than the reference pressure, the diffusion coefficients are computed according to

$$\ln D_{\alpha\beta}^{(P)} = \ln D_{\alpha\beta}^{(P_0)} \frac{P_0}{P}. \quad (\text{S9})$$

Note that Cantera [17] follows a different polynomial fitting method for the viscosity, thermal conductivity, and binary diffusion coefficients compared to SENGGA. Specifically, the polynomials take the form

$$\begin{aligned} \sqrt{\left(\frac{\eta_\alpha}{\sqrt{T}}\right)} &= \sum_{j=1}^J a_{\alpha,j} (\ln T)^{j-1}, \\ \frac{\lambda_\alpha}{\sqrt{T}} &= \sum_{j=1}^J b_{\alpha,j} (\ln T)^{j-1}, \\ \frac{D_{\alpha\beta}^{(P_0)}}{T^{3/2}} &= \sum_{j=1}^J d_{\alpha\beta,j} (\ln T)^{j-1}. \end{aligned} \quad (\text{S10})$$

This method was implemented in EMI-SENGGA and applied in all simulations presented in the paper since non-negligible differences in the concentrations of ionic species were observed between the two polynomial fitting methods when testing a 1D laminar CH₄-air flame (results are not presented here for the sake of conciseness).

S1.6. Ion transport model

The transport model for ionic species differs from that of neutral molecules. In this study, the ion transport model implemented in Cantera is also implemented in EMI-SENGGA. According to this ion transport model, the transport properties are computed as follows [17]:

- The Stockmayer-(n,6,4) model is used for collisions between charged and neutral species [18, 19, 20, 21, 22].
- For the computation of mixture-average diffusion coefficients and mobilities, only binary transport between neutral-neutral and ion-neutral species is considered. Interactions between ions are neglected.
- For the computation of mixture-averaged viscosity and thermal conductivity, only neutral species are included.
- For collisions between O₂ and O₂⁻, experimental collision data are used. The reason is that the Stockmayer-(n,6,4) model cannot accurately describe collisions involving those two molecules due to resonant charge transfers. The data is taken from Prager [22].

S2. Dimensional analysis

S2.1. Magnetostatics

For this analysis, we assume uniform μ and ϵ . First, we take the curl of Ampere's law, Eq. (1), which gives

$$\nabla \times (\nabla \times \mathbf{H}) = \epsilon \frac{\partial}{\partial t} (\nabla \times \mathbf{E}) + \nabla \times \mathbf{J}. \quad (\text{S11})$$

Then, we substitute the electric field from Faraday's law, Eq. (2), into Eq. (S11). Thus, we end up with a wave equation for the magnetic field, $\mathbf{H}$, in the form

$$\epsilon \mu \frac{\partial^2 \mathbf{H}}{\partial t^2} = \nabla^2 \mathbf{H} - \nabla (\nabla \cdot \mathbf{H}) + \nabla \times \mathbf{J}. \quad (\text{S12})$$

Since, for uniform μ , one has $\nabla \cdot \mathbf{H} = 0$, this equation can be further simplified to

$$\epsilon \mu \frac{\partial^2 \mathbf{H}}{\partial t^2} = \nabla^2 \mathbf{H} + \nabla \times \mathbf{J}, \quad (\text{S13})$$

which is a wave equation. For the time evolution to be negligible, the time derivative term should be negligible compared to $\nabla^2 \mathbf{H}$, i.e., the behaviour of the equation moves from a hyperbolic equation (i.e., wave equation) to an elliptic equation. This requires

$$\frac{\overline{H}}{L^2} \gg \frac{\epsilon \mu \overline{H}}{T^2} \longrightarrow T \gg \frac{L}{c}, \quad (\text{S14})$$

where $\overline{H}$ is the scale of the imposed magnetic field (in the following, the overline will be used to indicate the scale of the respective quantity), L is the length of the domain and $1/(\mu\epsilon)$ could be approximated as $c^2 = 1/(\mu_0\epsilon_0)$, i.e. the square of the speed of light in vacuum, given that our conditions are very close to the properties of a vacuum. This condition states that any process generating time-varying magnetic fields should be characterised by a time scale much larger than L/c . This guarantees that the magnetic field adapts almost "instantaneously" to any changes in the system configuration (e.g., currents). In our problem, the potential fluctuations of the magnetic field are due to time-varying currents generated by the chemical reactions. The time scale of ion/electron formation typically satisfies the condition of Eq. (S14).

However, this condition alone is not sufficient, since the scalar magnetic potential formulation used in this work also requires that

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \approx 0. \quad (\text{S15})$$

If the time derivative of the electric displacement is negligible compared to the free current density, which implies $\bar{\sigma}T/\epsilon \gg 1$, the second condition we need for our formulation to be valid is (negligible current-induced magnetic field)

$$\bar{H} \gg L\bar{J} \longrightarrow \frac{L\bar{J}}{\bar{H}} \ll 1, \quad (\text{S16})$$

which constrains the magnitude of the currents generated by the combustion process. Assuming that an electric field is only induced by the charges of the reacting flow, Gauss's law, i.e. $\nabla \cdot \boldsymbol{\mathcal{E}} = \rho_q/\epsilon$, gives the scaling $\bar{\mathcal{E}} \sim \bar{\rho}_q \delta/\epsilon$, with δ being the thickness of the flame, where most of the charges are present. From the current's definition, $\boldsymbol{J} = \sigma \boldsymbol{\mathcal{E}}$, we obtain the scaling $\bar{J} \sim \bar{\sigma} \bar{\mathcal{E}}$. Using these two relations, the condition of Eq. (S16) becomes $L\delta\bar{\sigma}\bar{\rho}_q/(\bar{H}\epsilon) \ll 1$. Alternatively, if an external potential is present, $\boldsymbol{\mathcal{E}} = -\nabla\Phi$ and Eq. (S16) becomes $\bar{\sigma}\Delta\bar{\Phi}/\bar{H} \ll 1$, where $\Delta\bar{\Phi}$ indicates the potential difference over the reference length scale L , i.e. $\bar{\mathcal{E}} \sim \Delta\bar{\Phi}/L$. Note that it has been assumed that the current density is dominated by electric drift, while the diffusion of charges and their advection due to the flow are neglected.

Using the above dimensionless numbers, i.e., Eqs. (S14) and (S16), the validity of the magnetostatic solver in the presence of charged species and currents can be estimated.

S2.2. Electrostatics

Similarly to the magnetostatics scaling presented in Section S2.1, we introduce below a dimensionless number for electrostatics. By taking the curl of Faraday's law, Eq. (2), and substituting Ampere's law, Eq. (1), we end up with the wave equation for the electric field in a linear medium (or vacuum), which reads

$$\nabla^2 \boldsymbol{\mathcal{E}} = \mu\epsilon \frac{\partial^2 \boldsymbol{\mathcal{E}}}{\partial t^2} + \frac{1}{\epsilon} \nabla \rho_q + \mu \frac{\partial \boldsymbol{J}}{\partial t}. \quad (\text{S17})$$

Electrostatics requires

$$\frac{\bar{\mathcal{E}}}{L^2} \gg \mu\epsilon \frac{\bar{\mathcal{E}}}{T^2} \longrightarrow T \gg \frac{L}{c}. \quad (\text{S18})$$

From charge conservation, this condition also implies that the term $(1/\epsilon)\nabla\rho_q$ is dominant over the term $\mu\partial\boldsymbol{J}/\partial t$ (same timescale for the time derivative is assumed). The condition ensures that the electrostatic field adjusts almost “instantaneously” to the charge distribution at each time instant.

Another condition for electrostatics and the use of the Poisson equation for the potential is that

$$\nabla \times \boldsymbol{\mathcal{E}} = -\frac{\partial \boldsymbol{B}}{\partial t} \approx 0. \quad (\text{S19})$$

This requires (negligible induced electric field)

$$\bar{\mathcal{E}} \gg \frac{L\bar{B}}{T}. \quad (\text{S20})$$

Assuming that the magnetic field is mainly due to currents (which requires $\bar{\sigma}T/\epsilon \gg 1$), from the Ampère law we can write $\bar{B} \sim L\mu\bar{J}$. Replacing $\bar{J}$ with $\bar{\sigma}\bar{\mathcal{E}}$ gives a dimensionless condition $L^2\mu\bar{\sigma}/T \ll 1$, where the charge density and species mobilities are contained within the electrical conductivity through Eq. (30) of the manuscript. Therefore, the electrical conductivity of the flow must satisfy

$$\bar{\sigma} \ll \frac{T}{L^2\mu} \quad (\text{S21})$$

for the electrostatics assumption to hold. Note that it has been assumed that the current density is dominated by electric drift, while the diffusion of charges and advection due to the flow are neglected.

S3. Results

S3.1. Validation of the electrostatic field implementation

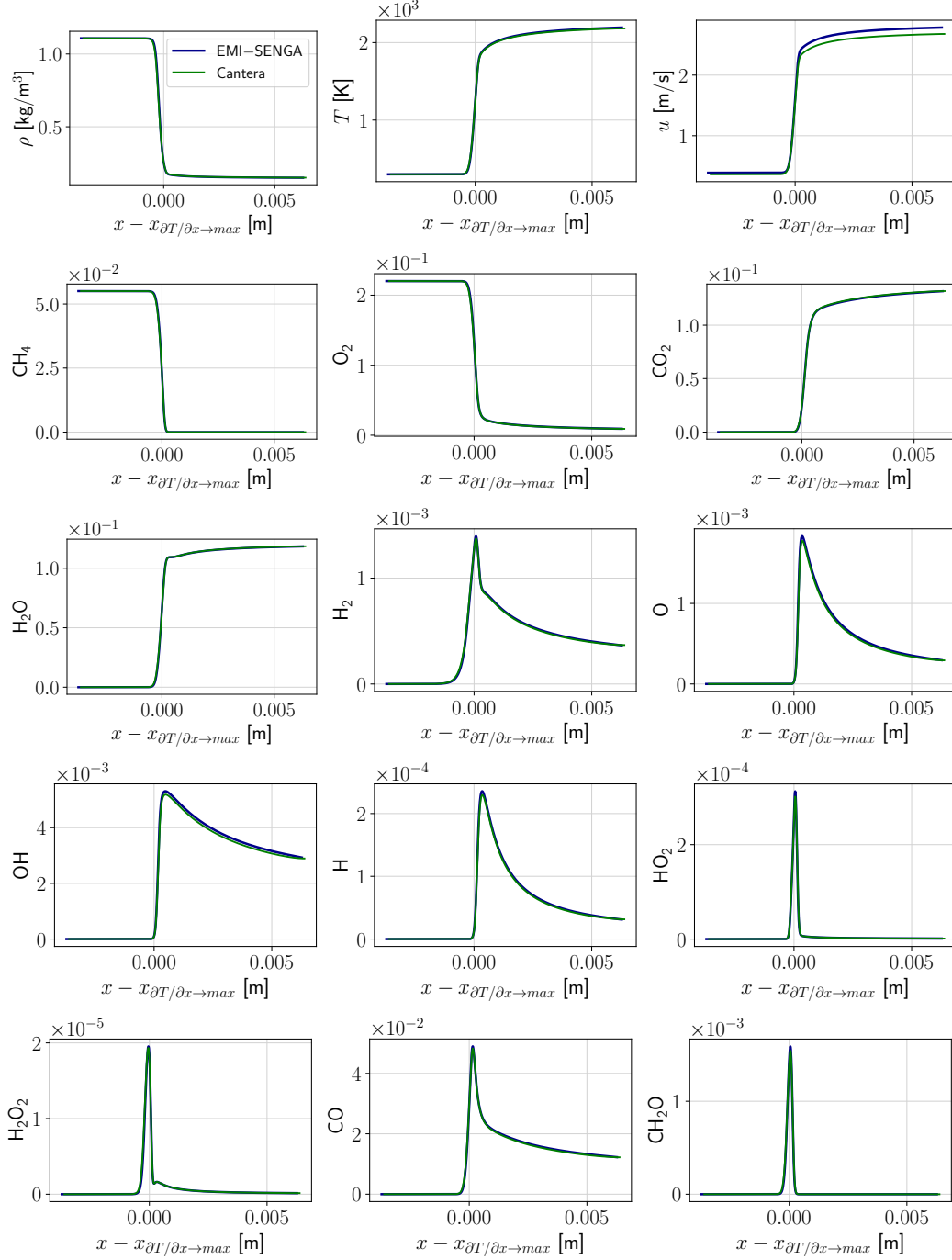


Figure S4: Comparison between Cantera and EMI-SENGA for selected quantities obtained with the ion transport model and with electrostatic interactions activated (continues to Fig. S5). Lines for species correspond to mass fractions.

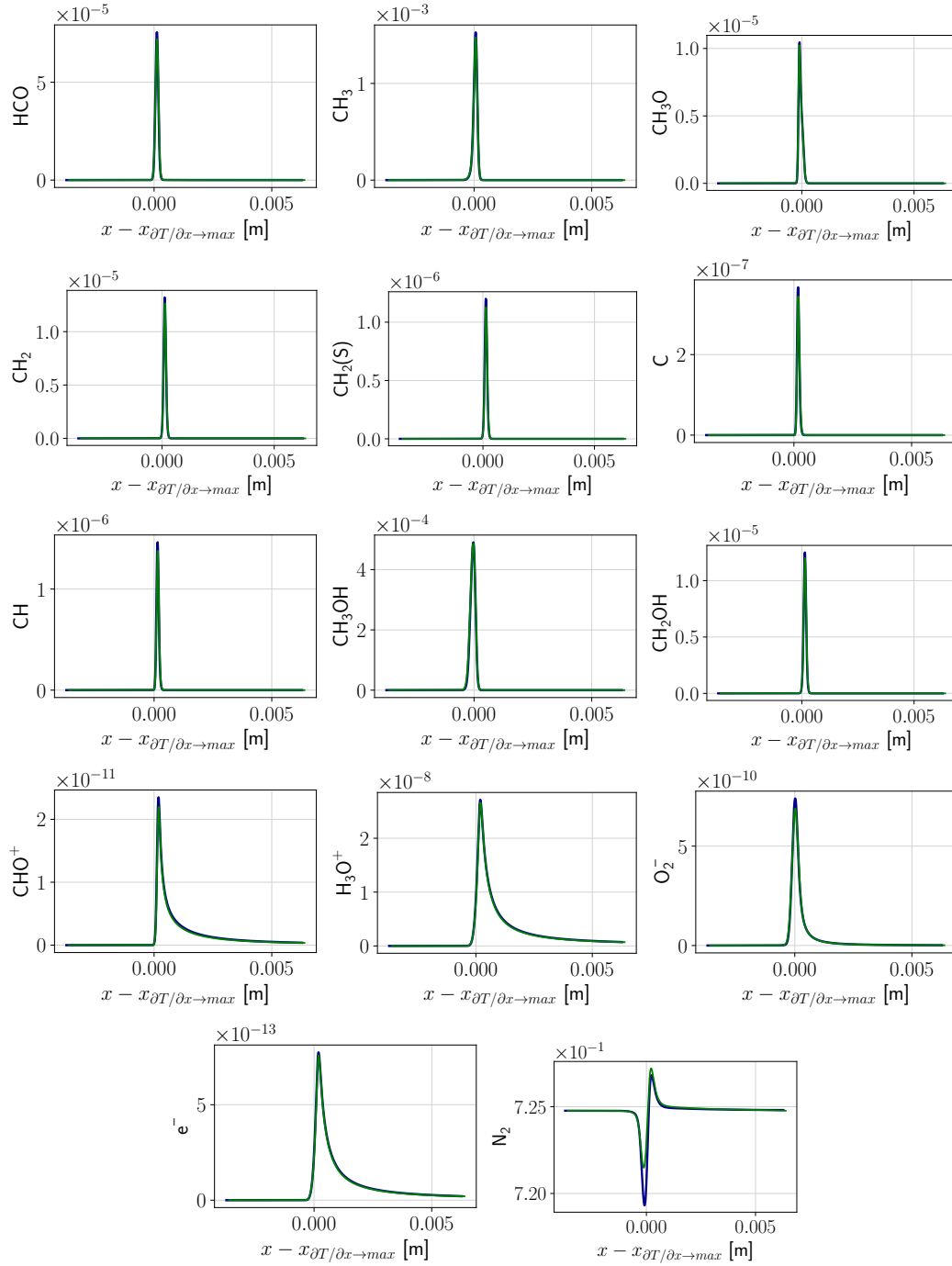


Figure S5: (Continued from Fig. S4) Comparison between Cantera and EMI-SENGA for selected quantities obtained with the ion transport model and with electrostatic interactions activated. Lines for species correspond to mass fractions.

S3.2. 1D laminar reacting flow under electrostatic fields

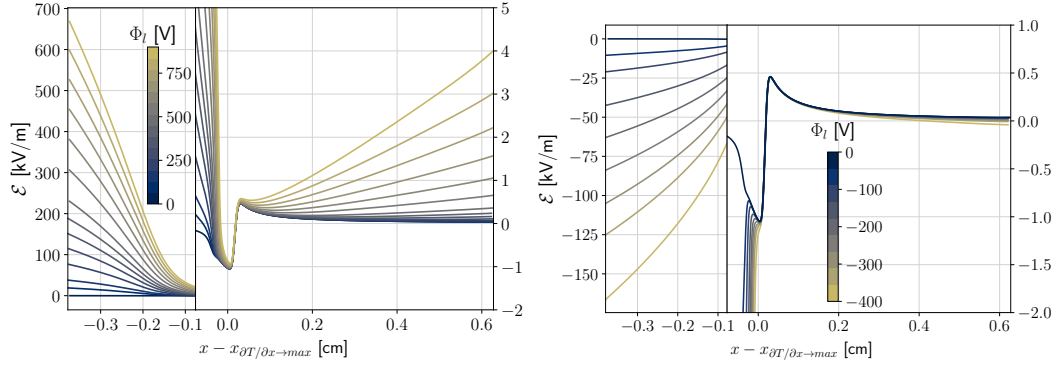


Figure S6: Electrostatic field for a left electrode with a positive (left) and negative (right) voltage. The right electrode is grounded.

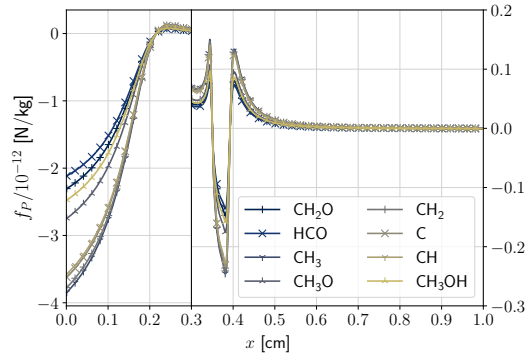


Figure S7: Polarization force on various neutral species for the case with $\Phi_l = 500$ V.

S3.3. 1D laminar reacting flow under magnetostatic fields

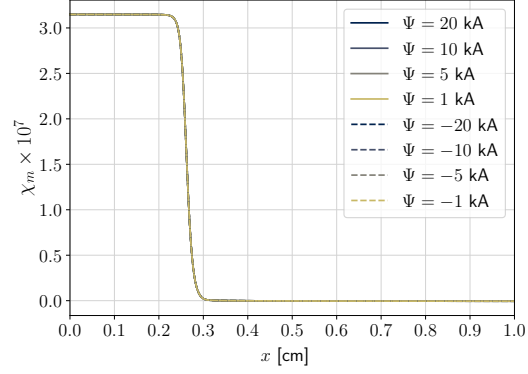


Figure S8: Magnetic susceptibility of the mixture.

S3.4. 2D laminar reacting flow under magnetostatic fields

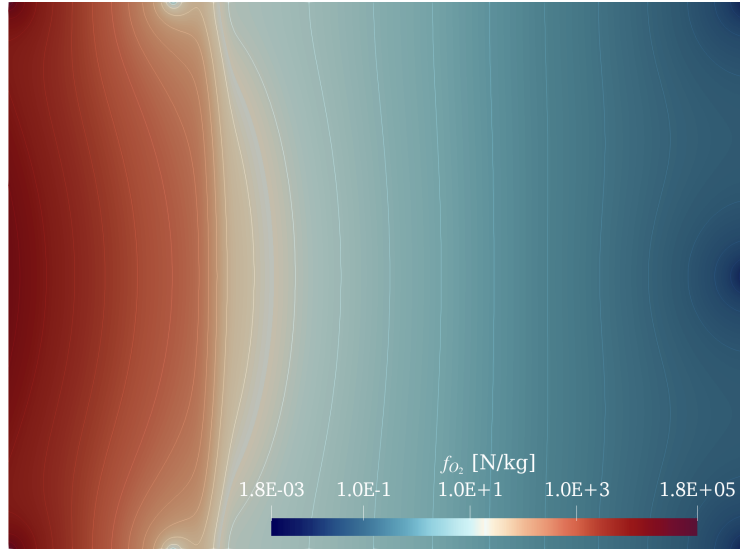


Figure S9: Magnitude of the magnetization force acting on O_2 molecules for the solid line Profile A of Fig. 9 of the main paper.

S3.5. Validation of the EMI-FDTD solver

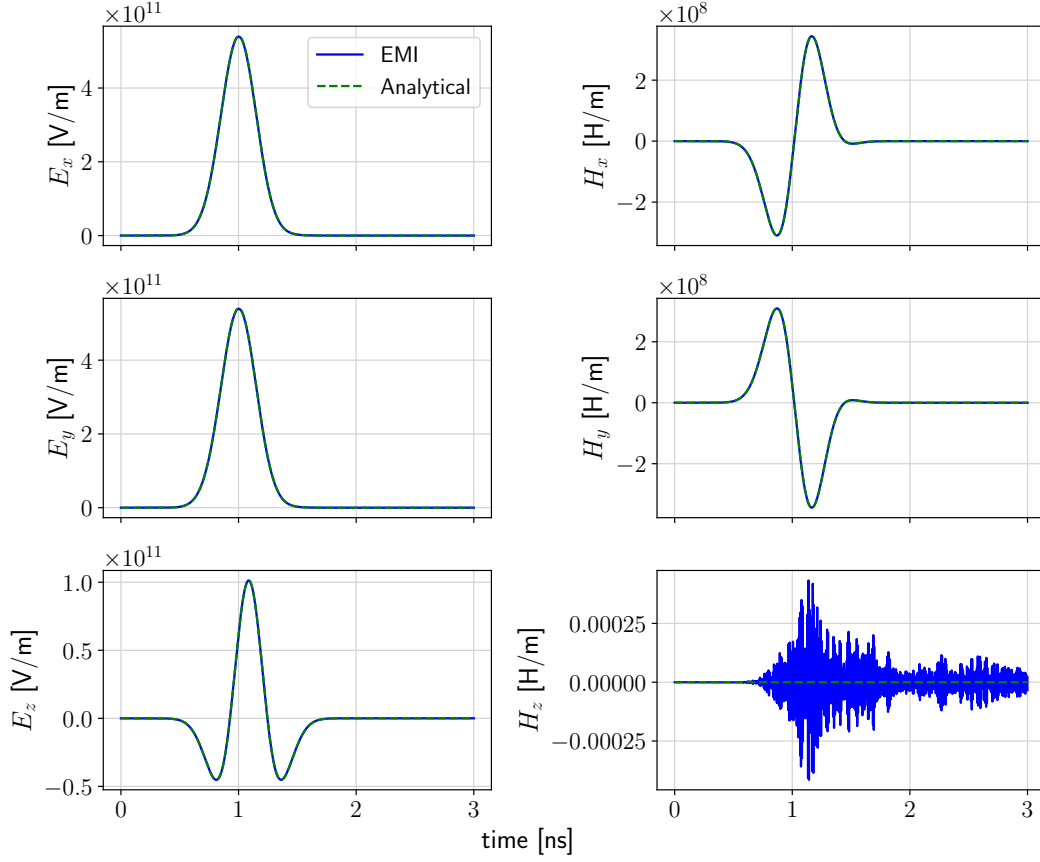


Figure S10: Comparison between EMI-FDTD and the analytical solution of Ref. [23] for a Hertzian dipole source with the current waveform given by the derivative of a Gaussian pulse.

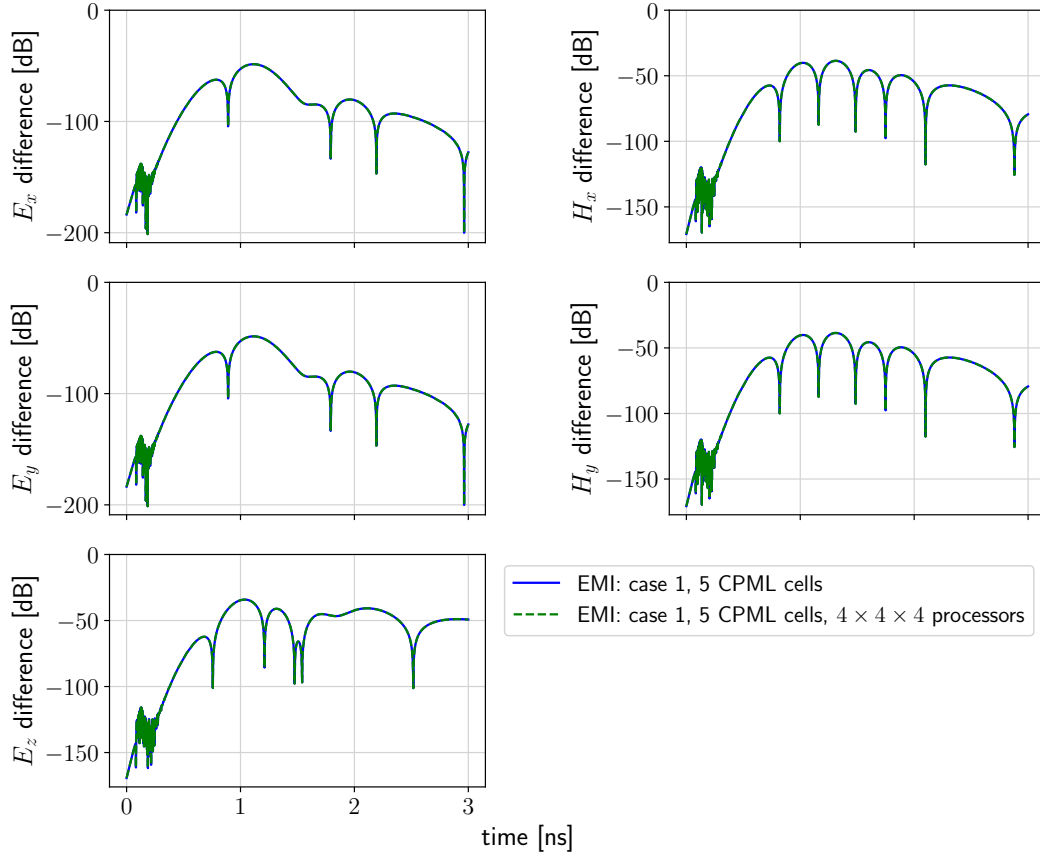


Figure S11: Evaluation of the parallelization strategy of EMI-FDTD.

S3.6. Evaluation of the electrostatic assumption in reacting flows

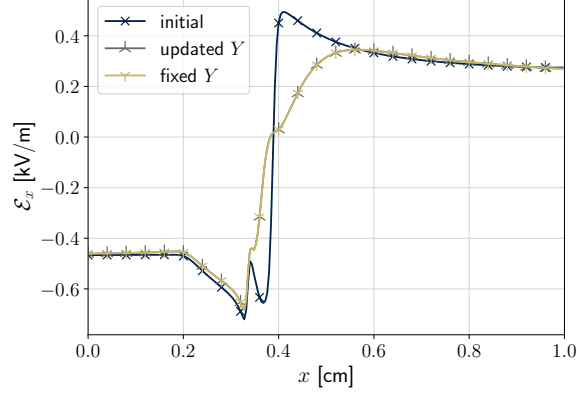


Figure S12: Comparison between the electric field at the beginning of the simulation and at 10 ns of simulated time. The “initial” case corresponds to the Y profile at the beginning of the simulation; “updated Y ” refers to the final profile, obtained after the advancement of the conservation equations solved by EMI-SENGA; and “fixed Y ” is the final profile when the conservation equations are not solved. Results are plotted for a line parallel to the x -direction and passing through the centre of the domain.

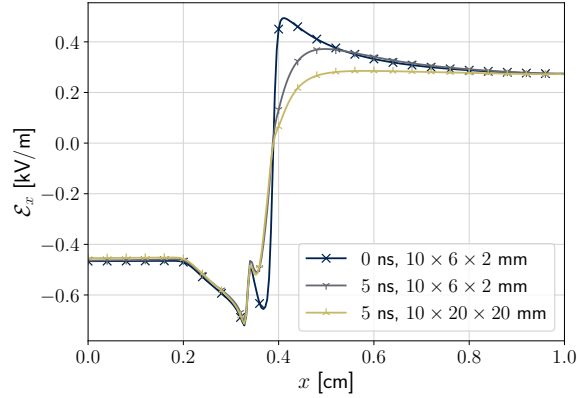


Figure S13: Comparison between the electric field at the beginning of the simulation and at 5 ns of simulated time for the baseline domain and for a bigger domain size. Results are plotted along a line parallel to the x -direction and passing through the centre of the domain.

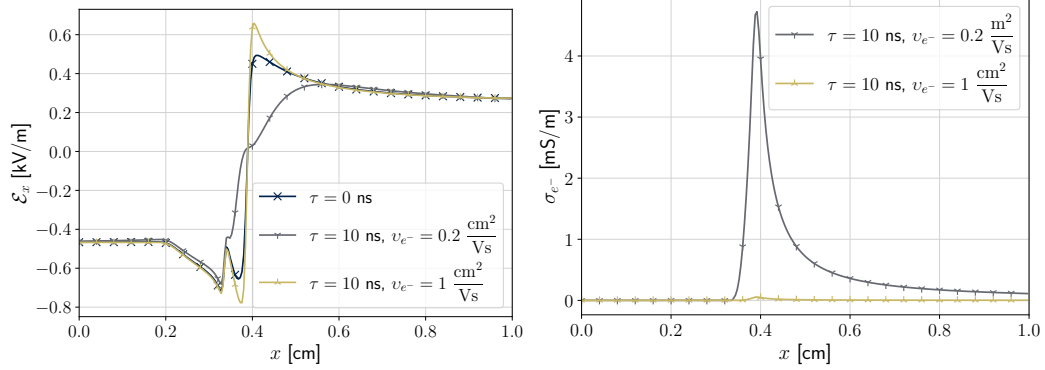


Figure S14: Electric field (left) and conductivity (right) under different electron's mobilities at 10 ns of simulated time.

S3.7. Grid convergence of FDTD solver

To ensure that the 2nd-order staggered grid of the FDTD solver does not affect the accuracy of the solution, we perform a grid convergence analysis. Specifically, we compute the Grid Convergence Index (GCI) according to the methodology detailed in Ref. [24].

A total of 3 different grids were investigated, with dimensions shown in Table S4. The coarse and fine grids have 40% less and more, respectively, number of cells in each direction compared to the standard grid. These grids provide the necessary resolution to accurately compute the GCI [24]. The simulation details are described in Section 3.6 of the paper, where the electron mobility is set to $1 \text{ cm}^2/(\text{Vs})$. The GCI is computed with respect to the two main parameters of interest, the electric field $|\mathcal{E}| = \sqrt{\mathcal{E}_x^2 + \mathcal{E}_y^2 + \mathcal{E}_z^2}$ and the magnetic field $|\mathbf{H}| = \sqrt{H_x^2 + H_y^2 + H_z^2}$.

The GCI results are shown in Table S4. Both GCIs are less than 2%, demonstrating that the grid resolution did not affect the electromagnetic field solution. Therefore, the results suggest that the second-order accuracy scheme used in this study does not affect the accuracy of the electromagnetic field propagation in the investigated configuration. As noted in the paper, stronger electromagnetic field gradients may require a higher-order accuracy.

Table S4: Grid configuration and results for the CGI evaluation.

Grids:			
Grid	Standard	Coarse	Fine
$[N_x, N_y, N_z]$	[250, 150, 50]	[150, 90, 30]	[350, 210, 70]
N_{procs}	125	27	343
Results:			
$CGI_{\mathcal{E}}$	1.39%		
CGI_H	1.87%		

S3.8. Electromagnetic wave sources on reacting flows

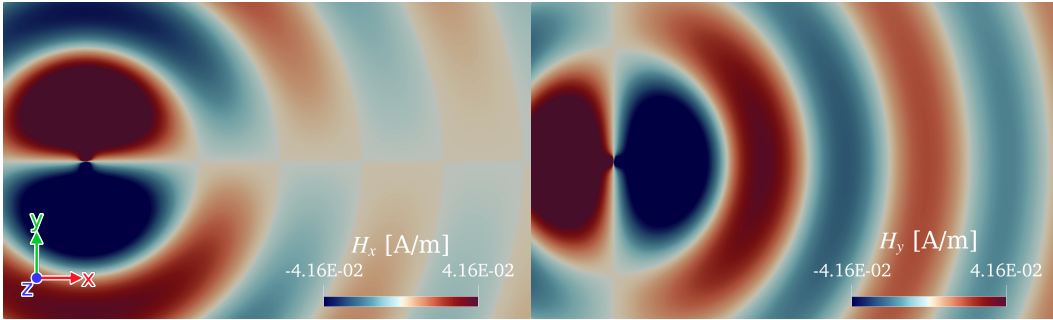


Figure S15: Selected magnetic field components under a sinusoidal wave source at 5 ns of simulated time. The amplitudes of the magnetic field components are an order of magnitude larger than the displayed colormap limits; the limits of the colormap were chosen to allow for the observation of the waveform. The fields are plotted in a slice normal to the z -direction and passing through the centre of the domain.

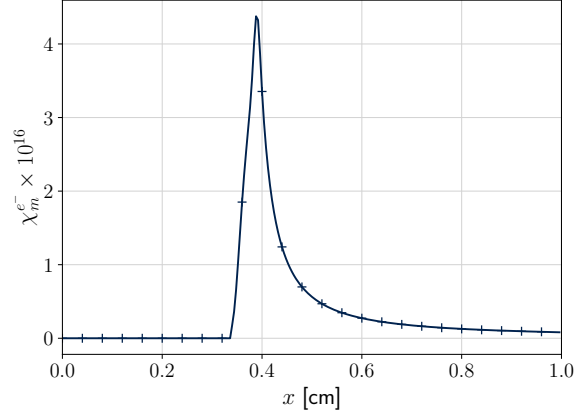


Figure S16: Magnetic susceptibility of electrons along a line parallel to the x -direction passing through the centre of the domain.

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