



# Project 051 Combustion Concepts for Next-generation Aircraft Engines

## Massachusetts Institute of Technology

### Project Lead Investigator

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#### Massachusetts Institute of Technology (MIT)

- P.I.: Dr. Raymond L. Speth
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- Period of Performance: February 5, 2020, to August 31, 2027 (reporting here with the exception of funding level and cost sharing only for the period October 1, 2024, to September 30, 2025)
- Tasks:
  1. Develop a nitrogen oxide (NO<sub>x</sub>) emissions model for a reacting jet-in-crossflow environment
  2. Modeling plasma-assisted combustion for NO<sub>x</sub> emissions reduction in aircraft gas turbines

### Project Funding Level

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### Investigation Team

Dr. Raymond L. Speth, (P.I.), Tasks 1 and 2  
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Yang Chen, (graduate student), Task 1  
Matthew Quiram, (graduate student), Task 2

### Project Overview

With advances in material technology in the past 50 years, aircraft engines with higher pressure and temperature ratios have been designed to improve the engine's total efficiency and reduce fuel consumption. However, the increase in combustor temperatures tends to produce higher NO<sub>x</sub> emissions, which account for a substantial portion of aviation's environmental impact. Therefore, novel low-emissions combustion technologies are needed for the reduction of aircraft engines' emissions, along with the high fuel efficiency of next generation aircraft and engine design.

The objective of the current project is thus to evaluate the performance of various novel combustion concepts in emissions and efficiency. This study would then facilitate the selection of promising high-performance concepts for further development, which would eventually lead to a reduced aviation impact on public health and climate. Throughout the current project, innovative numerical modeling techniques for emissions, combustion chemistry, and combustor internal aerodynamics are developed to enable efficient and accurate evaluation of the performance of different concepts.





The first model currently being developed is a Lagrangian diffusive strip  $\text{NO}_x$  emissions model for a reacting jet-in-crossflow, where the present focus is on integration of the chemistry and aerodynamics component models. This model will offer the benefits of simulating detailed  $\text{NO}_x$  formation mechanism, capturing the emissions impacts from aerodynamics, and a low computational cost for wide-range parametric studies. This technique fills the gap between the traditional modeling methods of chemical reactor network and computational fluid dynamics. Chemistry and flame solvers, including Cantera<sup>1</sup> (Goodwin et al., 2024) and Ember (Speth, 2017) are utilized in this development.

The second concept under investigation is plasma-assisted combustion for low- $\text{NO}_x$ , gas-turbine relevant Jet-A operation. In this work, non-thermal plasma discharges are integrated into combustor simulations to extend lean blow-off limits with the goal of reducing overall  $\text{NO}_x$  emissions. This requires the development of a Jet-A reaction mechanism that is tailored to account for  $\text{NO}_x$  formation and destruction in the presence of plasma. The resulting mechanism will be applied to Cantera-based reactor network and one-dimensional (1D) flame models that can handle the two-way coupling of electron energy distribution and electron impact reactions. By systematically comparing plasma and non-plasma cases, this work aims to identify the operating regimes in which plasma actuation enables leaner combustion with a net reduction in  $\text{NO}_x$ , as well as regimes where plasma is likely to increase  $\text{NO}_x$ .

## References

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- Speth, R. L. (2017). *Ember: a quasi-one-dimensional, unsteady flame solver* (Version 1.4.0). Zenodo, doi: 10.5281/zenodo.1004752. <https://github.com/speth/ember>

## Task 1 – Develop a $\text{NO}_x$ Emissions Model for a Reacting Jet-in-crossflow Environment

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### Objectives

Various emissions modeling techniques are utilized for the development of novel combustion concepts with low  $\text{NO}_x$  emissions. Among these techniques, chemical reactor network (CRN) methods have high fidelity in capturing detailed chemistry and low computational cost, allowing optimizing of a wide range of model design parameters. However, the simulation of aerodynamics effects on  $\text{NO}_x$  emissions, such as flame straining effects or multi-stream mixing effects, have been limited in the CRN approach. The aerodynamic effects in the CRN method are typically represented by different combinations of well-stirred reactors (WSR) that assume complete mixing and plug-flow reactors (PFR) that assume no mixing. Then, a weighted average of WSR and PFR components can be employed to approximate a finite-rate mixing process. This type of CRN representation usually requires a large amount of experimental data for model calibration as the representation lacks aerodynamics constraints. This data requirement of CRN models can thus limit their use in studying novel combustion concepts where little experimental information is available.

As a remedy, reacting-flow computational fluid dynamics (CFD) methods are employed to explore cutting-edge combustion concepts. CFD captures detailed aerodynamic constraints in multi-dimensional space such that aerodynamic effects on  $\text{NO}_x$  emissions can be simulated. However, for a typical Eulerian-grid-based CFD method, this requires a dense computational grid across multiple dimensions, resulting in a high computational cost. This computational cost generally makes only reduced-order chemistry mechanisms affordable for simulating both combustion chemistry and  $\text{NO}_x$  emissions. The reduced-order mechanisms can then undermine the accuracy of the simulations in capturing certain  $\text{NO}_x$  formation pathways like the prompt  $\text{NO}_x$  mechanism. The high computational cost of CFD methods can also limit the number of cases simulated, leading to only a small number of a combustor's design parameters being explorable in a CFD study.

The tradeoff between CFD and CRN methods can be observed in previous studies on  $\text{NO}_x$  emissions in a reacting-jet-in-crossflow (RJICF) environment. An RJICF is a two-stream mixing flow structure with typically one high-speed jet penetrating

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<sup>1</sup> Cantera is an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. Cantera is a sponsored project of NumFOCUS®, a 501(c) nonprofit charity in the United States. NumFOCUS is a registered trademark of NumFOCUS, Inc., Austin, Texas.



nearly perpendicularly into a lower speed crossflow. This flow structure is widely utilized in many low-emissions combustion concepts, such as the quench zone in a rich-quench-lean (RQL) combustor and the injection plate for hydrogen ( $H_2$ ) micro-mixing combustors. The quick mixing in an RJICF, attributable to its complex vortical structures, reduces  $NO_x$  emissions by shorting the high-temperature combustion time or quenching the high post-flame temperature. Previous studies thus investigated how different RJICFs' design features, such as jet momentum ratio and jet diameter, affect the mixing behavior and the subsequent  $NO_x$  emissions. The compromise in performance between a CFD and CRN method can be seen in these studies. CRN-based studies simulated the jet-and-crossflow mixing process with approximations ranging from an instantaneous mixing to a two-step piecewise-constant-rate mixing. However, detailed reaction mechanisms, such as the GRI-series with prompt and thermal  $NO_x$  formation pathways, were used, along with parametric studies across more than 20 test cases. In contrast, CFD-based studies modeled the detailed jet interactions with the complex vortex groups in RJICF, but the chemistry simulations were limited to only two-step reaction mechanisms or flamelet-based tabulated chemistry methods. Likely due to high computational cost, parametric studies with CFD were also limited to around one to five cases. Therefore, there exists value in developing a  $NO_x$  emissions model for RJICF that balances the high-fidelity chemistry available in a CRN with the detailed aerodynamic simulation available in CFD while maintaining moderate computational costs for parametric studies.

A Lagrangian diffusive strip (LDS) method potentially offers a balance between CFD and CRN methods. It is a chemical analogy to the momentum boundary layer method widely used to study the near-wing aerodynamics of an airplane. To capture the mixing process in RJICF, the LDS method models a 1D convection-diffusion-reaction process within chemical boundary layers between the jet and the crossflow. Each chemical boundary layer is then transported by an external flow field, approximated by a potential flow around a simplified representation of the RJICF's vortex groups. Detailed aerodynamic effects on  $NO_x$  formation can then be simulated by the potential flow field straining the  $NO_x$ -producing chemical boundary layers. With the assumption of an inviscid, incompressible external flow field, the computational cost of the LDS method can be dramatically lower than a traditional Eulerian CFD method that defines a computational grid throughout the whole flow domain. To further reduce the computational cost, the three-dimensional RJICF process is reduced to a two-dimensional simulation by assuming pure convection along the jet direction. The chemical boundary layers on the cross-sectional plane perpendicular to the jet centerline can then be integrated starting from the jet's root in a parabolic CFD fashion. The reduction in computational cost from the aerodynamics simplification is then used to accommodate detailed chemistry and a wide-ranging parametric study.

### **Milestones**

- Develop a finite volume formulation for the Ember transient flame solver to ensure conservation of specific quantities of interest.
- Develop an entrainment-dilation model to simulation the two-way coupling effect between the chemical boundary layer and the jet dynamics.
- Develop a chemical boundary layer re-segmentation function to maintain the stability of the simulation through adaptive grid refinement and small flow structure absorption.

### **Major Accomplishments**

- The finite volume Ember chemical solution reduces species conservation error from the original 10% after 10 ms of simulation down to below 0.2%.
- The jet dilation modeling captures the linear growth trend of the jet width for a free jet problem.
- The multi-segment merging and remeshing process allows stable jet simulation to 1 ms, capturing the major region of interest for  $NO_x$  emissions estimation.

### **Publications**

None.

### **Outreach Efforts**

Results were presented to the FAA ASCENT Project Manager during regular bi-weekly teleconferences.

### **Awards**

None.



## **Student Involvement**

This task was conducted by Yang Chen, working under the supervision of Dr. Jayant Sabnis and Dr. Raymond Speth.

## **Plans for Next Period**

- Incorporate the Ember chemical solver into the model to enable NO<sub>x</sub> emissions modeling after the non-reacting simulation of the RJICF model.
- Complete further model validation for the determination of correct vortex dynamics in the external flow and the correct heat release physics.

## **Task 2 – Modeling Plasma-assisted Combustion for NO<sub>x</sub> Emissions Reduction in Aircraft Gas Turbines**

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### **Objective**

Plasma-assisted combustion (PAC) has been shown to improve ignition and extend lean blow-off (LBO) limits in a range of fuel and combustor configurations (Pilla et al., 2006; Lacoste et al., 2013). In most practical implementations, plasma actuation is delivered through nanosecond repetitively pulsed discharges that deposit high electric field bursts on nanosecond-timescales driving non-thermal electron-impact chemistry. Several studies suggest that this electron-impact chemistry contributes to additional pathways for the formation of NO<sub>x</sub> (Xiong et al., 2019). In certain cases, this may outweigh the NO<sub>x</sub> benefits of leaner operation. Other experiments have demonstrated that it is possible to reduce NO<sub>x</sub> relative to a non-plasma baseline under specific operating conditions and discharge parameters (Shashavari et al., 2023). Thus, PAC's impact on NO<sub>x</sub> is an open design question, and a predictive modeling approach is needed to navigate this trade space.

Current PAC modeling work has focused on simple fuels (e.g., methane, hydrogen, or ammonia), which have an abundance of experimentally verified reaction data. However, the relevant fuel for practical aircraft turbine applications is a kerosene-like aviation fuel, and the goal of this work is to assess whether PAC can be used in a realistic combustor geometry and mission profile to lower net NO<sub>x</sub> emissions when both plasma-generated NO<sub>x</sub> and the benefits of leaner operation are taken into account. Addressing this question requires a modeling approach that combines a reduced Jet-A reaction mechanism tailored to NO<sub>x</sub> formation and destruction in the presence of non-thermal plasmas, with a two-way coupled representation of the electron energy distribution and plasma chemistry that can be used in reactor network and 1D flame models.

In this task, we build on previous development of plasma reaction capabilities within our primary combustion modeling tool, Cantera, and implement an electron energy distribution function (EEDF) computation using a two-term approximation of the Boltzmann equation. This allows the EEDF to evolve self-consistently with the gas state and provides more reliable electron-impact rate coefficients for reactions which contribute to NO<sub>x</sub> formation and destruction under the conditions relevant to aircraft gas turbines.

In parallel, we will develop a plasma-augmented reaction mechanism for a representative Jet-A surrogate that is specifically designed for zero and 1D NO<sub>x</sub> and PAC studies. Experimental electron-impact cross-sections and rate coefficients for reactions involving hydrocarbons larger than methane are sparse. Many of these must therefore be derived from scaling laws and, where these models are unavailable, emulate plasma discharge effects by applying calibrated multipliers to surrogate reactions. The mechanism will retain the reduced structure necessary for tractable reactor-network and 1D flame calculations, while incorporating additional excitation, ionization, dissociation, and quenching processes that are known to influence combustion properties and NO<sub>x</sub> formation and destruction.

Our team began by evaluating how combustion and plasma discharge parameters (e.g., equivalence ratio, inlet temperature, residence time, pulse frequency, and reduced electric field) affect NO<sub>x</sub>/carbon monoxide (CO) emissions in a simple well-stirred reactor for the aforementioned reaction mechanism. Building on the insights gathered from the well-stirred reactor model, we then extend the analysis to reactor network representations of staged combustor architectures to evaluate the effect of PAC on engine conditions representative of realistic operations (i.e., idle, approach, cruise, and takeoff). This would allow for the identification of the most favorable operating conditions and plasma discharge parameters.



Complementary 1D flame simulations can be used to resolve the local structure of PAC-stabilized flames, with and without plasma, to understand where and when  $\text{NO}_x$  is produced within the flame and post flame region. These calculations will clarify how pulsed discharges modify temperature profiles, radical pools, and residence times in high temperature zones, and how these changes translate into both LBO extension and  $\text{NO}_x$  trends. The combination of reactor networks and 1D flame models enables us to connect local plasma flame interaction physics to overall combustor emissions in a way that is directly relevant to engine design.

The aim of this work is to create combustion models that can quantify the trade-offs between plasma enhanced lean operability and  $\text{NO}_x$  emissions across the aircraft operating envelope. As well as the ability to determine the combinations of plasma and combustion parameters where plasma actuation offers a potential  $\text{NO}_x$  reduction benefit and where it is unlikely to be advantageous.

### **Milestones**

- Successful Implementation of two-term Boltzmann equation approximation in Cantera.
- Creation of a computationally stable reduced Jet-A- $\text{NO}_x$ -plasma reaction mechanism, built on the HyChem “A2NO $_x$ ” skeletal mechanism (Saggese et al., 2020).
- Adaptation of RQL combustor model to implement pulsed discharges in the primary zone.
- Creation of a well-stirred reactor simulation to evaluate  $\text{NO}_x$  production using various plasma discharge and combustion parameters.

### **Major Accomplishments**

- Validation of Cantera Boltzmann solver functionality against results from Pavan (2023).
- Functionality of Jet-A- $\text{NO}_x$ -plasma reaction mechanism within a well-stirred reactor with pulsed plasma discharges.

### **Publications**

None.

### **Outreach Efforts**

None.

### **Awards**

None.

### **Student Involvement**

This task was conducted by graduate student Matthew Quiram working under the supervision of Dr. Raymond Speth.

### **Plans for Next Period**

- Continue using the well-stirred reactor model to evaluate which combinations of plasma and combustion parameters may provide the greatest emissions benefit compared to the non-plasma baseline.
- Create a zero-dimensional reactor network simulation using a combustor architecture representative of an aircraft gas turbine that could use plasma assisted combustion to extend its LBO limit.
- Use the insights gathered from the well-stirred reactor simulations to help determine parameters and engine operating conditions which may provide a net reduction in  $\text{NO}_x$  emissions.

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