Lagrangian Particle Tracking Analysis of NO_x Emissions in Rotating Detonation Engines

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1 Abstract

NO_x emissions behavior was explored in high-fidelity simulations of RDEs using a simplified NO_x chemistry mechanism and Lagrangian Particle Tracking techniques. Simulations were performed with a Radial Air Inlet (RAI) RDE design using gaseous hydrogen for fuel and air for oxidizer. Particle properties within the combustor revealed a strong dependence of NO_x emissions levels to temperature, with significant NO_x production occurring only after an approximate temperature threshold of 1300 K was reached. Additionally, particles that aged while moving axially through the combustor appeared to increase their average temperature and subsequently their NO_x levels, whereas aging particles constrained near the chamber bottom experienced milder temperatures and NO_x production on average. A clear relationship between NO_x, temperature, and pressure was also seen in the data, with increasingly higher temperatures and pressures (indicative of locations close to the detonation wave) leading to higher NO_x levels. Overall, this analysis provides deeper insight into how fluid parcels experience flow behavior through detonative combustion in RDEs from the Lagrangian perspective and how this ultimately affects NO_x emissions in such systems.

2 Introduction

Modern combustion research has recently focused heavily on the concept of Rotating Detonation Engines (RDEs) due to their theoretical propensity to deliver up to 20% greater efficiency over traditional propulsion devices [1]. RDEs include a detonation wave propagating around an annular chamber consuming and burning fuel/oxidizer mixture for energy release. This energy release increases the dynamic pressure of the fluid to allow for greater expansion and work extraction from the system while also fueling the continued propagation of the detonation wave. The compact energy release RDEs provide [2] along with their capability to increase thermodynamic efficiency [3] make them viable options for power generation applications [4]. Emissions are also of great importance for such applications, specifically the emissions of nitrogen oxides or NO_x.

The unique detonation flow structure in RDEs is fundamentally different from the purely deflagrative processes seen in traditional gas turbines. Large fluctuations in temperature and pressure arise from the

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presence of detonation waves, and residence time within high temperature regions becomes an important factor for emissions mitigation due to the extreme sensitivity of NO_x to temperature. Past studies of a premixed 2D ideal RDE [5] show that although the extreme conditions within RDEs could possibly constitute higher emissions levels, only minor NO_x levels were observed with shorter residence times at high temperatures helping to reduce emissions. However, this study does not take into account the non-idealities incurred by practical RDEs from the separate injection of fuel and oxidizer, which can include high variability in local equivalence ratios and parasitic combustion [6, 7]. The non-premixed nature of practical RDEs, a necessary feature included to avoid flashback of detonations into fuel and oxidizer manifolds [2, 3], amplifies the importance of the injection process in defining overall RDE operation [8]. As such, if NO_x emissions are to be studied in RDE systems, the effect that non-idealities have on emissions becomes an important consideration.

This study explores the patterns of NO_x emissions in practical RDEs using an Eulerian numerical approach with the inclusion of Lagrangian Particle Tracking (LPT). LPT tracks fluid parcels and their properties as they move through the combustor, allowing for greater insight into how the parcels are affected by specific changes in flow characteristics. Within the context of RDEs, LPT allows for better understanding into how different fluid elements interact with detonation waves as they progress through the combustion process, as well as giving better insight into the relationship between NO_x formation, temperature, and residence time. The case ran in this study involves the use of a hydrogen-air mixture at stoichiometric conditions with a Radial Air Inlet (RAI) RDE configuration from the Air Force Research Laboratory (AFRL) [9]. High-fidelity numerical simulations using multi-step chemical kinetics are employed on this case to characterize NO_x emissions in RDEs. The next section provides further details of the configuration and numerical methods used.

3 Simulation Configuration Details

3.1 Configuration

The RDE configuration used in this study is the AFRL RAI RDE which is shown in Fig. 1. It contains 120 equally spaced discrete fuel injectors along with a continuous radial air injection slot around the annulus of the detonation chamber. This specific design has a 0.3 inch combustor annular gap and a 0.069 inch air injector gap. The main case ran in this study involves an air mass flow rate condition of 320 g/s at the air plenum inlet plane and a fuel mass flow rate of 9.3 g/s at the fuel plenum inlet plane. These flow rates are set so as to keep the global equivalence ratio at 1 for stoichiometric injection of hydrogen-air mixture.

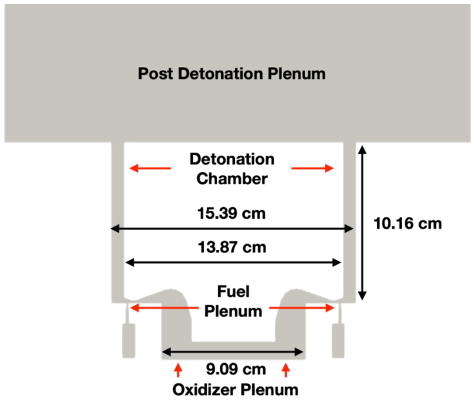

Figure 1: Cross-section schematic of AFRL RAI RDE configuration.

3.2 Numerical Approach

A high fidelity numerical approach is taken for the simulation in this study, wherein the conservation of mass, momentum, and energy equations, along with species conservation equations, are solved and the model is closed by the ideal gas equation of state. All boundary conditions involve adiabatic, no-slip walls, with a constant mass flow rate boundary condition imposed at the fuel and oxidizer inlet planes. Cantera [10] is used for the calculation of chemical kinetics, and a 13 species, 32 reaction modified Jachimowski mechanism is used to represent H_2-Air-NO_x chemistry [11]. The solver is a modification of the UMdetFOAM solver from the Advanced Propulsion Concepts Laboratory (APCL) at the University of Michigan (UM), which has been previously validated for a range of flows pertinent to RDE flow behavior [12]. Second order HLLC+MUSCL, second order Runge Kutta, and KNP are used for the spatial, temporal, and diffusion schemes respectively. LPT is implemented into the solver for the purpose of tracking fluid element properties through space and time during the course of the regular Eulerian phase simulation. Particle properties are set so that the particles are mass-less and therefore do not affect the underlying Eulerian flowfield in any manner. In this way the particles assume no drag, are perfectly elastic, and take on the underlying Eulerian velocity field directly, resulting in an instantaneous particle response to fluid changes and a Stokes number of essentially 0. The underlying unstructured mesh contains 2×10^{-4} m resolution in the detonation chamber, resulting in roughly 48×10^6 control volumes in the overall mesh.

The simulation is initiated from a quasi-steady state of statistically stationary combustion in the RDE using H_2-Air-NO_x chemistry. Roughly 5000 particles are injected over the course of two wave cycles (0.48 ms), with the bulk of particles randomly injected along a radially-facing ring at a radius of 0.06 m inside the air injection slot and additional particles randomly injected at the exit planes of fuel injectors entering the detonation chamber. Particles assume the underlying Eulerian flow velocity of the cells in which they reside, and additional properties such as temperature, pressure, and the like are tracked at these particle locations and recorded at an interval of 0.01 ms.

4 Results

4.1 Lagrangian Analysis of NO_x Formation in RDEs

Lagrangian particle properties plotted against axial position and residence time within the combustor are shown in Fig. 2. The particles plotted here are ones that have aged at least 1 full cycle (0.24 ms) after injection. It is seen here that the longer the particles reside in the combustor the temperatures they experience become higher in general. This result stands to reason, as the data shows particles that have aged for at least 1 full cycle, so the particles should have experienced some effect of the detonation wave and resulting combustion process. In addition, most of the particles that initially experience high temperatures within the detonation chamber begin to move axially towards the exit of the chamber shortly thereafter. This behavior is also expected, as the product gases should expand axially after being processed through detonation waves. The interesting discovery from this data, however, is that the intensity of NO_x is tied to a rather linear relationship between axial position and residence time. In other words, as NO_x is formed within the RDE it mostly ages with increasing axial position towards the exit and doesn't accumulate as much near the bottom of the detonation chamber. As such, formation of NO_x is seen to be activated by high temperatures from detonation processes and then it exits the detonation chamber thereafter.

With regards to how promptly the particles exited the chamber, 31.3% of particles aging at least 1 full cycle exited the combustor within the full 2 cycles of simulation time, whereas 55.4% of particles made

it at least halfway axially through the combustor and 13.3% didn't make it halfway axially. These statistics confirm the strong influence of axial expansion seen in product gases behind the detonation waves, as not many particles remain constrained near the chamber bottom through at least 1 full cycle. The particles that are constrained near the chamber bottom also experience generally lower temperatures and NO_x levels, with average temperatures and NO_x levels here amounting to 71.5% and 56.5% of the average values seen in particles reaching the combustor exit respectively. This indicates that the gases constrained near the chamber bottom while also aging for at least 1 cycle are most likely products of incomplete combustion, either representing partially burned or unburned reactants at cooler temperatures than product gases that experienced more complete combustion.

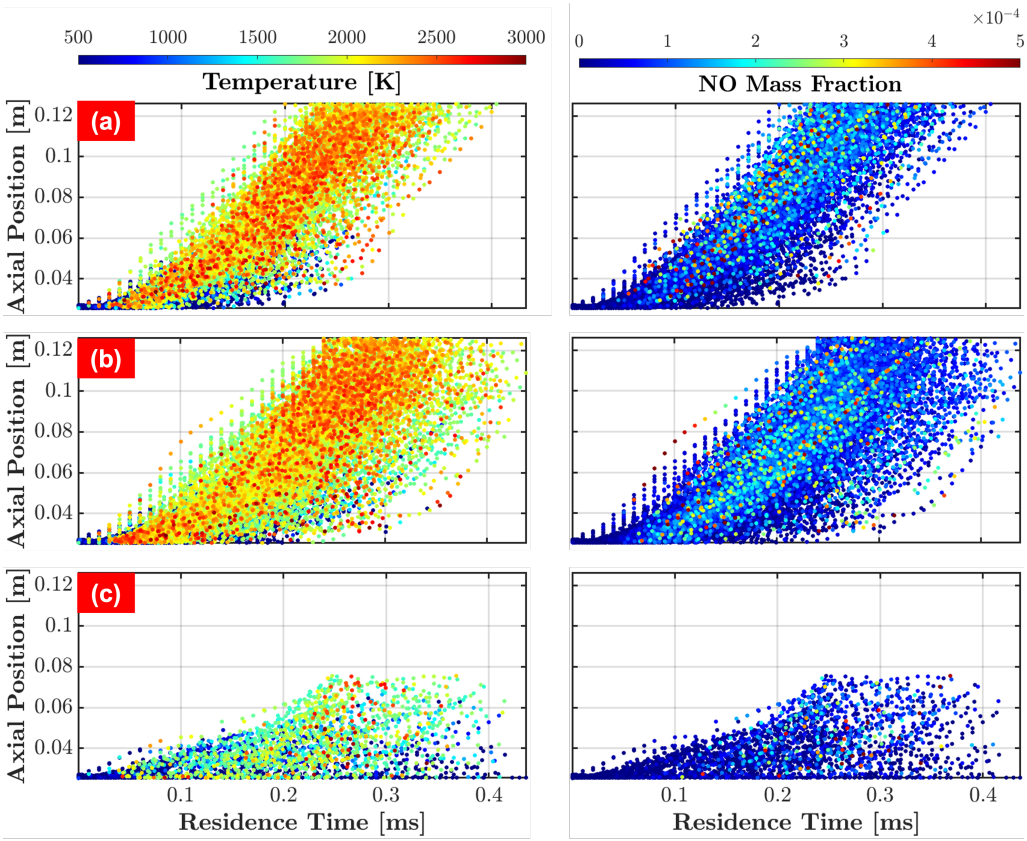

Figure 2: Temperature and NO mass fraction for particles experiencing at least 1 full cycle of residence time (0.24 ms) divided into particles that have (a) axially reached the exit plane of the combustor, (b) axially reached between the midpoint and exit plane of the combustor, and (c) did not axially reach the midpoint of the combustor.

Figure 3 shows temperature, pressure, and NO mass fraction at all recorded positions for all Lagrangian particles. A strong correlation between temperature and NO mass fraction is seen, with NO_x levels rising dramatically after a certain temperature threshold is met. This threshold appears to have two levels, with an initial spike in NO_x seen at roughly 1300 K and another spike in NO_x seen at roughly 1700 K. Emissions levels remain steadily high above this temperature. Considering that the average temperatures of the particles making it at least halfway axially through the chamber are above 1300 K and average NO_x levels are highest here, this threshold value makes sense. The inverse of this result is also true, with particles not reaching the axial midpoint of the chamber experiencing average temperatures below 1300 K and lower resulting NO_x levels. Another interesting observation from the plot is the relationship between temperature and pressure. For higher temperature particles the pressure becomes

increasingly higher, leaving an empty space at the bottom right corner of the plot indicating no particles experiencing extremely high temperature, low pressure conditions. As temperature values continue to increase, pressures seem to rise exponentially and NO_x levels remain high. These extreme temperature and pressure conditions are indicative of conditions near the detonation front and signal immediate NO_x production within the detonation wave itself. The particles that still maintain relatively high NO_x levels as temperature and pressure are lowered and fall into a more linear relationship most likely reside in the post-detonation region where product gases begin expanding and deflagrative processes continue. This region of higher temperatures (1700 K to 2500 K) and lower pressures seems to contain the majority of high-NO_x particles, which further suggests that these particles reside in the post-detonation region as opposed to near the detonation front since the azimuthal length of the post-detonation region is much longer than that of the detonation wave itself and thus contains more particles. The steadily high NO_x levels across the entire range of high temperatures and varying pressures, however, suggests initial formation of NO_x within the detonation wave, followed by either additional NO_x formation in the post-detonation region from deflagrative processes or simple axial transport of the initially formed NO_x during product gas expansion.

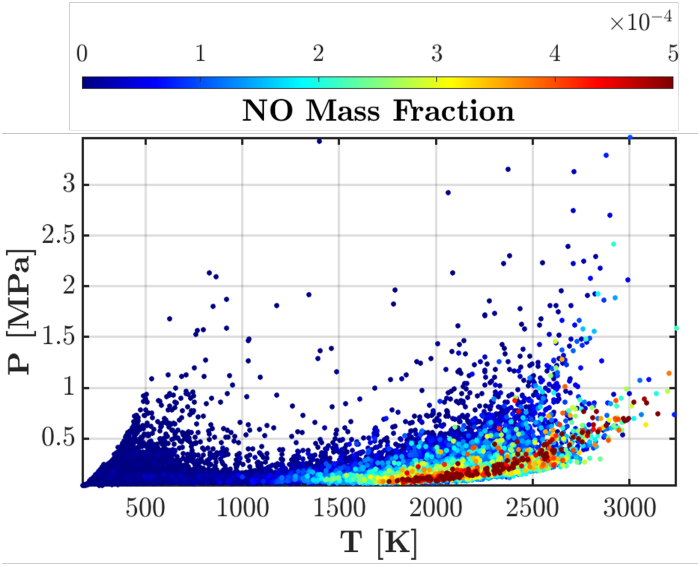

Figure 3: Pressure vs temperature colored by corresponding NO mass fraction for all particle measurements.

5 Conclusions

One main case was studied to evaluate NO_x production in a Radial Air Inlet (RAI) RDE configration within the context of Lagrangian Particle Tracking (LPT) analysis. Stoichiometric hydrogen-air conditions were used along with a simplified NO_x chemistry mechanism that primarily described thermal NO_x production. Constant mass flow rate boundary conditions of 320 g/s oxidizer flow and 9.3 g/s fuel flow were used which provided flow characteristics of 1 wave in the system with a cycle time of roughly 0.24 ms.

The results showed that NO_x production was tied to two major parameters, temperature and residence time in the combustor. Most particles aging through 1 full cycle reached at least halfway axially through the combustor and experienced high enough temperatures to activate NO_x production, generally after a threshold temperature of 1300 K was reached. Particles not reaching the halfway point axially after at least 1 cycle were considered to be partially burned or unburned reactants and had lower resulting

temperatures and NO_x levels. The obvious connection between temperature and NO_x was also seen, with an additional correlation between temperature and pressure signaling locations where detonation waves resided. NO_x remained high in these areas due to the sudden increase in temperature and pressure activating chemical reactions to allow it to form.

Future work seeks to expand Lagrangian analysis of NO_x emissions in RDEs to multiple geometric cases with varying operating parameters. This will allow for clearer relationships to be formed between how RDEs are setup and the effect these setups have on emissions levels. Additionally, future work looks to refine the particle tracking method used so that more properties can be tracked and better statistics can be calculated from injecting greater amounts of particles. Lastly, more detailed descriptions of NO_x chemistry would like to be used to observe the role minor NO_x formation pathways have in the combustion process for RDEs.

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