

Towards Modeling Exhaust Gas Emissions from Rotating Detonation Engines

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1 Introduction

ENGINES based on the inherent higher thermodynamic efficiency of the detonation cycle have been desirable for many years. Within the last 15 years, there has been a considerable amount of research into developing engines utilizing detonation waves for air-breathing propulsion, to the point where practical propulsion engines are being developed and tested¹. A promising detonation propulsion concept is the Rotating Detonation Engine, or RDE. The RDE is a type of Continuous-Detonation-Engine (CDE), where the detonation is initiated once and remains while the engine is running. It uses an annular ring combustion chamber. A premixed or non-premixed gas is injected axially at the head-end of the combustion chamber, combusted through a detonation wave that propagates circumferentially around the chamber, and then is exhausted out the far end of the chamber. The RDE has several attractive features compared with other detonation engine concepts, however, it does have technical challenges. For instance, at start-up, a detonation wave must be initiated in a single direction, whereas most initiators will propagate a detonation wave in both directions from the initiation site. Since the detonation wave continually runs near the head-end section of the combustion chamber, the inlet micro-nozzles are subjected to intense pressures and temperatures which may limit their life, or cause back flow into the mixture plenum. Conditions within the combustion chamber, too, are less well understood than conditions within a Pulse Detonation Engine (PDE), so that designing a combustion chamber to withstand the forces and heat-fluxes typical in an RDE may be more problematic. The exhaust gas flow and more specifically, the emissions from these engines is an area that has not received much attention. This is the specific topic of interest of the investigation reported in this paper.

The feasibility of the RDE has been experimentally shown at the Lavrentyev Institute of Hydrodynamics². Additionally, there have recently been several numerical investigations into RDEs³⁻⁷ as well as experiments with different configurations⁸⁻¹¹ for both hydrogen and hydrocarbon fuels. The numerical investigations have typically been two-dimensional with hydrogen-air or hydrogen-oxygen, although preliminary three-dimensional results have also been demonstrated⁵. The numerical studies have focused on an overall description of the flow-field within an RDE combustion chamber^{3,6}. The experimental studies have been focused mainly on mapping out operational regimes for different configurations, however, more recent setups may allow for more detailed study⁹. We have developed a similar code for simulating two-dimensional and three-dimensional RDE combustion chambers using the same algorithms that have been applied very successfully for our PDE and general detonation research¹²⁻¹⁷. Previous results from this code have examined the role of plenum pressure and back pressure on performance^{18,19}, basic combustion chamber geometry on performance²⁰, and the effect of the injection system on the fill region and pressure feedback²¹.

A basic RDE is shown in Figure 1. The combustion chamber is an annular ring, where the mean direction of flow is from the head end (bottom in figure) to the exit plane (top). The micro-nozzles flow in a premixture of

fuel and air or oxygen, and a detonation propagates circumferentially around the combustion chamber consuming the freshly injected mixture. The gas then expands azimuthally and axially, and can be either subsonic or supersonic, depending on the back pressure at the outlet plane. The flow has a very strong circumferential aspect due to the detonation wave propagation. Because the radial dimension is typically small compared to the azimuthal and axial dimension, there is generally little variation radially within the flow. The RDE can thus be “unrolled” into two dimensions in many circumstances. The main features of an RDE have been discussed previously in our papers¹⁹ and have also been discussed by others⁷, and so will not be summarized here. More detailed analysis of the flow-field from our simulations has also been conducted to better understand thermodynamics and energy transfer within the RDE combustion chamber^{23,24}.

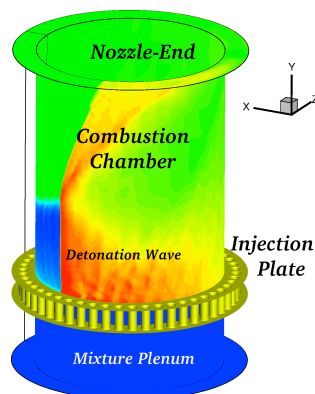


Fig 1. Representative three-dimensional solution in a Generic RDE device.

Similar to the PDE, one of the main features of an RDE is that the outflow is unsteady. Unlike the PDE, however, this unsteadiness is at a much higher frequency and appears much better behaved than a PDE. To obtain optimum performance, understanding how this unsteadiness interacts with either turbine blades or with the nozzle is essential for realizing the potential of the RDE. This paper presents preliminary work on understanding the exhaust plume of a baseline RDE, and how this exhaust plume effects the flow field inside the RDE. First we compare simulations with and without an exhaust plenum added to the simulation, to help validate the RDE model and boundary conditions used in previous simulations. Second, the plume is characterized for several different configurations, and last, a conical nozzle is attached to the centerbody to investigate the effect on the plume and RDE flow field. In the short term, being able to model the exhaust plume may help to validate this and other RDE models since the exhaust plume is much easier to experimentally quantify than the flow inside the RDE combustion chamber. Longer term benefits include understanding how to design an appropriate turbine or nozzle to handle the unsteadiness in the RDE. Some previous work has been done on RDE nozzles by Yi *et al*.²⁵ Our main focus of this work is not on specific nozzle shape or design, but more on characterizing the effect of a large exhaust plenum on the combustion chamber flow and RDE exhaust characteristics. In addition, the chemistry model is modified so that the late-time recombination kinetics and its impact on exhaust gas emissions can be estimated.

2 Rotating Detonation Engine Model

The current focus of numerical work is on extending the flow-field from the RDE combustion chamber to the exhaust plenum. The annular combustion chamber of an RDE is characterized by an inner and outer diameter D_i and D_o and a chamber length, L . For the injection wall, premixed hydrogen-air is injected into the combustion chamber at the head-end or injection face through very small micro-injectors. We specify an area ratio between the total micro-injector throat area and the total injector face area, $a = A_i / A_w$. For this work, all the RDE simulations are three-dimensional simulations. An exhaust plenum has been added to the end of the combustion chamber domain. The head-end of the exhaust plenum, as well as the sides, are all inviscid walls, and the exhaust end of the plenum has far-field boundary conditions. The walls are placed far enough from the combustion chamber so as not to effect the RDE exhaust characteristics.

The conservation equations solved in both the combustion chamber and exhaust plenum are the standard Euler equations, with an additional conservation equation for reactant. For this work, we use the ideal injection source term described in detail in Ref. 21. While not as accurate as modeling the injectors directly, this provides

us with a steady and stable injection system where the general time-averaged features match nicely with more detailed injection studies. This allows us to focus more closely on the exhaust plenum.

3 Solution Procedure

We base the solution procedure on two different codes developed in house at the Naval Research Laboratory. The first code, RDE3D, has been used extensively for the previous RDE simulations, and has been shown to produce good results for the combustion chamber geometries that have been studied to date. The second code, RDEPlenum3D, is a new code based on the same solvers as the RDE3D code, but solves separate domains for the combustion chamber and the plenum and links them together through interpolation in an overlap region. This gives us a great deal of flexibility in specification of the grids for the RDE and plenum, while introducing only minimal errors through the interpolation.

The solution procedure for the conservation equations is the FCT-algorithm of Boris and Book²⁹ which is especially well suited for high-speed flows. The version of the algorithm used for the RDE3D code is described in detail in NRL/MR/6410--93-7192³⁰ and will not be repeated here for brevity. The chemical source term appearing in the reactant conservation equation is computed through the chemical integrator CHEMEQ2³¹. These algorithms have been used extensively for characterization of PDEs, and have been shown to be both accurate and efficient for unsteady reacting flows. The current numerical procedure uses domain decomposition for parallelization. The full domain is broken into subdomains using the algorithm developed for the PARTI library³² and the MPI message-passing library³³. For obstructions within the flow-field, we use the Virtual-Cell-Embedding (VCE) method originally developed by Landsberg and Boris³⁴. This method is used for specifying the injector face and micro-injectors that separate the mixture plenum and the combustion chamber. When computing gas fluxes, processor communication is done between the subdomains for overlap regions such that fluxes retain their higher-order accuracy at subdomain boundaries. This method is very efficient and scalable for explicit calculations. These numerical procedures are encapsulated into the Detonate3D solver. The RDE3D program is an extension of this solver with additional boundary conditions and data manipulations specific to RDE's (such as the ideal injection source, averaging procedures, mass flow rate and force calculations). Current results have been run using up to 144 cores on a 3 GHz Core 2 Xeon cluster with 12 cores per node and 12 nodes.

For the RDE/plenum calculations, we wrote a new program called RDEPlenum3D. The new program is almost entirely based on both the RDE3D and the Detonate3D solvers. We calculate two separate domains: the annular combustion chamber domain, using the cylindrical three-dimensional grid of the RDE3D solver; and the exhaust plenum domain, using a rectilinear three-dimensional grid of the Detonate3D solver. There is a small area of overlap between the two domains, where the grid in the "buffer" region in the RDE3D solution¹⁹ overlaps the exhaust plenum grid. The two solution procedures are coupled together in this region by interpolating between the overlapped grids. An example of this combined domain is given in Figure 2. Since both grids are regular and stationary with respect to each other, interpolation is easily found and can be stored for future use. The exhaust plenum is made large enough such that the boundaries have little effect on the exhaust of the RDE. One of the complexities of this approach is that both domains have been separately decomposed for parallel computation. Therefore, a complex communication schedule must be developed to transfer information from the combustion chamber solution to the plenum solution efficiently, accounting for the decomposed nature of each grid. This results in considerable book keeping, but does not significantly impact the efficiency of the solver or the quality of the solution as long as the overlap region is not too significant. An additional complexity of the combined-domain solution is the mixed coordinate systems between the RDE and plenum. Because the combustion chamber solution is in cylindrical coordinates and the Plenum solution is in rectilinear coordinates, care must be taken to transfer the momentum vector between the coordinate systems after each interpolation is done. This transformation is also stored for every interpolated point so that it is not recomputed.

The grid shown in Figure 2 is much coarser and the plenum walls are much closer to the RDE than what is used for actual simulations. One can see that the overlap area is small between the two grids. Since the solution procedure uses a two-step Runge-Kutta time-stepping algorithm, and the FCT algorithm itself requires three overlap cells to retain their higher-order accuracy, we set the overlap to six cells and do the interpolation only once per overall time-step. The time-step is set based on the detonation wave and so is very small, thus the temporal errors introduced at this interface are small.

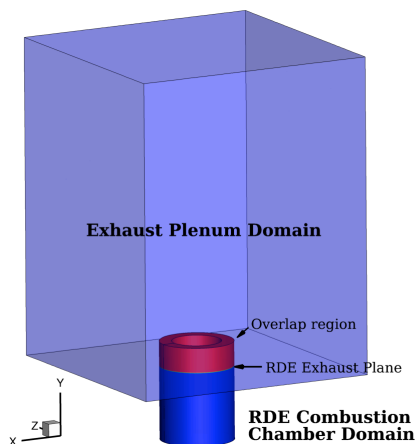
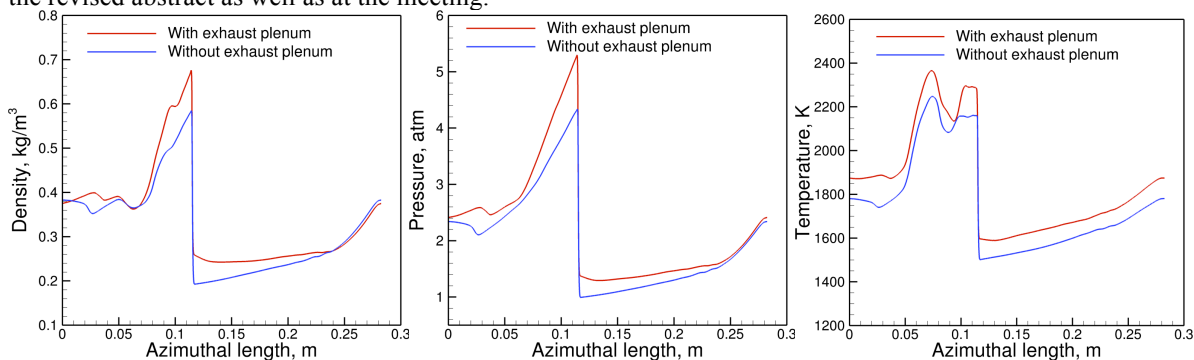


Figure 2. Example of dual domain for RDEPlenum3D simulation.

4 Results and Discussion

The addition of the exhaust plenum appears to have only a minimal effect on the temperature and pressure fields within the combustion chamber, however, we expect the conditions right at the RDE exhaust plane to be more variable. For the simulation with the exhaust plenum, the flow has the ability to expand radially compared to the more constrained solution without the exhaust plenum. This is shown in Figure 3, where we examine averaged solution profiles at the exhaust plane. We begin to see some significant differences between the two solutions. Interestingly, the simulation with the exhaust plenum has slightly elevated pressures and temperatures, and slightly lower axial velocities compared to our previous simulations without the exhaust plenum. This is most likely due to the simulation driving the pressure to the back-pressure in the subsonic regions at the exit boundary for the case without the exhaust plenum. Because we do not force this when simulating the exhaust plenum, the pressure is able to rise more near the exhaust plane. Another interesting difference between the two simulations is the difference in the averaged radial velocity. For the exhaust plenum, clearly there is some flow towards the centerbody, due to the recirculation region that is set up just above of the combustion chamber exhaust plane (although this is small compared to axial and azimuthal velocities). For the previous solutions without the exhaust plenum, the flow is constrained within the radial range of the combustion chamber, which is in this case between 40 mm and 50 mm.

Currently, a detailed kinetic model has been included to account for the late-time exhaust gas recombination chemistry effects. The general features of the RDE remain unchanged. However there is some additional heat release resulting in a 5-6% increase in specific impulse when compared to the simulations ignoring the exhaust gas chemistry. Further details, along with specific observations on the exhaust gas emissions will be presented in the revised abstract as well as at the meeting.



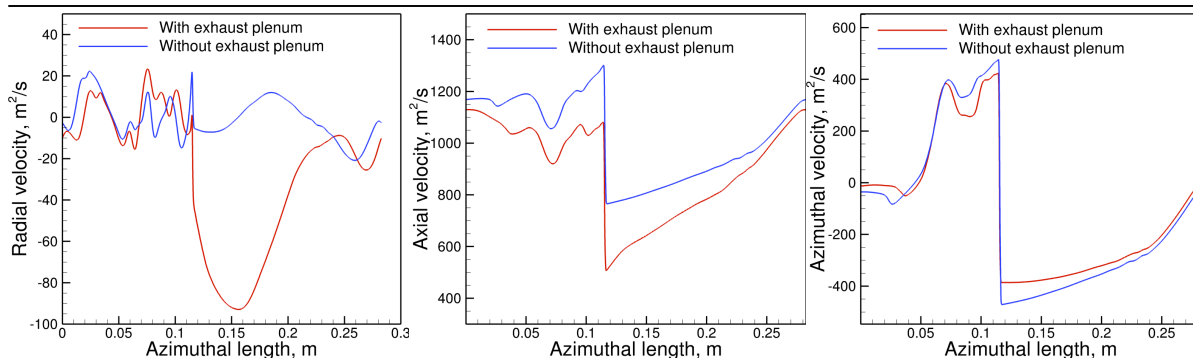


Figure 3. Combustion chamber exhaust profiles from averaged solution, comparing simulations with and without the exhaust plenum.

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