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A modeling strategy for transitory injection simulation in Rotating Detonation Engines

Pierre HELLARD, Thomas GAILLARD, Dmitry DAVIDENKO DMPE, ONERA, Université Paris Saclay F-91123 Palaiseau - France

Abstract

The efficiency of a Rotating Detonation Engine (RDE) strongly depends on the transitory injection process of fresh reactants in the combustion chamber: poor propellant mixing induces losses of combustion efficiency and consequently low detonation speed and unstable detonation propagation. Moreover, dilution of fresh reactants with burnt gases during the injection, increases the deflagration losses and decreases the pressure gain provided by the detonation. Numerical simulation can help to design an efficient injector to reduce these losses. Such simulation must reproduce the unsteady behavior of the transitory injection close to the injection wall. In particular, the injection of fresh gases is temporarily blocked due to the high pressure of burnt gases right behind the detonation front. The following reinjection of fresh propellants takes place during a short time period, therefore the optimization of this process represents a complicated technical problem. This study proposes an approach to model a single injection cycle taking into account the effect of the burnt gases expansion past a detonation wave near the injection wall. RDE injectors usually comprise slots or periodic elements such as repeated holes along the circumference of the annular combustion chamber. To reduce the computational cost of the CFD simulations used for the injector optimization, only one injection element of the whole injector is considered. The modeling strategy consists in using a custom initial condition, which permits to model the expansion process of burnt gases after the passage of a detonation wave. The effect of the initial condition parameters are discussed in this study. Propellant injection and mixing interactions are simulated with the LES approach on a fine mesh. Simulation results for different injector configurations are presented including the one experimentally studied at Nagoya University [1].

1 Introduction

In the 1960s, Voitsekhovskii [2] proposed the concept of an RDE in which one or more detonations rotate in an annular combustion chamber, continuously fed with fresh gases. The detonation consumes the reactive layer of fresh gases injected during a period between two successive detonation waves. Using detonation instead of deflagration theoretically leads to an engine efficiency increase compared to conventional engines. Despite encouraging results [3][4][5], no experimental studies have shown a concrete efficiency increase with RDE to the authors knowledge.

Numerical tools can help to investigate new RDE configurations, which could lead to a performance increase. During the early stages of development of an RDE, empirical laws [6] and reduced models [7] can highlight important parameters of an RDE that could lead to stable operation, high thrust efficiency and pressure gain. Nevertheless, these models cannot characterize the mixing of fresh propellants in the chamber, which is a key factor of the RDE efficiency [8][9]. More complex 3D simulations of the whole RDE can be performed to study the mixing in the engine and to confirm the engine efficiency, but these simulations are too expensive to be used as a pre-design tool.

Previous studies have proposed to use "cold gas injection" simulation (or continuous injection simulation) to analyze the mixing of fresh propellants in the chamber [10][11]. In such simulations, fuel and oxidizer are injected continuously in the chamber, and burnt gases are not taken into account. A cold flow simulation can give insight to design an efficient injection system for an RDE, but it cannot capture the real axial stratification of the fuel and oxidizer, obtained in simulations of operating RDE [12][13][14]. Such stratification is mainly due to asynchronous recovery of the fuel and oxidizer injection after the passage of a detonation wave followed by the burnt gases expansion. This axial stratification decreases combustion efficiency and the engine performance.

In [15], a methodology was proposed to model the burnt gases expansion in an RDE. This simulation strategy, named hereafter as reinjection simulation, is applied in this paper to the RDE of Nagoya University [1] and the RDE numerically studied at ONERA. Reinjection simulations rely on a custom initial condition to model the burnt gas expansion. In the following, the effects of the initial condition parameters are studied. This can help to correctly set the initial condition of the simulation, to obtain the same dynamic injector response as in an experimental RDE, which will help to analyse the injection system quality.

2 Simulation methodology

The Large Eddy Simulations (LES) discussed in the following were performed with the multiphysics software CEDRE developed at ONERA [16]. The compressible Navier-Stokes equations are solved with the CHARME solver. The MUSCL (Monotonic Upstream Scheme for Conservation Laws) interpolation scheme associated with the Van Leer slope limiter is used to obtain second-order accuracy on the convective fluxes. A central-difference second-order scheme is used to compute the viscous fluxes. Time integration is performed with the first-order Euler implicit scheme, with a time step of 10 ηs . The Smagorinsky model is chosen to account for the effect of subgrid scales of flow turbulence.

2.1 Computational domain

The first case studied is the annular chamber of the RDE designed and operated at Nagoya University [1]. The RDE inner and outer diameters are 62 mm and 78 mm respectively, resulting in a 8 mm channel width, while the length of the chamber is 70 mm. A converging-diverging nozzle is attached at the exit of the combustion chamber. The contraction ratio of the throat is 2.5. In the present

simulation, the nozzle is not accounted for since its effect is also modeled by the initial condition. On the other hand, the length of the combustion chamber is greatly increased to reduce the potential reflective effect from the outlet boundary condition on the injection plane.

 C_2H_4 and O_2 are injected through 120 injection elements (see figure 1) to obtain a global equivalence ratio of 0.9, like in [1]. One injection element is composed of two perpendicular injection tubes of 1 mm in diameter. The two tubes in one injection element are radially aligned to provide a direct impact of the unlike jets. Only one injection element is considered, thus reducing the computational cost of the simulations. The numerical study [10] validated this approximation on a different RDE and for cold flow simulations. The mesh is composed of approximately 1.5 million tetrahedrons, with a minimum size of 100 µm in the mixing zone. The mesh cell size is gradually increased along the chamber height. The present mesh refinement is comparable to previous RDE simulations [17][18].

The second geometry studied is a hypothetical annular RDE (named as ONERA RDE in the following), in which the injection element described in the patent [19] is installed. H₂ and O₂ are used as propellants for this RDE. As for the previous case, the mesh is composed of 100 µm tetrahedrons in the mixing zone.



Figure 1: Sectional view of the computational domain corresponding to Nagoya RDE (left) and to ONERA RDE (right)

Concerning the boundary conditions, non-slip condition is set on all the walls. Walls are also set as adiabatic. The outlet is set as supersonic. The mass flux and total temperature are imposed at the inlet of the injection tubes. Periodic boundary conditions are imposed on the radial planes, at halfdistance between the neighboring injection elements. In the Nagoya RDE, only one detonation wave, propagating at 1197 m/s was obtained experimentally, resulting in a $\tau_1 = 170$ µs period. This time period corresponds to the time available for injection, and thus to the duration of the corresponding reinjection simulations. There is no experimental data for the ONERA RDE. A time period of $\tau_2 =$ 20 µs is supposed in the following for this RDE. It corresponds to the time period obtained in the numerical study [20], in which the injection element of the patent [19] was also used.

Only the effect of the initial condition is considered in this study, assuming no reaction between the propellants and burnt gases during the reinjection process.

2.2 Initial Condition

As mentioned before, the reinjection simulation methodology uses a custom initial condition to model the expansion of the burnt gases in the chamber. The initial condition is obtained from the resolution of a Riemann problem. The initial states of the Riemann problem are defined as follows (see figure 2): the lower state is usually represented by the CJ conditions, while the upper state considers an isentropic expansion from the CJ conditions to a certain axial Mach number. Hence, the lower state models the burnt gases produced just after the detonation passage over one element, while the upper state accounts for the expanded detonation products from the previous detonation. The bottom of the chamber, also referred to as the injection plane, is located at the lower boundary (y = 0 in figure 2). Therefore, the location of the discontinuity h_D can be seen as the height of the detonation wave.



Figure 2: Scheme of the Riemann problem solved to obtain the initial condition for reinjection simulations



Figure 3: Temperature field in a 2D simulation of an RDE. Streamlines in the frame moving with the detonation are shown in black

The Riemann problem solution provided by an in-house code permits to determine the point where the head of the expansion fans reaches the bottom boundary (position $(x_1, y=0)$ in figure 2). At this coordinate, the solution is extracted along y and applied to the LES simulations as an initial condition in the RDE chamber. Concerning the initial condition in the injection tube of the LES simulation, it is previously obtained with a cold flow simulation. More details on reinjection simulations can be found in [15].

3 Results and discussion

3.1 2D simulations of the RDE operation

Pressure profiles extracted from 2D simulations of an RDE, with uniformly distributed injection of premixed propellants, will be used hereafter as a reference result to describe the expansion process. This section aims at analyzing the results obtained from these 2D simulations. Mainly, the effect of the number of detonation waves assumed in the entire RDE chamber, directly linked to the spatial period in the 2D simulations, will be studied. The numerical methods and meshes used for these simulations have been detailed in [14], and an example of a simulated flowfield is shown in figure 3.

Figure 4 shows pressure profiles along the injection plane obtained from three 2D simulations, with the same mass flux of propellants (H₂/O₂). In this figure, the dimensionless abscissa x^* is the circumferential position x divided by the spatial period between detonation waves, noted L in the following. The detonation is located at $x^* = \frac{x}{L} = 0$.

The only parameter that differs in these simulations is the number of detonation waves assumed in the RDE and hence, the spatial period L. Nevertheless, the three pressure profiles are almost perfectly superimposed, meaning that for 2D premixed simulations, the period L does not have an impact on the pressure profile in the engine if the dimensionless coordinate x^* is used. This similarity was also mentioned in [21] concerning simulations using Euler equations.

Thanks to this result, 2D simulations can be performed on a small computational domain (i.e. a small spatial period), leading to lower computational cost. The pressure profile describing the expansion process for any selected number of waves can then be derived from such a 2D simulation.

3.2 Reinjection simulations

3.2.1 Effect of the Riemann problem states

The effect of the two states of the Riemann problem is investigated on the Nagoya RDE. In an RDE, a detonation wave does not propagate at the theoretical CJ speed and it does not produce the theoretical CJ pressure, mainly because of the heterogeneities in the fresh mixture layer consumed by the detonation. Therefore, two cases are compared in figure 5: the first one in which the states of the Riemann problem are determined from the exact CJ conditions (Case 1), and the second one in which the states are determined from a deteriorated CJ condition (Case 2), obtained from the inhouse code *DetonHeter*, that takes into account the unmixedness of fresh propellants. The corresponding upper and lower initial states of the Riemann problem are summarized in table 1 for the two cases.

Since the initial condition of Case 2 is obtained from a deteriorated CJ condition, the initial pressure is far below the pressure of Case 1.



Figure 4: Pressure profiles along the injection plane of a RDE chamber from 2D premixed simulations



Figure 5: Pressure profiles at the injection plane for two reinjection simulations, using different conditions for the Riemann problem, and comparison to the experimental pressure of the Nagoya RDE

	Lower state		Upper state	
	Pressure (bar)	Temperature (K)	Pressure (bar)	Temperature (K)
Case 1	48.9	3982	14.3	3147
Case 2	12.1	3728	3.5	2924

Table 1: Pressure and temperature of the states defining the Riemann problem

Pressure in Case 2 decreases slower than in Case 1, and reaches its final value around $t = 100 \mu s$, while pressure in Case 1 decreases faster until it reaches a steady value around $t = 25 \mu s$. Thus, the conditions of the lower and upper states have a strong impact on the simulation. The mean pressure in these two simulations is either too high (5.4 bar in Case 1) or too low (1.2 bar in Case 2) compared to the experimental pressure (approximately 3.7 bar in [1]).

3.2.2 Effect of the upper state Mach number

The second parameter studied here is the upper state Mach number $(M_{y,up})$, which is linked to the expansion of the burnt gases produced by the detonation wave. The pressure profiles at the injection plane in the reinjection simulations are plotted in figure 6 for three different values of $M_{y,up}$.

From the results shown in figure 6, $M_{y,up}$ has an effect on the final pressure: when $M_{y,up}$ is reduced, burnt gases expansion is reduced as well and the pressure at the injection plane has a higher final value. In addition, the pressure profiles shown here are quite different from the expected exponential decay illustrated in figure 4. Consequently, $M_{y,up}$ is not a suitable parameter to control the shape of the pressure profile in the chamber but it is linked to the final pressure at the injection plane.

Figure 6: Pressure profiles at the injection plane for the three reinjection simulations using different upper state Mach numbers $M_{y,up}$

Figure 7: Instantaneous fields of Z_{excess} in the mid-plane of the Nagoya injection element at $t = \tau_1$ for two upper state Mach numbers $M_{y,up}$

The effect of $M_{y,up}$ is also shown in figure 7 with the field of Z_{excess} . If Z_{excess} is positive (respectively negative), it corresponds to the volume fraction of C_2H_4 (respectively O_2) in excess relative to

stoichiometry. The two fields obtained at the end of the reinjection period τ_1 are very different from each other. Since the final pressure in the chamber increases when $M_{y,up}$ is reduced, the velocity of the propellant jets in the chamber is also reduced for the same mass flux. Thus, the fresh gases have more time to mix close to the injection plane. This leads to a better mixing in the case of $M_{y,up} = 1$ as shown in figure 7, on the right. Also in the same reinjection simulation, the O₂ jet impinges the inner wall of the engine, creating a lean mixture close to it. This behavior is in agreement with the experiment, in which a part of the wall coating in the experimental chamber was oxidized during the RDE operation [1].

3.2.3 Effect of the discontinuity position

Hereafter, the effect of the discontinuity height h_D is studied for the ONERA RDE. For this case, a 2D simulation of the engine has been performed, and is used as the reference pressure profile (see "2D premixed" in figure 8). Two values for h_D are tested in the reinjection simulations: 3 mm and 10 mm. The pressure profiles obtained from these two reinjection simulations are compared with the pressure profile of the 2D premixed case in figure 8.

It can be seen in figure 8 that h_D has an impact only on the rate of the pressure decay. In fact, initial pressure is the same, but increasing h_D slows down the expansion of burnt gases at the injection plane of the RDE chamber. Therefore, h_D seems to be a key parameter to set a proper initial condition that can correctly model the effect of burnt gas expansion.

Figure 8: Pressure profiles at the injection plane for the 2D simulation (solid line) and three reinjection simulations (dashed and dot-dashed lines), with various h_D

Figure 9: Pressure profiles at the injection plane plotted against x^+ for the two reinjection simulations

Now, a strategy to predict the correct value of h_D is proposed. As for figure 4, the idea is to find a dimensionless coordinate to compare the pressure profiles obtained from reinjection simulations. The Riemann problem is supposed to model the discontinuity located at h_D , separating burnt gases produced by a detonation, and the expanded burnt gases produced by the previous detonation. This discontinuity position is therefore linked to the thickness of the fresh mixture layer located in front of the detonation wave. If the period between two detonation waves increases, there is more time to inject propellants and the thickness of the fresh layer grows. Therefore, it can be assumed that, like the thickness of the fresh layer, h_D is proportional to the time period between detonations (τ). Also, the temporal and the spatial periods are linked as $L = \tau \times V_D$, where V_D is the detonation speed in the laboratory reference frame. Hence, the thickness of the fresh gases layer is proportional to the spatial period (equation (1)), as experimentally shown in [6][22].

$$h_D \propto L$$
 (1)

It was shown previously that the pressure profiles of a 2D simulation with different numbers of waves in the RDE chamber depends only on the dimensionless variable $x^* = \frac{x}{L}$. Thus, by using equation (1) it comes:

$$x^* = \frac{x}{L} \propto \frac{x}{h_D} \tag{2}$$

Then, using the coordinate change $t = \frac{x}{V_D}$ in equation (2) leads to the following equation:

$$x^* \propto \frac{t \times V_D}{h_D} = x^+ \tag{3}$$

Pressure at the injection plane of the RDE chamber is plotted against the dimensionless variable x^+ for the two previous reinjection simulations in figure 9. The two curves are perfectly superimposed. Thus, it is possible to predict the pressure profile for a reinjection simulation. In fact, one reinjection simulation (obtained with an assumed discontinuity height $h_{D,1}$) allows to plot the pressure profile $P(x_1^+ = \frac{tV_D}{h_{D,1}})$. Then, it is possible to reconstruct the pressure profile P(t) that will be obtained for a different value of the discontinuity height $h_{D,2}$ with equation:

$$t = \frac{x_1^+ h_{D,2}}{V_D}$$
(4)

To illustrate the previous method, the pressure profile of an optimum height ($h_D = 6.5$ mm) that will lead to a pressure profile close to the one of the 2D simulation is plotted in green dashed-dotted line in figure 8.

Finally, using this method to the previous reinjection simulation Case 2 (Nagoya RDE), leads to a h_D of approximately 60 mm to get the experimental mean pressure in the simulation. This value seems very high compared to the previous 6.5 mm obtained for the ONERA RDE. This difference is due to the longer time period of the Nagoya RDE (170 µs) compared to the assumed ONERA RDE period (20 µs), which creates a thicker mixing layer (and thus a larger h_D). Another reason can be that the deteriorated CJ condition used in Case 2 for the initial state of the Riemann problem has a too low pressure compared to the experiment. The initial condition of the Riemann problem is therefore once again very important.

4 Conclusion

The reinjection simulation methodology has been applied to two RDE configurations and the effect of the initial condition parameters on the pressure profile decay at the injection plane have been studied. The conditions of the lower and upper states of the Riemann problem have to be set carefully since they have an important impact on the initial and final pressures at the injector exit plane. The upper state Mach number controls the final pressure in the chamber: a lower Mach number stops the burnt gases expansion sooner. The rate of the pressure decrease is mainly controlled by the location of the discontinuity imposed in the Riemann problem. The farther the discontinuity is located, the slower is the pressure decay. A method to accurately impose this height has been proposed to correctly set the initial condition. The present method can therefore be used to help designing an efficient injection system that reduces the axial stratification of fuel and oxidizer. Future work will focus on the validation of reinjection simulations with comparison to 3D simulations of an RDE chamber.

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