A model for multi-wave dynamics in a rotating detonation engine

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1 Introduction

The rotating detonation combustor (RDC) is an unconventional engine design employing detonative combustion, in contrast to traditional deflagration-based engines. The greater power density of detonation-based combustion compared to traditional combustors may allow for more compact engines. The detonation velocity is matched precisely to the rate of reactant injection in the quasi-steady case; such a case is illustrated in Figure 1. One objective of recent work has been to characterize the regime in which this classical picture is accurate, and to account for the operating conditions which would lead to different wave propagation modes, e.g. those with counter-rotating waves, such as have been observed experimentally.

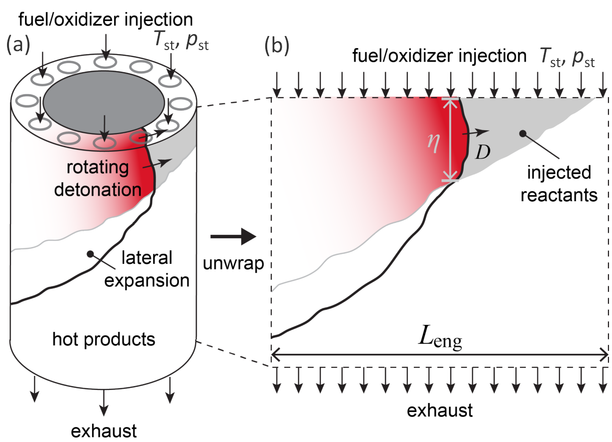

Figure 1: Schematic representation of the essentials of a rotating detonation combustor. In (a) the annular shape of the chamber is visualized. In (b) this chamber is unwrapped into a 2D domain, where the shape of the rotating detonation waves is better visible. A rotating detonation is propagating around the annular combustion chamber, consuming the injected reactants.

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Various works have attempted to provide models to understand these multi-wave phenomena focusing on either simplifying dynamical models of RDE operation or developing criteria for predicting which modes will be stable. Zhao and Zhang [1] have proposed that plenum pressure acts as the effective bifurcation parameter, while Teng et al. [2] identified the stagnation temperature and reaction-rate constant as key parameters. A model proposed by Connolly-Boutin et al. [3], based on a minimum mass-flow rate as a criterion for successful operation, has shown good agreement with experiment in predicting when stable rotating detonation operation is established. The above mentioned studies have focused on developing models to gain insight in RDE operation. However, these theoretical efforts do not provide the capability to predict which wave mode will be observed solely based upon the input of mixture properties and engine parameters. This leads to the research question that this study aims to answer:

”How do varying plenum stagnation temperature and combustion chamber perimeter influence rotating detonation wave (RDW) modes in an RDC?”

This study conducts a computational exploration of the parameter space of an RDE to determine when certain wave modes are observed. The two parameters that are varied in this study are the engine perimeter and the stagnation temperature in the plenum. By changing the engine perimeter, the area-normalized mass flow rate is varied, while changing the stagnation temperature allows for exploration of the influence of chemical sensitivity on RDE operation. Next to the computational exploration, a theoretical model is developed that aims to predict the viable operating wave modes as a function of the varied parameters. This theoretical model utilizes three important time scales that are present in an RDE. The numerically investigated temperature range is set where the theoretical model predicts interesting co-rotating or counter-rotating waves. This variation of temperature can also be seen as a proxy for the effect of heating through for example the recuperation of the injected mixture, or through contact with hot walls. The results of the theoretical model will be compared to the results of the computational simulations.

2 Problem statement and model description

An overview for the approach that is used in this study is presented in Fig. 2. The goal is to develop an explanatory theoretical model that predicts for what mixture properties and engine size, which wave modes can be observed in an RDE. This model will be compared to a set of numerical simulations where the annular combustion chamber of an RDE is unwrapped into a 2D domain. In these simulations, the plenum stagnation temperature and the engine perimeter will be varied. The theoretical model will be based on the comparison of three important typical timescales that are present in an RDE. For these timescales, this model proposes two criterion: the *critical layer thickness criterion* and the *Induction-time criterion*. For these criteria it is required to know for each set of parameters what is the critical layer thickness and when the injected mixture will auto-induct. Yielding confinement simulations will be conducted to estimate what is the critical layer thickness for each set of investigated parameters. A chemical model is needed to make predictions on the auto-induction time of the injected mixture. This chemical model will also be the basis for both the numerical RDE simulations as well as the numerical yielding confinement simulations, where it will capture the detonation wave behavior under different conditions. This chemical model will need to be validated using numerical simulations where there are no losses, so that detonations under ideal circumstances are modelled. These results are compared to experimental data to see how the chemical model performs.

2.1 Chemical model

The chemical model that is used is a two-step Arrhenius model containing an induction and an exothermic reaction. Such simplified model is needed to reduce the computational costs that are required for simulations with detailed chemistry. These detailed models track several species and step reactions, which for this research is unnecessary. Additionally, an induction time (and length) scale before the onset of exothermic reactions can be clearly defined, facilitating the development of the theoretical model. For the two-step model, kinetic parameters are calibrated based on the ZND profile using detailed chemistry for the stoichiometric H_2-air mixture [4] at different initial conditions. The two-step model and the procedure for the calibration of the kinetic parameters are detailed in [5].

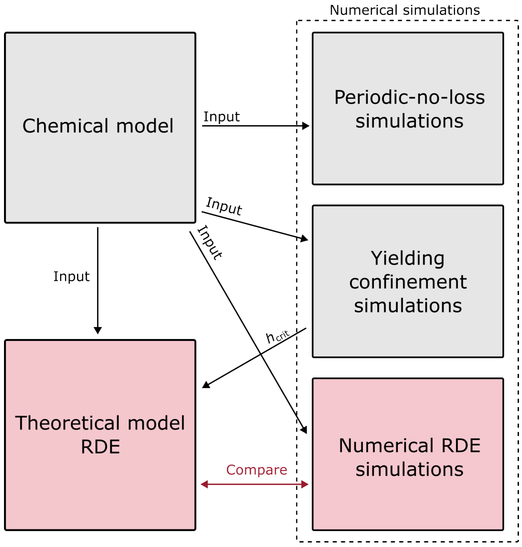

Figure 2: Research strategy.

2.2 Numerical RDE simuations

The reactive system consists of an inviscid, calorically perfect gas (i.e., with a constant specific heat ratio γ). The gasdynamics of this system are described by the two-dimensional reactive Euler equations in a lab-fixed reference frame. The boundary conditions and initial configuration for the numerical simulations of RDE considered in this study are described in detail in [5].

2.3 Theoretical model of RDE

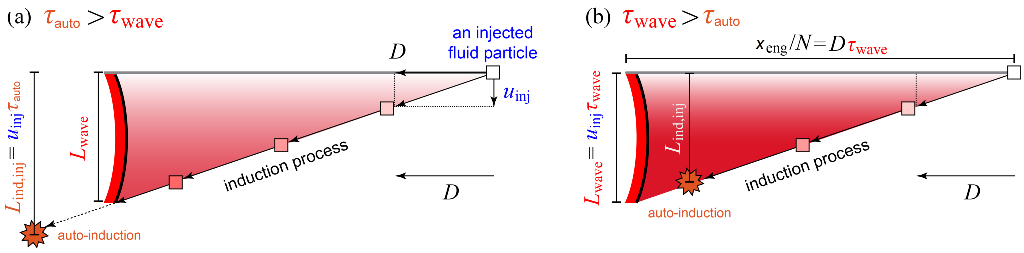

Figure 3: Illustration of the induction progress profile in an idealised rotating detonation wave. White regions are uninducted, black regions are fully inducted. (a) Induction time is significantly longer than the wave-period. Heat-release occurs solely as a result of the detonation-wave. (b) Induction time is of the same order as the wave-period; the mixture in front of the detonation wave has nearly completed the inductive reaction, even prior to being shocked. In this regime, injected mixture may autoignite, especially if shocked by some perturbation.

The model developed here compares two independent timescales present in the RDE in order to predict mode feasibility: the timescale induced by the chemical reaction is taken to be the induction time of the mixture, τ_{ind}; the geometry-induced timescale is taken to be τ_{wave}.

Criterion I: Induction Timescale Criterion

For fixed plenum conditions T_{pl}, p_{pl}, we assume for simplicity sonic injection at an area ratio of 1; this fully defines the pre-shock state of the injected reactants T_{inj}, p_{inj}. The RDE will be unable to sustain a co-rotating mode if reactants undergo exothermic reaction prior to being hit by the detonation; the timescale for induction at constant temperature T_{inj} may be determined by integrating the transport equation of the induction-progress variable:

$$\xi(\tau_{\text{ind}}) - \xi(0) = \int_0^{\tau_{\text{ind}}} \omega(T_{\text{inj}})\text{d}t \tag{1}$$

$$\tau_{\text{ind}}(T) = \omega(T)^{-1} = k_{\text{I}}^{-1}\text{exp}\left[-\frac{E_{\text{I}}}{RT_{\text{S}}}\left(1 - \frac{T_{\text{S}}}{T_{\text{inj}}}\right)\right] \tag{2}$$

For descriptive convenience, the induction time is left as a function of temperature; the familiar induction time associated with a ZND detonation is thus $\tau_{\text{ind,ZND}} = \tau_{\text{ind}}(T_{\text{vN}})$, while the induction time of the injected reactants is $\tau_{\text{ind,inj}} = \tau_{\text{ind}}(T_{\text{inj}})$. If the time between passages of detonation waves is greater than this induction time, it is predicted that the reactants will react exothermically before they are reached by the detonation; in such a case the quasi-steady co-rotating mode is expected to be unobservable.

Criterion II: Critical Layer Thickness Criterion

Accounting for the possibility of multiple co-rotating detonations, we may write the time available for refilling of reactant after a wave passes as

$$\tau_{\text{wave}} = \frac{L_{\text{eng}}}{ND} \tag{3}$$

with L_{eng} the domain-length (i.e. the engine perimeter), and D the detonation velocity. In the case of a single wave, this is equal to the period of the detonation wave; this period decreases in proportion to the number of waves. It is well-documented that detonation-waves of finite-thickness exhibit a velocity-deficit relative to the CJ velocity [?]. The use of a velocity-deficit curve allows us to predict when a detonation wave will fail due to propagating into a layer of less than the critical-layer thickness. In the RDE the wave-velocity and layer-thickness are uniquely intertwined. In order to make progress, use may be made of a velocity-deficit curve; for the present purpose, it suffices to note that these curves may be reasonably approximated via functions

$$\frac{D}{D_{\text{CJ}}} = 1 - \beta\left(\frac{L_{\text{ind}}(T_{\text{pl}})}{L_{\text{wave}}}\right) \tag{4}$$

With L_{wave} the layer thickness and β a fitting coefficient. Further, this equation holds *only* in the region where L_{wave} is greater than $L_{\text{wave,crit}}$, the critical layer thickness. It is expected that the detonation will fail when this is not the case. The induction length is inserted to normalise the scaling of this thickness at different plenum temperatures. Values of β may be estimated through various methods - here they were estimated from numerical experiments involving reactive layers bounded by inert gas at the predicted post-expansion temperature.

Next, neglecting the backflow induced by a passing detonation wave, and assuming the velocity of the wave is constant, $L_{\text{wave}} = u_{\text{inj}}\tau_{\text{wave}}$. This results in an equation for the wave-period which may solved self-consistently for the velocity-deficit adjusted period of the detonation wave. We thus define $\tau_{\text{layer}} = \frac{L_{\text{wave,crit}}}{u_{\text{inj}}}$, the time which is required for the reactant to refill sufficiently to sustain a detonation.

Finally, the simplified criterion for feasibility of a co-rotating mode based on plenum conditions may be presented:

$$\frac{\tau_{\text{ind}}}{\tau_{\text{wave}}} < \text{const.} \tag{5}$$

$$\frac{\tau_{\text{layer}}}{\tau_{\text{wave}}} > 1 \tag{6}$$

A priori it is expected that this constant should be unity; in order to account for the observation that nearly inducted mixtures are more unstable even below this point, this constant is left as the sole fit-parameter of this model. In general, a co-rotating mode of the RDE may undergo transition for a variety of reasons, including insufficiency of the mixing time, autoignition of the reactants, and insufficient size of the reactive layer to sustain a detonation. For the present model, transition due to autoignition of the reactants is taken as the main cause of transition between modes, although extension to other mechanisms of transition simply requires an expression for the associated time-scale τ_{crit} as a function of the relevant parameters.

3 Comparison between numerical simulation and theoretical results

The results of RDW propagation modes predicted by the theoretical models are plotted in 4(a). Distinct curves in the plot correspond to different numbers of co-rotating waves; here only those for 1, 2, and 3 co-rotating modes are drawn for clarity. It is predicted that, for the corresponding curve, a mode with N co-rotating waves will not be observable *above* the appropriate line. In a similar manner, the lower set of curves correspond, for each possible mode with N co-rotating waves, to failure of the detonation due to insufficient refilling time. It is predicted that a mode with N co-rotating waves will not be observable *below* or *to the left of* the corresponding line. For the critical layer lines, back flow induced by a passing detonation is neglected. If this would be taken into account, the ratio in 6 would have to be significantly larger than one, causing the critical layer criterion lines to shift to the right.

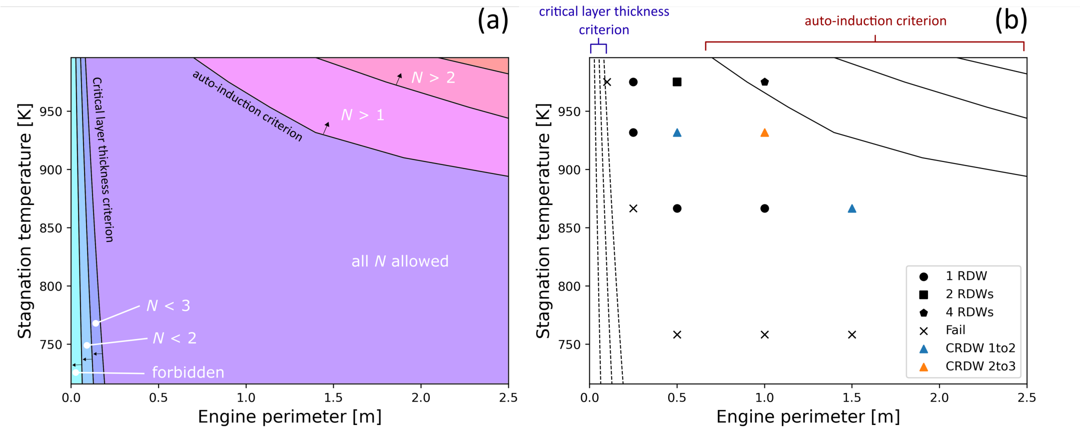

Figure 4: (a) Regime diagram of different RDW propagation modes predicted by the theoretical model for the competing timescales and (b) compared with the results from numerical RDE simulations (plotted as markers).

The results of RDW propagation mode from numerical simulations for varying stagnation temperature and engine perimeter are summarized in 4(b), where the results are compared to the predictions made by the theoretical model. The numerical simulation results are laid over the critical layer thickness criterion lines and the auto-induction criterion lines from 4(a).

It can be seen that qualitatively the numerical results seem to agree with the theoretical model predictions. For insufficient layer thickness the detonation will fail and closer to the auto-induction line multiple waves seem to be allowed. It seems that the lines resulting from the theoretical criteria should shift closer to each other to match the results from the numerical simulations. The cases for $T_{\text{st}} = 758\,\text{K}$ all seem to fail. For all these simulations it is observed that the initial high pressure zone is unable to create a detonation wave in the developing reactive layer. It is thus not certain what would result if initially there would be a detonation, but there may be a possibility that detonation can be sustained if a different method of initiation is used. It is suggested that the CRDW modes can be seen as transitioning modes between stable N-modes. It is thus predicted that for higher plenum stagnation temperatures and/or larger engine perimeters 5 RDWs are observed, or a 4-to-5-RDW mode containing CRDWs. In between the simulated cases, it is expected that stable 3 RDW mode is observed and the 3-to-4-RDW mode containing CRDWs.

4 Concluding Remarks

In summary, a model has been developed which predicts what modes of RDE operation will be feasible for a given combination of plenum temperature, T_{pl} and engine perimeter, L_{eng}. Two criteria are proposed to dictate stability of a given mode: the time between passage of detonation waves τ_{wave} must be shorter than the time the injected reactants take to complete their induction period, τ_{ind}, otherwise autoignition will occur and the mode will not be sustainable; further, the time between passages of the detonation, τ_{wave}, must be sufficiently long that enough reactant is injected to surpass the critical layer thickness of the detonation. This model is compared to CFD simulations of the reactive Euler equations, using a simplified 2-step chemistry model. The simulations are found to be in qualitatively good agreement with the theoretical model predictions. Additional features will be considered in an improved theoretical model to reduce the quantitative discrepancies and presented in the full paper.

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