State-to-State Model for Rotating Detonation Combustors

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1 Introduction

One of the critical aspects of rotating detonation combustor/engine (RDE/RDC) development, and perhaps limiting so far, is the development of appropriate metrics to define operation and performance. This may be limiting in laboratory experiments, but it is certainly so in more relevant and practical configurations. Perhaps the identification of operation mode of a particular configuration operated under certain operating conditions is more straightforward, and some strategies and methods have been identified in previous works [1–6]. These methods are now beginning to shed light on combustion dynamics.

The quantification of performance is certainly more challenging because of at least three factors. Firstly, the inlet and outlet properties (p, T, velocity and composition) are not spatially and temporally uniform. This requires that spatially and temporally resolved measurements, or at least phase-average measurements, are obtained. This also requires that an additional suitable averaging operation of these properties be conducted to define mean (bulk) performance metrics (e.g., I_{sp}). This aspect is important for both time averaging (e.g., to determine phase-average properties) and spatial averaging (e.g., to find bulk properties) [7, 8]. This aspect is even more challenging if one considers that there might not be a linear relationship between measurable quantities (e.g., wave speed, CTAP, temperature) and performance metric (e.g., total pressure gain), making the use of averaged properties for analysis dubious and justifying the need for time- and space-resolved measurements.

Secondly, the unsteady (quasi-periodic) nature of the problem makes the use of steady state ideas of performance quite a challenge. In some prior work the concept of rothalpy, useful in the analysis of turbomachinery, has been explored as a means to analyze the problem in a steady state sense in a frame rotating with the detonation wave and has provided a useful framework for analysis [9]. The unsteadiness time scale and amplitude are also significant, which impose limitations on measurement instrumentation. Finally, an overall understanding and quantification of the various processes that contribute to losses is still lacking. This prevents relating losses to operating and design conditions, somewhat hindering progress toward highly performing designs. As a result, understanding gain (or lack thereof) in both a global and local sense, and its variation with operating conditions and mode of operation, still remains an elusive task, but a critical one to solve.

To date, there is no accepted approach to fully quantify the overall performance of a detonation-based combustor, either indirectly from measurements of observables (e.g., pressure measurements) or directly from a measure of the pressure rise (gain) across the combustor. Even if thrust measurements are taken, it might be difficult to related them across systems and operating principles (i.e., deflagration- vs. detonation-based systems). In addition, reliance only on global metrics like thrust does not necessarily inform about the breakdown of losses, the understanding of which is what will enable us to offer performing designs. The methods proposed by Kaemming and Paxson. [10] based on the concept of equivalent available pressure (EAP), is a valuable approach, although its implementation from experimental data does suffer from some of the challenges identified previously. This concept defines pressure gains in terms of a steady state equivalent pressure that is available to do work or provide thrust. This definition allows for the comparison of systems based on different operating principles. They define EAP in two different forms: (a) an EAP equivalent to the measured thrust or work extracted, which includes the effect of downstream components; and (b) an EAP equivalent to the thrust or work that would be extracted if the working fluid were expanded to ambient pressure, which accounts only for the contribution of the combustor. This latter form is defined as the EAPi to differentiate it from the former EAP and it is preferred to evaluate the combustor performance in isolation from downstream components. The problem of matching combustor to downstream component is however a problem in and of itself. However, the use of EAPi from experimental measurements is somewhat challenging as it requires to have thrust measurements (with flow expanded to ambient) and/or total pressure at the exit (so expansion to ambient can be conducted in analysis). In experiments, however, it is challenging to conduct a total pressure measurement [11] and thrust measurements can be affected by nozzle design and base pressure effects (especially at low pressure ratio operations). The recent work by Bach et al. [12] summarises current measurements of pressure gain derived from EAP through thrust measurements and the few attempts at direct measurement of pressure gain through total pressure measurements from pitot tubes at the exit. To overcome some of these limitations, but also to expand on this basic idea in ways that allow us to include and quantify all loss mechanisms, we are developing a methodology to evaluate loss and pressure gain that is based on a combination of state and thrust measurements in the RDC, interpreted through a phenomenological model of the thermodynamic processes the flow undergoes from inlet to exit, although in a simplified form. Because the model is based on a (thermodynamic) state-to-state description of the flow evolution in the RDC connected by elementary processes, the model is intrinsically a lump-state model, and it may provide only a global and qualitative engineering insight to the performance of RDCs and its dependence on operating details. The goal of this work is to develop the model, demonstrate its use for parametric studies on hypothetical systems and apply the model to measurement on existing RDCs to attempt validation of the model.

2 Description of model

The essence of the approach for estimating gain is based on thermodynamic cycle models similar to the early reduced order models of RDCs for performance estimation [7, 9, 11, 13–16], but is augmented by combining a phenomenological understanding of the various processes that occur in the detonation channel.

The current form of the state-to-state thermodynamic model is shown in figure 1, which describes the various thermodynamic states that a fluid particle undergoes on a representative fluid pathline as it moves from the inlet to the exit. The representation is meant to be in the laboratory frame of reference. The indicated pathline is only notional. In fact, it is well known that different fluid particles undergo different paths and processes. In essence, what is indicated here is somewhat similar to the analysis conducted in past work [7, 9, 13], but with the addition of a few intermediate states to describe additional processes the fluid undergoes. Most of these processes are meant to represent loss mechanisms.

With reference to figure 1, we can consider that a fluid element undergoes the following processes, which are described by suitable parameters:

- $2.0 \rightarrow 3.1$: Initially the inlet processes the working fluid from the air plenum into the detonation channel, and it is characterized by a pressure loss (efficiency) $\eta_i = p_{o,3.1}/p_{o,2.0} < 1$. This represent a stagnation loss caused by the aerodynamics of the inlet.

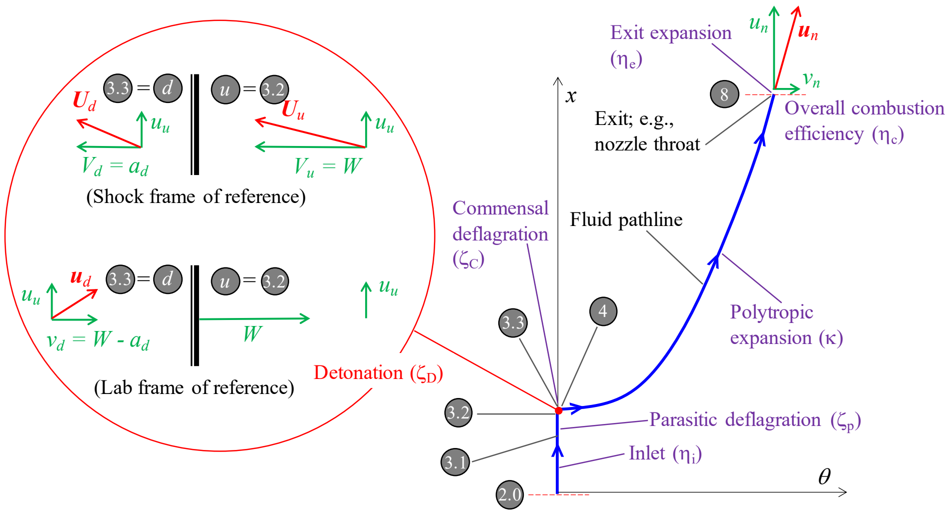

Figure 1: Notional diagram of thermodynamic processes and states that a fluid element might undergo during a detonation cycle from inlet to exit.

- $3.1 \rightarrow 3.2$: Parasitic combustion occurs where a fraction ζ_p of the total available heat of the mixture is released prior to the arrival of the detonation wave through deflagration. This is associated with a change in the conditions seen by the approaching detonation wave [17, 18]. The onset of parasitic combustion could be due to different mechanisms, such as ignition of the fresh mixture at the boundary between the fresh fill region and the hot post-combustion gases of the previous cycle or due to otherwise entrainment of hot gases into the fresh fill mixture. Parasitic deflagration can be a significant fraction of the total heat release associated with the fuel [18]. The presence of parasitic combustion is essentially a loss mechanism, because it prevents the realization of the full potential gain that could be achieved at the wave if the parasitic combustion did not exist. In practice, this will result in a lower pressure and temperature ratio across the detonation wave. To first order, this is associated with a lower shock compression at the wave because of the lower effective Mach number of the wave (relative to the partially deflagrated mixture).

- $3.2 \rightarrow 3.3$: Detonation, approaching with a speed W (less than D_{CJ}), arrives and processes the flow to state 3.3. This releases only a fraction ζ_D of the total available heat release [18], because of mixture or heat release leakage, for example due to incomplete mixing [19, 20]. Since only a fraction ζ_D of the available heat is released, the pressure rise across the detonation wave and the increase in total enthalpy due to increase in kinetic energy associated with the induced (azimuthal) velocity behind the wave are penalized (i.e., are less than what could otherwise be). Strictly speaking this is not a loss, but it is a reduction in the gain that can be achieved. In practice, state 3.3 is the C-J state corresponding to the upstream state 3.2 and ζ_D.

- $3.3 \rightarrow 3.4$: Commensal combustion after the detonation wave occurs where a fraction ζ_C of the total available heat is released through deflagration. This is another loss due to deflagration. Although in the schematic diagram this process (and also the previously discussed processes) is shown localized at the wave, commensal combustion could occur with a certain spatial and temporal distribution that is not localized at the detonation wave as the flow expands further past the wave.

- $3.4 \rightarrow 8.0$: Because of the large pressure difference between the detonation channel and the exit conditions, the flow expands axially toward the exit following an expansion process. Here the expansion is modeled as a simple polytropic expansion of index κ. This representation allows us to introduce loss mechanisms in the expansion to the exit. For example, we can represent the process according to the polytropic

$$pv^{\kappa} = C$$

(where C is a constant) and the polytropic index κ can be written as

$$\kappa = (1 - \gamma)K + \gamma$$

where γ is the ratio of specific heats and the factor K is defined as

$$K = \frac{\Delta q}{\Delta w},$$

with Δq and Δw being the heat and work exchanged during the expansion, respectively. The factor K can be considered to be a loss factor. More precisely, it represent the relative change of the heat exchanged to that of the work done during an expansion. If $K = 0$, the polytropic process represents an isentropic expansion; if $K = 1$ an isothermal expansion; and if $K < 0$ it indicates that while the flow is expanded, both work and heat are removed from the system. This latter case can be interpreted as representing a combination of heat loss to the wall, work loss due to frictional forces, and work expansion to turn the flow axially.

- $8.0 \rightarrow$: The flow is ultimately exhausted from the combustor (i.e., past the nozzle) while retaining an amount ζ_e of incomplete combustion. Essentially this implies that not all of the fuel that leaks through detonation wave is converted to products through commensal combustion, but instead, a fraction is not completely converted and contributes to having a combustion efficiency at the exit of less than 100%. By definition of the processed described here,

$$\zeta_p + \zeta_D + \zeta_C + \zeta_e = 1.$$

  A nozzle expansion efficiency η_e can also be included.

The model is only approximate as it completely neglects that different fluid elements experience different degrees of these processes. Thus, these intermediate states and process parameters are to be interpreted as lump parameters or parameters integrated in time (over a cycle) and in space. Thus, they may have only a purely engineering role and can be used solely to gather general and qualitative trends. The intermediate states may then assume only a lump thermodynamic state meaning, and it may be somewhat disconnected from the local gas dynamic state. However, additional details on individual processes may be added as more descriptive representations are introduced, such as the more descriptive yet still reduced-order model of inlet dynamics and partially-stirred reactor fill zone developed by Bedick *et al.* [21]. Improving the representation of the individual processes is work in progress for the complete manuscript. In addition, constrains may be introduced, such as conservation of mass or choked conditions at the exit of the RDC.

Given inlet and operating conditions, and given that the intermediate states can be evaluated as described above, performance metrics can be defined. One metric of interest here is the overall pressure gain (inlet to exit), which can be defined in terms of the pressure gain factor G:

$$G \equiv \frac{p_{o,8.0}}{p_{o,2.0}} - 1 = \frac{p_{o,8.0}}{p_{o,3.4}} \frac{p_{o,3.4}}{p_{o,3.3}} \frac{p_{o,3.3}}{p_{o,3.2}} \frac{p_{o,3.2}}{p_{o,3.1}} \frac{p_{o,3.1}}{p_{o,2.0}} - 1 \tag{1}$$

which is positive if an overall gain is achieved, negative otherwise. Because the intermediate states depends on the parameters describing the connecting processes, then the gain factor is a function of these model parameters:

$$G = \tilde{G}(\underline{\beta}; \underline{q})$$

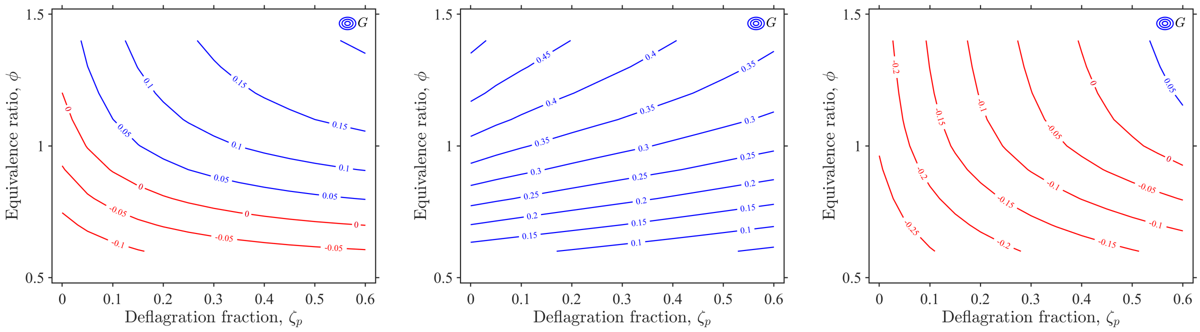

Figure 2: Gain factor G evaluated with simplified model with $\eta_i = 0.6$ and representative value of K: (a) $K = 0$ (isentropic expansion), (b) $K = 1$ (isothermal expansion), and (c) $K = -2$ (expansion with loss).

where $\underline{\beta}$ represents the vector of model parameters, $\underline{\beta} = \{\eta_i, \zeta_p, \zeta_D, \zeta_C, K, \zeta_e, \eta_e\}$, and $\underline{q}$ the vector of inflow conditions.

Assuming for simplicity $\zeta_e = 0$, i.e., complete combustion, and $K = 0$, i.e., isentropic expansion past the detonation wave, equation 1 can also be reduced in the following form:

$$G = \eta_e(G_{CJ} + 1)\eta_i - 1 \tag{2}$$

where G_{CJ} represents the gain factor achieved at the detonation wave, and includes the losses imposed by both parasitic deflagration and incomplete heat release across the detonation wave (i.e., $\zeta_C \neq 0$). Thus:

$$G_{CJ} = \tilde{G}_{CJ}(\zeta_p, \zeta_D).$$

Although the result is obvious if one considers the definition of the gain factor, equation 2 emphasizes that there is a linear relationship between achieved gain G and inlet and expansion nozzle losses. This linear relationship can in fact be verified by our direct measurement of thrust, from which a pressure gain can be estimated from the calculation of the EAP [22].

For the model to be applicable, for example for the evaluation of G, several parameters defining the elementary processes need to be defined; specifically: η_i, ζ_p, ζ_D, ζ_C, ζ_e, K, η_e; as well as some operating conditions, such as the plenum pressure, the peak pressure in the detonation channel and the exit pressure. As the model is refined and developed further, other additional quantities might be required. The quantities identified so far are quantities that can directly or indirectly be inferred. For example, the quantification of heat release distribution for H2/air operation can be approximated by using a measure of the OH* chemiluminescence emission, as we have done in the past [18, 23]. Static and dynamic pressure measurements in the: plenums, detonation channel, and nozzle throat; are required to either constrain the model or define some of the loss parameters (efficiencies, such as the inlet efficiency or pressure drop η_i). These measurements are available in the databases we are constructing.

3 Application of the framework to idealized cases

Although the framework described here has similarities to analyses proposed in the literature, it expands upon them by including a description and parametrization of loss mechanisms. Although it might not be readily obvious in the definition of G above, each of the loss term identified here enters in the definition of the intermediate states. To give a numerical example of the framework to estimate the gain factor, consider the results of figure 2 for a hypothetical H2/air operation under different conditions without an exit throat. These plots describe isocountour line of the gain factor as a function of equivalence ratio and parasitic deflagration fraction ζ_p assuming $\eta_i = 0.6$, $\zeta_C = \zeta_e = 0$, and various values of K. Negative gain factors are shown as red lines while positive gain is shown as blue lines. Intermediate states were computed using a combination of chemical equilibrium solvers for detonation waves and deflagration (based on Cantera and NASA CEA). Variation in thermodynamic properties were accounted for. The contribution of parasitic combustion on the detonation wave was modeled using an approach similar to what used in our previous work [17]. Cases with $K = 0$ and $K = 1$ are shown for comparison, but it is the case with $K < 0$ that is more relevant here ($K = -2$ is perhaps a case with an unrealistically high value, but we do not know this a priori now) because it represents a case where there is heat and possibly a work loss during the expansion through the detonation channel. The isothermal case ($K = 1$) may be used to represent a case where deflagration occurs while the flow expands toward the exit past the detonation wave. From the results of figure 2, we can observe that once some losses are included, the predicted gain factor is always negative (red) indicating a net loss. By balancing the various loss mechanism, this framework allows to evaluate different scenarios and configurations.

4 Ongoing Work

What presented here is the initial framework of the model that identifies the main components, states, elementary processes and models to describe them. The model is and will remain a state-to-state model, although the description will be developed further to introduce additional details or more descriptive models [21]. Work will continue on refining the model and applying it to existing systems tested in our laboratory. The model will be exercised to conduct trade studies and identify sensitivities to loss factors. Existing measurements will also be used to validate and expand on the model. The final manuscript will present the models, including the description of the elementary processes, in details, and it will present the trade and validation studies.

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References

[1] Bohon, M., Bluemner, R., Paschereit, C., and Gutmark, E., "High-speed imaging of wave modes in an RDC," *Experimental Thermal and Fluid Science*, Vol. 102, apr 2019, pp. 28–37.

[2] Bluemner, R., Bohon, M., Paschereit, C. O., and Gutmark, E. J., "Dynamics of Counter-Rotating Wave Modes in an RDC," *2018 Joint Propulsion Conference*, American Institute of Aeronautics and Astronautics, jul 2018.

[3] Chacon, F. and Gamba, M., "Detonation Wave Dynamics in a Rotating Detonation Engine," *AIAA Scitech 2019 Forum*, American Institute of Aeronautics and Astronautics, jan 2019.

[4] Rankin, B. A., Richardson, D. R., Caswell, A. W., Naples, A. G., Hoke, J. L., and Schauer, F. R., "Chemiluminescence imaging of an optically accessible non-premixed rotating detonation engine," *Combustion and Flame*, Vol. 176, feb 2017, pp. 12–22.

[5] Anand, V., George, A. S., and Gutmark, E., "Amplitude modulated instability in reactants plenum of a rotating detonation combustor," *International Journal of Hydrogen Energy*, Vol. 42, No. 17, apr 2017, pp. 12629–12644.

[6] George, A. C. S., Anand, V., Driscoll, R. B., and Gutmark, E. J., "A Correlation-Based Method to Quantify the Operating State in a Rotating Detonation Combustor," *54th AIAA Aerospace Sciences Meeting*, American Institute of Aeronautics and Astronautics, jan 2016.

[7] Kaemming, T., Fotia, M. L., Hoke, J., and Schauer, F., "Thermodynamic Modeling of a Rotating Detonation Engine Through a Reduced-Order Approach," *Journal of Propulsion and Power*, Vol. 33, No. 5, sep 2017, pp. 1170–1178.

[8] Paxson, D. E. and Kaemming, T., "Influence of Unsteadiness on the Analysis of Pressure Gain Combustion Devices," *Journal of Propulsion and Power*, Vol. 30, No. 2, mar 2014, pp. 377–383.

[9] Nordeen, C. A., Schwer, D., Schauer, F., Hoke, J., Barber, T., and Cetegen, B., "Thermodynamic model of a rotating detonation engine," *Combustion, Explosion, and Shock Waves*, Vol. 50, No. 5, Sep 2014, pp. 568–577.

[10] Kaemming, T. A. and Paxson, D. E., "Determining the Pressure Gain of Pressure Gain Combustion," *2018 Joint Propulsion Conference*, American Institute of Aeronautics and Astronautics, July 2018.

[11] Bach, E., Bohon, M., Paschereit, C. O., and Stathopoulos, P., "Development of an Instrumented Guide Vane Set for RDC Exhaust Flow Characterization," *2018 Joint Propulsion Conference*, American Institute of Aeronautics and Astronautics, jul 2018.

[12] Bach, E., Paschereit, C. O., Stathopoulos, P., and Bohon, M., "RDC Operation and Performance with Varying Air Injector Pressure Loss," Jan 2020.

[13] Braun, E. M., Lu, F. K., Wilson, D. R., and Camberos, J. A., "Airbreathing rotating detonation wave engine cycle analysis," *Aerospace Science and Technology*, Vol. 27, No. 1, jun 2013, pp. 201–208.

[14] Mizener, A. R. and Lu, F. K., "Preliminary Parametric Analysis of a Rotating Detonation Engine by Analytical Methods," *52nd AIAA/SAE/ASEE Joint Propulsion Conference*, American Institute of Aeronautics and Astronautics, jul 2016.

[15] Shepherd, J. E. and Kasahara, J., "Analytical Models for the Thrust of a Rotating Detonation Engine," *GALCIT Report FM2017.001*, GALCIT, 2017.

[16] Paxson, D. E. and Perkins, H. D., "A Simple Model for Rotating Detonation Rocket Engine Sizing and Performance Estimates," *AIAA Scitech 2021 Forum*, American Institute of Aeronautics and Astronautics, Jan. 2021.

[17] Chacon, F. and Gamba, M., "Study of Parasitic Combustion in an Optically Accessible Continuous Wave Rotating Detonation Engine," *AIAA Scitech 2019 Forum*, American Institute of Aeronautics and Astronautics, jan 2019.

[18] Feleo, A., France, J., White, L. W., and Gamba, M., "Evaluation of OH Emission for Determining Operation of a Rotating Detonation Engine," *AIAA Scitech 2019 Forum*, American Institute of Aeronautics and Astronautics, jan 2019.

[19] Prakash, S., Fievet, R., and Raman, V., "Analysis of the detonation wave structure in a linearized rotating detonation engine," *Submitted to AIAA Journal*, 2019.

[20] Sato, T., Voelkel, S., and Raman, V., "Detailed Chemical Kinetics Based Simulation of Detonation-Containing Flows," *Volume 4A: Combustion, Fuels, and Emissions*, ASME, jun 2018.

[21] Bedick, C., Ferguson, D. H., and Strakey, P., "Validation and Application of a Reduced-Order Rotating Detonation Engine Inlet and Fill Zone Model," *AIAA Scitech 2021 Forum*, American Institute of Aeronautics and Astronautics, Jan. 2021.

[22] Feleo, A., Chacon, F., and Gamba, M., "Uncertainties in Thrust and EAP Measurements of a Rotating Detonation Combustor with Axial Air Inlet," *AIAA Propulsion and Energy 2020 Forum*, American Institute of Aeronautics and Astronautics, Aug. 2020.

[23] Feleo, A., Chacon, F., and Gamba, M., "Effects of Heat Release Distribution on Detonation Properties in a H2/Air Rotating Detonation Combustor from OH* Chemiluminesence," *2019 AIAA Propulsion and Energy Forum*, 2019.