Combustion instability modeling using multi-mode flame transfer functions and a nonlinear Euler solver

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Abstract
Modern methods for predicting combustion dynamics in high-pressure combustors range from high-fidelity simulations of sub-scale model combustors, mostly for validation purposes or detailed investigations of physics, to linearized, acoustics-based analysis of full-scale practical combustors. Whereas the high-fidelity simulations presumably capture the detailed physics of mixing and heat addition, computational requirements preclude their application for practical design analysis. The linear models that are used during design typically use flame transfer functions that relate the unsteady heat addition $q'$ to oscillations in velocity and pressure ($u'$ and $p'$) that are obtained from the wave equation. These flame transfer functions can be empirically determined from measurements or derived from theory and analysis. This paper describes a hybrid approach that uses high-fidelity simulations to generate flame transfer functions along with nonlinear Euler CFD to predict the combustor flowfield. A model rocket combustor that presented a self-excited combustion instability with pressure oscillations on the order of 10% of mean pressure is used for demonstration. Spatially distributed flame transfer functions are extracted from a high-fidelity simulation of the combustor and then used in a nonlinear Euler CFD model of the combustor to verify the approach. It is shown that the reduced-fidelity model can reproduce the unsteady behavior of the single element combustor that was both measured in the experiment and predicted by a high-fidelity simulation reasonably well.

Keywords
Combustion instability, rocket combustor, spatially distributed flame transfer functions, nonlinear Euler solver, non-premixed flow

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1. Introduction
Combustion instability is due to coupling between heat release, hydrodynamics, and acoustics. It is observed in many combustor systems, including rocket engines, gas turbine engines, and blast furnace and heating units. Thanks to the advancements in modern computing technologies, high-fidelity modeling approaches like Large Eddy Simulation (LES) and Detached Eddy Simulation (DES) can be applied to the complex problem of combustion dynamics, and provide many valuable insights into the coupling physics. Although high-fidelity simulations are becoming routine for laboratory-scale combustors, their use for modeling full-scale devices is still far out of reach. Therefore, for engineering applications, reduced-fidelity models like Helmholtz solvers are mostly used. This paper explores a hybrid, reduced-fidelity model that targets full-scale prediction. It uses results from a high-fidelity simulation to provide a model of the coupling between heat release, hydrodynamics, and acoustics.
release and acoustic fluctuations, and a nonlinear Euler CFD model to calculate the gas dynamic field and its response to unsteady heat release. This combination presumably captures most of the physics of the reacting flow along with nonlinear wave dynamics. The approach was demonstrated using a model rocket combustor that presented self-excited instabilities in a moderately nonlinear regime where pressure oscillations were on the order of 10% of mean pressure.

For increased physical insights and applicability, an engineering-level model should account for the acoustic modes in the combustor, realistic boundary conditions at the inlet and exit of the combustor, and the coupling between hydrodynamics, heat release and flowfield fluctuations. The nonlinear Euler equations are used here to mitigate the limitations of acoustics-based models related to nonlinear gas dynamics and flow boundary conditions.

Capturing the relationship between heat release and flow fluctuations in the chamber is key for accurate combustion instability modeling. One popular approach is the so-called Flame Transfer Function (FTF), and its nonlinear, amplitude-dependent counterpart the Flame Describing Function (FDF), which correlates unsteady heat release fluctuations to incoming pressure and velocity variations.

Flame transfer functions have been used extensively to study combustion instabilities in both laminar and turbulent premixed flames. They can be measured from experiments, in terms of a global flame transfer function in which the FTF is obtained from time-dependent, volume-integrated measurements of flame emission, and the velocity at the inlet of the combustor. The flame transfer function data obtained from the experiments are further used to develop a flame transfer function dispersion relation. Numerous studies dedicated to the influence of various flow parameters on the flame are found in the literature. Preetham and Lieuwen investigated the effects of flame structure on FTF and Duchaine et al. investigated the effects of flame speed, the expansion angle of burnt gases, inlet air temperature, inlet duct temperature, and combustor wall temperature on a laminar premixed flame. Beyond the global FTF approach, some studies have been dedicated to obtaining local flame transfer function from experiments. Kim et al. showed that, for the conditions of their study, the global flame transfer function can accurately predict the resonant modes and growth rates if the flame length is less than 10% of the acoustic wavelength. Otherwise, the local flame transfer function was found to be more accurate. The work presented in this paper explores the application of the FTF to a non-premixed flame in a rocket combustor where the reaction zone is distributed and extends far downstream in the combustor. The length of the reaction zone is typically higher than 10% of the acoustic wavelength. Hence, spatially distributed local flame transfer functions were used for this study.

High-fidelity simulations offer the advantage of highly-resolved flow fields for the extraction of FTFs and FDFs. Most of the previous studies can be categorized into two basic approaches: a frequency-domain approach, in which the global FTF obtained from the ratio of the Fourier transform of the global heat release fluctuations to the Fourier transform of pressure or velocity fluctuations; and an impulse response function approach, in which the FTF in the frequency-domain is obtained by taking Z-transform of the impulse response function extracted from a correlation of data in the time-domain.

The impulse function approach of extracting flame transfer functions from simulations was mainly used to integrate the developed FTF with acoustic solvers. Scarpato et al. investigated a reheat-combustor considering flame as a multiple input single output system and multiple input multiple output system using the Wiener-Hopf method to unlink the coupling between the effects of various flow parameters on combustion instability. The main assumption of the Wiener-Hopf method is that the system is linear, which is true at small fluctuations levels and is most applicable to gas turbine systems, but questionable for rocket combustors with heat release rates three-orders-of-magnitude greater than airbreathing counterparts, and pressure oscillation amplitudes that commonly exceed a few percent of the mean pressure.

The extraction and application of FTFs to non-premixed flames, like those in rocket combustors, are very limited. A recent attempt using the quasi one-dimensional Euler equations and n time-lag model yielded positive results but showed how several issues related to non-premixed flow mixing and flame characteristics can be suppressed in the 1-d approach. It should be noted that in rocket combustors, pressure oscillations with amplitudes that are within +/− 5% of mean pressure have historically been considered stable, and nonlinearities can quickly arise due to extreme rates of heat addition. The flame is highly distributed and intermittent, and reactions extend far downstream in the combustor.

For non-premixed flames where the mixing rapidly changes with the flow fluctuation levels, the acoustic solvers cannot account for the local variation of the fluid properties that may be necessary for accurate prediction. It is, however, important to note that the acoustic solvers can account for fluid properties through a pre-defined profile or source terms to account for mean flow gradients. These approximations are usually sufficient for premixed cases.
exhibiting relatively low amplitudes of the pressure fluctuations and therefore have a low impact on local fluid properties. The present work uses multi-dimensional nonlinear Euler equations together with spatially distributed local flame transfer functions to improve the local sensitivity of the modeling of the coupling between heat release, hydrodynamics, and pressure fluctuations.

The nonlinear Euler equations can capture the steep fronted waves and account for the effects of compressibility and complicated geometries, but viscous effects may need to be evaluated for their impact on the prediction. Multi-dimensional nonlinear Euler equations also allow the use of spatially dependent FTFs and modeling of transverse instabilities in rectangular and cylindrical chambers with multiple elements. They also allow for accurate treatment of nonlinear effects that result in limit cycle behavior and boundary conditions that are practical, and equivalent to those used in the high-fidelity simulations used to produce the FTF. Further, using nonlinear Euler equations allows physical insights to the entire flow field beyond what is provided by the acoustic solvers.

The motivation behind the development of this tool is to be able to predict combustion instabilities in a full-scale multi-injector rocket combustor using the high-fidelity simulation data of a single-injector or few-injectors systems. The underlying idea of this tool involves two steps. The first step is to use the high-fidelity simulation of a single-injector system and extract the FTFs/FDFs. The second step is to integrate the FTFs/FDFs with reduced-fidelity NLE solver to predict combustion instability in full-scale multi-injector rocket combustor. The FTFs/FDFs used in this approach are spatially resolved and are extracted on a point-by-point basis from the high-fidelity simulation. The underlying assumption for this approach is that the geometric influences of a single element are preserved in its full-scale utilization. It is possible that the full-scale system exhibiting transverse waves differs from the single element. Such a case can be handled by simulating a few elements in addition to the single-element simulation.

The computational savings of our approach come from the fact that expensive simulations involving the filtered, reacting Navier-Stokes equations with multiple species are restricted to the first stage where a single-element or few-element combustor is used to extract the FTFs/FDFs. In contrast, the full-scale multi-injector combustor, along with the geometric complexity of the combustor, is solved efficiently in a nonlinear Euler solver using the FTFs obtained in the second stage to represent all the injectors of the multi-injector combustor. In general, the first stage involves a high-fidelity three-dimensional detailed chemistry large eddy or detached eddy simulation while the second stage utilizes the FTFs/FDFs within a nonlinear Euler solver. For the purpose of the work presented in this paper, we utilize a two-dimensional hybrid RANS/LES simulation of the representative single-element combustor to extract the FTFs/FDFs. It is important to note that the proposed tool does not impose any restrictions on the type of high-fidelity simulation performed (LES, DES, etc.) to extract the FTFs.

The main objective of the current paper is to demonstrate a reduced-fidelity modeling approach for modeling combustion instability problems. The work presented in this paper is the first step towards developing a new tool that can predict combustion instabilities in practical systems. In this approach, the multi-mode FTFs/FDFs extracted from the high-fidelity simulations of a reduced-scale system are used to account for distributed unsteady heat release. The results presented in this paper show that the proposed reduced-fidelity model can reproduce the longitudinal combustion instability that was measured in a self-excited rocket combustor, and predicted by a high-fidelity simulation of the combustor. In this paper, we show the approach used to extract the spatially distributed local flame transfer functions from high-fidelity simulation results using Dynamic Mode Decomposition (DMD), and their integration with the nonlinear Euler equations. We also evaluate the capability of extracted FTFs to reproduce the self-excited combustion dynamics in a single element rocket combustor flow and conduct a limited sensitivity analysis on the effects of the number of modeled modes, grid resolution, and the number of sampling points from the simulation.

The remainder of this paper is organized as follows: In section 2, the formulation of a modeling framework is introduced. In section 3, the approach to extract flame transfer functions from a high-fidelity simulation by applying the DMD technique is presented. In section 4, verification of the proposed approach using a Rijke tube is presented. In section 5, the results of an analysis of the model sensitivity to the number of modes used in the FTF, the number of sampling points used in the Fourier transform of the unsteady heat release calculation, and the mesh size are presented. Summary, and conclusions are presented in section 6. A detailed framework of high-fidelity simulations is presented in Appendix 1.

2. Framework for integrating flame transfer function with nonlinear euler equations

To implement the FTF, a nonlinear Euler (NLE) solver with three species — oxidizer, fuel, and products was chosen. In the case of high-fidelity simulation, the
multi-species equations together with the computationally expensive reaction rates calculated at every time step are solved as shown in Appendix 1. However, in the proposed NLE framework only three species are being solved and their reaction rates are obtained from the time-averaged reference hybrid RANS/LES solution. This eliminates the need to compute the computationally expensive source terms of the species equations shown in Appendix 1. The governing equations that are being solved are

\[
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = H_{\text{mean}} + H_q
\]

where

\[
Q = \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho h_0 - p \\
\rho Y_f \\
\rho Y_{ox}
\end{pmatrix}, \quad E = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho u h_0 \\
\rho u Y_f \\
\rho u Y_{ox}
\end{pmatrix}, \quad F = \begin{pmatrix}
\rho v \\
\rho uv \\
\rho v^2 + p \\
\rho v h_0 \\
\rho v Y_f \\
\rho v Y_{ox}
\end{pmatrix}, \quad H_{\text{mean}} = \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
\omega_f \\
\omega_{ox}
\end{pmatrix}, \quad H_q = \begin{pmatrix}
0 \\
0 \\
0 \\
q''''(\hat{x}, t) \\
0 \\
0
\end{pmatrix}
\]

where $H_{\text{mean}}$ is the mean source term, $H_q$ is the unsteady source term, $\rho$ is the density, $u$ and $v$ are the components of velocity in $x$ and $y$ direction respectively, $h_0$ is the stagnation enthalpy, $p$ is the pressure, $Y_f$ and $Y_{ox}$ are the mass fraction of fuel and oxidizer respectively, $\omega_f$, $\omega_{ox}$ are the mean species destruction rates obtained by time-averaging hybrid RANS/LES simulation data, and $q''''(\hat{x}, t)$ is the fluctuating heat release per unit volume.

The fluctuating heat release, $q''''(\hat{x}, t)$, is obtained by performing inverse Fourier transform on the product of the FTF, $FTF(\hat{x}, \omega)$ and pressure fluctuations in the frequency-domain, $p'(\hat{x}, \omega)$, obtained by performing Fourier transform on the time-domain data of NLE simulation,

\[
q''''(\hat{x}, t) = F^{-1}(p'(\hat{x}, \omega) \ast FTF(\hat{x}, \omega))
\]

where $F^{-1}$ is the inverse Fourier transform. The FTF, $FTF(\hat{x}, \omega)$ is spatially distributed and calculated on a point-by-point basis (i.e. each spatial point is calculated independently of the others). The procedure followed in integrating the flame transfer function with the nonlinear Euler solver assumes that the time-averaged species destruction/production rates obtained from hybrid RANS/LES simulation will maintain proper mean conditions in the nonlinear Euler simulation. The integration procedure of the nonlinear Euler solver and the FTF mainly involves four steps:

1. Extract the flame transfer function from the high-fidelity simulation data of the combustor under study.
2. Obtain the time-averaged species destruction rates from the high-fidelity simulation and add them to the nonlinear Euler equations as source terms to species equations.
3. Initiate the NLE simulation using the time-averaged hybrid RANS/LES solution and run the simulation to record the pressure data necessary to activate the FTF.
4. Once pressure data of the NLE simulation are obtained, activate the FTF, and continue the NLE simulation.

In step-3 of the procedure outlined above, the NLE simulation without the FTF was run for 4 ms to record the pressure data of the NLE simulation. For the baseline simulation of the CVRC presented in section 4, the recorded time-domain pressure data of the NLE simulation was converted into the frequency-domain by choosing 1024 pressure points at equal intervals of time from the recorded data. The effect of number of the pressure points used for the conversion of time-domain pressure data into frequency-domain on the prediction capability of the proposed intermediate fidelity model is presented in section 5. A moving window of 4 ms of pressure data in the time-domain was used throughout the NLE simulation to obtain the pressure data in the frequency-domain at every time step, which is necessary to calculate corresponding heat release fluctuations in the time-domain. The approach to obtain the FTF from high-fidelity simulations is presented in the next section.

3. Extraction of flame transfer function from high-fidelity simulations

The flame transfer function (FTF), is a linear function that uses pressure and/or velocity fluctuations as an input and gives heat release fluctuations as the output. It is used in reduced-fidelity models to account for unsteady combustion by characterizing the response of the flame to pressure or velocity fluctuations. In the present work, pressure is used as the reference fluctuating input. The FTF is associated with a gain $G(\hat{x}, \omega)$ and
phase $\phi(\bar{x}, \omega)$ to transform the input fluctuations to a corresponding heat input fluctuation with appropriate magnitude and phase. Using pressure as the fluctuating parameter, the spatially resolved FTF, $FTF(\bar{x}, \omega)$, can be mathematically expressed as

$$FTF(\bar{x}, \omega) = \frac{q'''(\bar{x}, \omega)}{p'(\bar{x}, \omega)} = G(\bar{x}, \omega)e^{i\phi(\bar{x}, \omega)}$$ \hspace{3cm} (4)$$

The above expression can be interpreted as, when pressure fluctuations $p'$ at frequency $\omega$ are input through the FTF, the output will be heat release fluctuations $q'''$ at the same frequency. The ratio of magnitudes of heat release and pressure fluctuations at a particular frequency and location gives gain $G(\bar{x}, \omega)$ of the FTF and the difference of phases between the heat release and pressure fluctuations at that frequency and location gives the local phase of FTF, $\phi(\bar{x}, \omega)$. The Dynamic Mode Decomposition (DMD) technique\textsuperscript{35,38} can be applied to the reference pressure fluctuations and heat release fluctuations in the time-domain to isolate the frequency content. DMD is a dimensionality reduction technique similar to well established Proper Orthogonal Decomposition (POD)\textsuperscript{39,40} which reduces a high dimensional complex raw data set into lower dimensions (modes) that represent dominant features of the raw data set. POD reduces the raw data based on optimality to obtain a reduced set that best represents the original data set. POD organizes the reduced data set based on the energy content of each mode. Each POD mode comprises multiple frequencies. In contrast, DMD assumes a linear relationship in time between the snapshots of raw data and thereby reduces the raw data set into modes that are associated with a distinct frequency. This feature of DMD helps to identify the relation between variables at a particular frequency. Unlike the traditional post-processing techniques such as band-pass filtering which require a priori knowledge of the dominant frequencies and are susceptible to the various parameters used for the filtering, the decomposition techniques provide a systematic approach to identify the dominant features of the system, hence DMD was used to extract the FTF from hybrid RANS/LES data. Mathematically, it can be expressed as,

$$FTF(\bar{x}, \omega) = \frac{|q'''(\bar{x}, \omega)|e^{i\phi_{q'''}(\bar{x}, \omega)}}{|p'(\bar{x}, \omega)|e^{i\phi_p(\bar{x}, \omega)}} = G(\bar{x}, \omega)e^{i\phi(\bar{x}, \omega)}$$ \hspace{3cm} (5)$$

where $|q'''(\bar{x}, \omega)|$ and $|p'(\bar{x}, \omega)|$ are the magnitude of heat release and pressure fluctuations, and

$$\phi(\bar{x}, \omega) = \phi_{q'''}(\bar{x}, \omega) - \phi_p(\bar{x}, \omega)$$ \hspace{3cm} (6)$$

where $\phi_{q'''}(\bar{x}, \omega)$ and $\phi_p(\bar{x}, \omega)$ are the phase of heat release and pressure fluctuations in the frequency-domain.

Through the above procedure, the local magnitude of the FTF and phase difference between the heat release and reference (pressure) fluctuations can be obtained. This approach results in a spatially resolved FTF in the frequency-domain. For reference fluctuations at frequencies that lie outside the frequency range associated with the FTFs developed, the output heat release fluctuations will be zero. To obtain the heat release fluctuations that interact with the combustor instability modes, FTFs need to be extracted at each frequency that corresponds to a mode of interest.

The FTFs are valid at the frequency and the amplitude for which they were extracted. The prediction of combustion instabilities, therefore, requires the FTFs to be extracted at varying amplitudes and frequencies. The purpose of this paper is to demonstrate the extraction, implementation and challenges in a spatially distributed FTF using decomposition techniques in a known model rocket combuster. It is thus deemed sufficient to extract the FTF at the limit cycle amplitude of the reference simulation and at the resonant frequencies observed through decomposition. It should be stressed here that the validity of this technique relies on close correspondence between the flow-field obtained in the original simulation and the NLE-FTF solution.

It is possible to extend the proposed approach to a single element embedded in a multi-element combuster for the purpose of FTF extraction. Such a multi-element combuster may not necessarily be the full combuster but should allow for interactions between the adjoining elements to capture the influence of important physics. It is further possible to impose the acoustic field through boundary conditions such as described in the literature.\textsuperscript{41,42} The FTFs extracted from several such simulations can be combined for the purpose of producing an effective FDF for a single element. Including the effects of resonators or other acoustic devices is possible in this manner and it is an important advantage of the proposed approach. A primary limitation that needs to be recognized here is the geometric influence of the injector, which is assumed to be invariant between the single injector and a multi-injector combuster. A new injector will, therefore, require a new FDF to be formulated before attempting the full combuster simulation with the proposed approach.

4. Application of the NLE-FTF reduced-fidelity model

Verification using Rijke tube test case

The proposed approach of extracting the FTF and integrating it with the nonlinear Euler solver was
verified using a Rijke tube test case. A Rijke tube of length 0.5 m and radius 0.0225 m was considered. In this test case, unsteady heat release was added 0.125 m from the inlet of the tube following a simple linear dependence model

$$q'(t) = np'(t)$$  \hspace{1cm} (7)

where $q'$ is the heat release fluctuations in W, $n$ is the interaction index, and $p'$ is the pressure fluctuations in Pa. The linear model implemented is similar to the so-called $n - \tau$ model proposed by Crocco and Cheng with zero time-lag. For this study, $n = 2.8e-5$ W/Pa was chosen. The heat addition zone was spread across a length of 9 mm. Pressure boundary conditions were imposed at the inlet and outlet of the surrounding domain as shown in Figure 1. For all calculations and results reported henceforth, the interior tube is considered.

The peak-to-peak pressure oscillations observed in the limit cycle are found to be 10.5% of the mean pressure. A single dominating mode at 650 Hz corresponding to the first longitudinal mode of the tube was observed from the DMD power spectrum. Following the procedure outlined in section 3, the flame transfer function corresponding to 650 Hz was extracted. The gain of the extracted flame transfer function multiplied by the volume was found to be $2.8e-5$ W/Pa, equal to the $n$ of the linear model imposed, and the phase lag was found to be zero. This verified that the approach followed to extract the gain and phase of the FTF is mathematically correct.

The FTF was integrated with the nonlinear Euler solver following the procedure outlined in section 2. A comparison of the limit cycle pressure and Power Spectral Density (PSD) between the original simulation and the simulation with FTF is shown in Figure 2. A very good agreement between the limit cycle pressure fluctuations and PSDs was observed. Also, a very good agreement in terms of the mean pressure and temperature was observed between the original simulation and the simulation with FTF.

From the results obtained, it can be inferred that the approach proposed to extract the spatially distributed local flame transfer function and its integration with nonlinear Euler solver is verified. Successful verification of the proposed approach motivated its application to a model rocket combustor that demonstrates repeatable self-excited instability.

**Application to the continuously variable resonant combustor**

The Continuously Variable Resonant Combustor (CVRC) is a single element combustor with a gas-gas coaxial injector that is capable of exhibiting self-excited longitudinal instabilities and has been used as a benchmark case for model validation. The schematic of the CVRC is shown in Figure 3. The CVRC has a variable-length oxidizer post which can be adjusted by using the electro-mechanical actuator connected to the inlet of the oxidizer post. The inlet is choked to maintain a constant mass flow rate and provides an inlet boundary condition that can be modeled or simulated. The exit of the oxidizer post is matched to a dump combustor of length 0.381 m, which ends in a choked
The oxidizer post length can be varied from 0.089 m to 0.1905 m either continuously during an experiment or can be fixed at a particular post length of interest. The CVRC uses 90% hydrogen peroxide as the oxidizer, which when passed over a catalyst bed decomposes into 42.35% oxygen and 57.65% water vapor at 1030 K. Methane at 298 K is used as the fuel. The CVRC is operated at an equivalence ratio of 0.8. The test conditions are summarized in Table 1.

The CVRC exhibits repeatable self-excited instabilities at a limit cycle amplitude that is dependent on the oxidizer post length. Linear growth rates can be measured for fixed-post-length cases. The lowest limit cycle amplitudes corresponded to an oxidizer post length of 0.089 m, with peak-to-peak pressure fluctuations around 8% of the mean pressure. The most unstable case was observed when the oxidizer post length was 0.1397 m, with peak-to-peak pressure fluctuations around 40% of the mean pressure. At oxidizer post length 0.1905 m, the system was found stable during some runs and unstable during the rest. For this work, the repeatable weakly nonlinear case was chosen, i.e. 0.089 m oxidizer post length case. In this case, oscillations corresponding to the first three longitudinal modes can be seen from a spectral analysis of the pressure signal. Henceforth, the reference case will be referred to as CVRC 0.089 m oxidizer post length case.

The base-line simulation of the CVRC 0.089 m oxidizer post length case, two-dimensional axisymmetric hybrid RANS/LES simulation, was performed using an in-house finite volume solver GEMSMA which solves continuity, Navier-Stokes, energy and species equations using a dual-time formulation, implicit second-order time discretization, and second-order spatial discretization scheme.46 In the current work, the base-line simulation is referred to as the high-fidelity simulation to maintain generality. The hybrid RANS/LES approach uses the two-equation $k-\omega$ turbulence model to model the flow in regions where turbulence length scale cannot be resolved and in the rest of the domain it switches to LES mode. The computational mesh used for these simulations has 100k nodes. The computational setup of the CVRC and the mesh near the dump plane is shown in Figure 4. Both the oxidizer and fuel inlets were modeled as the constant mass flow boundaries and the exit of the chamber was modeled using the static pressure boundary. In terms of species mass fraction, the fuel inlet was modeled as 100% CH$_4$ and the oxidizer inlet was modeled as 42% O$_2$ and 58% H$_2$O. The chemical kinetics were modeled using a single step global chemistry reaction:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O.$$  

Flame transfer functions of the CVRC

The dynamic mode decomposition power spectrum of pressure and heat release signals of the CVRC 0.089 m oxidizer post length case obtained from the high-fidelity simulation is shown in Figure 5. The DMD spectrum of pressure shows that the first three dominant modes were observed at 1700 Hz, 2750 Hz, and 3375 Hz, whereas the DMD spectrum of heat release

![Figure 3. Experimental setup of the Continuously Variable Resonance Combustor (CVRC).](image-url)
shows only two dominating modes at 1700 Hz and 3375 Hz.

Following the approach outlined in section 2, the flame transfer functions corresponding to the first three dominant modes of the pressure, 1700 Hz, 2750 Hz, and 3375 Hz were extracted from the hybrid RANS/LES simulation data. In this work, the FTF is defined based on the pressure fluctuations as outlined in section 3. Hence, in this baseline simulation, the most dominant modes observed in the DMD power spectrum of pressure are included in the FTF. The effect of the modes included in the FTF on the prediction capability of the proposed intermediate fidelity model is presented in section 5. The gain of the flame transfer function, which is the ratio of heat release and pressure fluctuations, and phase of the flame transfer function, which is obtained by cross-correlation of pressure and heat release fluctuations, for the first three dominant modes is shown in Figure 6. The phase is insignificant in the regions with a relatively small gain. Hence, for better clarity, all the phase plots presented in this paper are filtered based on the normalized gain of the FTF and are referred to as gain-weighted phase plots. The gain of the FTFs appears to be more distributed for low energy modes and concentrated for the high energy modes. It is expected, since the gain of FTF is the ratio of heat release and pressure fluctuations. Higher heat release and lower pressure fluctuation levels lead to higher FTF gain and vice versa. The presence of high FTF gain at the pressure node locations, where small amounts of heat addition are much larger than the small pressure fluctuations that exist there, can be explained by the same reason.

The phase difference results show that the temporal coupling between heat release and pressure fluctuations varies across modes. The phase difference plot for the 1700 Hz mode shows a very strong coupling between the heat release and pressure fluctuations compared to other modes. It is evident from Figure 6 that both the FTF gain and phase difference are distributed.

**NLE-FTF simulation of the CVRC**

The DMD power spectrum of the heat release signals in Figure 5 shows only four dominant modes at 1700 Hz, 3375 Hz, 5075 Hz, and 5275 Hz. Hence, the cut-off frequency for the FTF extraction was chosen to be 5275 Hz. However, within the cut-off frequency, an additional dominant mode was observed in the DMD power spectrum of the pressure signals at 2750 Hz. A study on the effect of the number of modes included in the FTF revealed that the peak-to-peak amplitude of pressure oscillations observed in the NLE-FTF simulation results agreed best with the reference simulation when the modes 1700 Hz, 2750 Hz, and 3375 Hz were included in the FTF. Hence, the NLE-FTF simulation of the CVRC with 1700 Hz, 2750 Hz, and 3375 Hz modes included in the FTF is chosen in this section to provide an in-depth discussion of the NLE-FTF simulation results. A detailed discussion about the sensitivity of the NLE-FTF simulation to the modes included in the FTF is presented in section 5. Once the FTFs corresponding to the 1700 Hz, 2750 Hz, and 3375 Hz modes were extracted, the NLE-FTF simulation of the CVRC was performed as outlined in section 2. To eliminate any mesh size-related uncertainties, the same mesh that was used in the hybrid RANS/LES simulations was used for the NLE simulations. The NLE-FTF simulation was initialized...
using the time-averaged hybrid RANS/LES solution and the time-averaged species production rates of the reference high-fidelity simulation were imposed as the species source terms in the NLE simulation. The non-premixed and highly energetic nature of rocket combustion results in a very unsteady flame, and superimposing steady heat addition on the time-averaged solution results in unrealistic local temperatures. Hence, the heat addition approach was modified through a variable gain approach, in which the imposed species destruction rates from the time-averaged solution of the original simulation were modified to account for the local cell constituents and were then multiplied by a gain defined as the ratio of the instantaneous steady heat added in the NLE simulation to the mean heat added in the reference hybrid RANS/LES simulation,

$$\text{Gain}(t) = \frac{\dot{q}_{\text{ref}}}{\dot{q}_{\text{NLE}}(t)}$$  \hspace{1cm} (9)

where $\dot{q}_{\text{ref}}$ is the mean integrated heat release rate of the reference simulation and $\dot{q}_{\text{NLE}}(t)$ is the instantaneous integrated heat release rate of the NLE simulation.

$$\dot{\omega}_f(\vec{x}, t) = \text{Gain}(t) \ast \dot{\omega}_{f,\text{lim}}(\vec{x}, t)$$  \hspace{1cm} (10)

where $\dot{\omega}_f(\vec{x}, t)$ is the instantaneous local fuel destruction rate of the NLE simulation and $\dot{\omega}_{f,\text{lim}}(\vec{x}, t)$ is the local time-averaged fuel destruction rate obtained from the hybrid RANS/LES simulation and adjusted for local cell constituents. Using this dynamic gain approach correct mean conditions at every time step of the NLE-FTF simulation and at varying flow fluctuation levels required for using the FTF were obtained.

The FTF is activated once pressure data is obtained in the NLE simulation as outlined in section 2 and the NLE-FTF simulation is continued thereafter. The pressure trace measured close to the aft end of the combustor, at 0.368 m downstream of the dump plane is compared in Figure 7. The pressure trace in the NLE-FTF simulation shows a steady growth before reaching a limit cycle due to the linear relationship between unsteady heat release and pressure imposed by the FTF. However, the hybrid RANS/LES simulation reaches a limit cycle within 10 ms; we believe this is largely due to the way the LES simulation is initiated. Comparisons between the pressure-time traces at limit cycle conditions and PSDs from the NLE-FTF and reference high-fidelity simulations are shown in Figure 8.

The peak-to-peak pressure oscillations in the limit cycle of NLE-FTF simulation were found to be 10.8% of the mean pressure, agreeing well with the reference of 10.5% predicted by the hybrid RANS/LES simulation. However, the NLE-FTF pressure trace appears to be more sinusoidal compared to the hybrid RANS/LES simulation pressure trace which contains much sharper peaks. This difference between the NLE-FTF and the reference simulation is expected since only three FTFs corresponding to the first three dominant modes were used. It should be noted that the thermal conductivity and viscosity effects are not...
included in the NLE solver. The PSD comparison between the NLE-FTF and high-fidelity simulations shows that the dominant 1L mode (1700 Hz) and 2L mode (3375 Hz) are reproduced by the NLE solver to a good extent. Some discrepancy was observed in capturing the 2750 Hz mode. The FTF’s included were based on the first three dominant modes observed in the DMD spectrum of the pressure. However, the DMD spectrum of heat release showed only two dominant modes corresponding to the first and third dominant modes of the pressure. The absence of the effects of heat release at frequencies other than the three modes considered could be a reason for the discrepancy observed in the NLE simulation.

A typical pressure cycle of the NLE-FTF and hybrid RANS/LES simulation is compared in Figure 9. The NLE-FTF simulation is seen to generally match the wave motion in the chamber and oxidizer post as seen from the hybrid RANS/LES. The points of the analyzed cycle are numbered on the pressure trace shown in Figure 8(a). The cycle begins with high pressure at the aft end of the combustor in both the sets of results. The correspondence observed at the second point of the cycle between the low-pressure region within the oxidizer post suggests the similarities of the physics being modeled. The heat release in the case of NLE-FTF is dependent on the fluctuating pressure, which serves as an input to the FTF. The FTF in addition to the mean species consumption rate, approximates the unsteady heat release in the hybrid RANS/LES and due to the limited number of modes used in its construction, the differences in the pressure contours are discernible. The third point of the cycle, which shows the peak pressure at the head end of the combustor shows this difference. Since the heat release at the head end during the limit cycle conditions is the primary driving mechanism, the differences in the rest of the pressure cycle are expected.

The fuel mass fraction cycle obtained is shown in Figure 9. The periodic combustion observed during the limit cycle in the hybrid RANS/LES is mimicked in the NLE-FTF approach. The mean species destruction rates imposed are limited according to the local mixture conditions, which allows the accumulation of the fuel. The FTF based heat release, while accounting for the fluctuating part ensures the total fuel consumption. With this approach, the start of the fuel consumption during the initial two points of the cycle followed by maximum fuel destruction during the third point and beginning of the fuel accumulation for the next cycle can be seen in the last two points of the cycle from both sets of the results.

The corresponding temperature cycle is shown in Figure 10. The NLE-FTF simulation has a wider range of temperatures compared to the hybrid RANS/LES simulation. This is due to the unsteady heat release, which does not depend on the local cell constituents, instead, rely on the unsteady pressure at that location. After reaching the limit cycle condition, the same amount of heat is added and removed during the compression and expansion halves of the cycle, which maintains the correct mean temperature and hence the correct mean speed of sound. The frequencies obtained in the NLE-FTF simulation therefore closely match those observed with the hybrid RANS/LES results, as shown in Figure 8.

The cycle analysis and PSD comparison show that the NLE-FTF simulation is able to reproduce the major flow characteristics. From the perspective of the limit cycle comparison, the NLE-FTF simulation
Figure 9. Comparison of axisymmetric two-dimensional pressure and fuel mass fraction contours pressure between the hybrid RANS/LES and NLE-FTF simulations for one pressure cycle. The numbering 1 to 5 corresponds to the points in the cycle shown in Figure 8(a).

Figure 10. Comparison of axisymmetric two-dimensional temperature contours between the hybrid RANS/LES and NLE-FTF simulations for one pressure cycle. The numbering 1 to 5 corresponds to the points in the cycle shown in Figure 8(a).
was able to reproduce the high-fidelity solution to a good extent. It suggests that the proposed approach of the spatially resolved FTF’s extracted from the high-fidelity hybrid RANS/LES simulation together with a nonlinear Euler solver can reproduce the behavior of a rocket combustor to a good extent both in terms of mean variables and limit cycle statistics. Although the results obtained motivate the extension of this approach to a multi-element system, the next imperative is to understand the effects of the model control parameters on its predictive capability.

5. Sensitivity analysis of the NLE-FTF model

The CVRC results presented in section 4 were obtained using the FTFs corresponding to first three dominant modes observed in the DMD power spectrum of pressure, using the same mesh as the reference hybrid RANS/LES simulation and 1024 pressure data points were used in the Fourier transform calculation of the unsteady heat release. The control parameters such as the number of modes in the FTF, the number of sample points used for the Fourier transform, and the mesh size may influence the prediction capability of the NLE-FTF model to a certain extent. To establish the utility and generality of the model, we characterize the effects of these control parameters on its predictive capability. Hence a sensitivity analysis of the proposed NLE-FTF reduced-fidelity model was performed using the CVRC 0.089 m post length case. The number of modes considered for FTF extraction to use in the NLE-FTF simulation were varied from one to five, the number of pressure data points used for the unsteady heat release calculation was varied from 128 to 1024, and the mesh size was varied from 20,000 to 100,000 nodes.

Number of modes in the flame transfer function

Five cases were studied by varying the number of modes included in the flame transfer function used in the reduced-fidelity simulation. The mode selection/ordering for each case is based on the following logic: select a cut-off frequency and 1. include FTFs corresponding to the dominant frequency peaks observed in the heat release DMD spectrum within that cut-off frequency (case-1, case-2, and case-4). 2. include FTFs corresponding to the dominant frequency peaks observed in both the pressure and heat release DMD spectra within that cut-off frequency (case-1, case-3, and case-5). The cut-off frequency for case-1 is 1700 Hz, for case-2 and case-3 it is 3400 Hz, and for case-4 and case-5 it is 5275 Hz. To avoid any inconsistencies due to mesh size, all the cases were run using the same mesh used for the reference hybrid RANS/NLE simulation.

First, the results of NLE-FTF simulation are compared to the results of hybrid RANS/LES simulation from which the FTFs were extracted. A comparison of the limit cycle pressure trace between the hybrid RANS/LES simulation and reduced-fidelity NLE simulations with a varying number of modes in the FTF is shown in Figure 11. From the plot, it can be seen that the limit cycle pressure traces of all the NLE-FTF simulations except the 1-mode and 5-mode NLE-FTF simulation are in close agreement with each other and agree with the reference high-fidelity simulation data to a good extent. The average peak-to-peak pressure oscillations in the reference high-fidelity simulation

Figure 11. Comparison of (a) limit cycle pressure trace and (b) PSDs between the NLE-FTF simulations with a varying number of modes and the hybrid RANS/LES simulation.
measured over the entire limit cycle are 10.5% of the mean pressure. In the reduced-fidelity simulation, the average peak-to-peak pressure oscillations of the 1-mode, 2-mode, 3-mode, 4-mode FTF and 5-mode FTF simulations are 14.0%, 13.5%, 10.8%, 12.0%, and 14.5% respectively.\textsuperscript{48} The limit cycle amplitudes observed in the experiment, hybrid RANS/LES simulation, and the reduced-fidelity simulations are summarized in Table 2.

From the results, it can be seen that agreement between the NLE-FTF and reference simulation improves as the number of dominant heat release modes in the FTF are increased from 1 to 3 (case-1, case-2, and case-4). However, the NLE-FTF simulations with the 5-mode FTF, case-5, showed a slightly higher level of fluctuations than the case-4. We conjecture that the discrepancy in the limit cycle amplitude of the 5-mode FTF simulation is due to the presence of a pressure node in the heat release zone for the high-frequency modes and the inclusion of 2750 Hz mode that is not dominant in the heat release spectra but only in the pressure spectra. Among the five cases, the peak-to-peak pressure oscillations in the limit cycle of NLE-FTF simulation with the 3-mode FTF agreed best with the hybrid RANS/LES simulation.

As is evident from Figure 11(a), the hybrid RANS/LES simulation exhibited much sharper peaks compared to the NLE-FTF simulation. The NLE-FTF simulation with the least number of modes in the FTF exhibited more sinusoidal behavior (broad peaks) than others. This behavior may be due to the approximation of heat release oscillations as the sum of a limited number of sine waves. It can be observed from the plots that the pressure peaks are becoming much sharper as the number of modes in the FTF are increasing. A near-exact match of wave shape may be possible if even more modes are included in the FTF formulation. However, this is prevented by the presence of a pressure node in the heat release zone of the high-frequency modes.

A comparison of PSDs between the hybrid RANS/LES simulation and the NLE-FTF simulations is shown in Figure 11(b). From the plot, it can be seen that the NLE-FTF simulations mostly reproduced the modes that were included in the FTF of that particular simulation. The 1-mode FTF simulation reproduced only the first longitudinal mode, which was overestimated. No other dominant peaks corresponding to the higher longitudinal modes were observed. The 2-mode FTF simulation reproduced the first longitudinal mode (1L) to a good extent and slightly underestimated the second longitudinal mode (2L). Similar to the 1-mode FTF simulation, no other peaks corresponding to the higher longitudinal modes were observed. The 3-mode FTF simulation reproduced the first longitudinal mode to a good extent, but underestimated both the 2750 Hz mode and the second longitudinal mode. The 4-mode FTF simulation reproduced the first and second longitudinal modes to a good extent but over-estimated the 3L mode. Similarly, the 5-mode FTF simulation reproduced the first and second longitudinal modes to a good extent but over-estimated the 3L mode. In addition, the 5-mode FTF simulation also reproduced the 2750 Hz mode to a good extent. Although the 4- and 5-mode FTF simulations have slightly over-estimated the limit cycle amplitudes, the overshoot appears to be mainly due to incorrect prediction of the 3L mode. Both 4-, and 5-mode FTF simulations have reproduced the 1L, and 2L modes more accurately than other FTF simulations.

As mentioned earlier, the spatially distinct pressure node of the high-frequency mode in comparison with the heat release node is believed to be partly responsible for this over-prediction of the 3L mode by the 4-, and 5-mode FTF simulations. The pressure and the heat release mode shapes corresponding to the 5075 Hz mode of the 4 modes FTF simulation are shown in Figure 12. The FTF, being the ratio of heat release fluctuations and pressure fluctuations, can have a very large value as a consequence. The gain of the FTF of 5075 Hz is shown in Figure 13. From the

| Case                  | Modes included in the FTF | peak-to-peak limit cycle amplitude (% of mean pressure) |
|-----------------------|---------------------------|--------------------------------------------------------|
| Experiment            |                           | 8.5%                                                   |
| Hybrid RANS/LES simulation |                       | 10.5%                                                  |
| 1 mode FTF simulation | 1700 Hz                   | 14.0%                                                  |
| 2 modes FTF simulation| 1700 Hz, 3375 Hz          | 13.5%                                                  |
| 3 modes FTF simulation| 1700 Hz, 2750 Hz, & 3375 Hz| 10.8%                                                  |
| 4 modes FTF simulation| 1700 Hz, 3375 Hz, 5075 Hz, & 5275 Hz | 12.0%                                                  |
| 5 modes FTF simulation| 1700 Hz, 2750 Hz, 3375 Hz, 5075 Hz, & 5275 Hz | 14.5%                                                  |
plot, it can be seen that the gain of the FTF is very high at the location of the pressure node, which probably leads to non-physical heat addition/removal in the NLE-FTF simulation.

To address this issue arising due to the mode shape of the 5075 Hz mode, an engineering approach is proposed wherein, the length scale of the pressure node is altered by selecting a lower cut-off of 10% for defining the pressure mode shape. The resulting pressure node appears to be spread over a longer length scale, thus avoiding the sharp peaks in the FTF magnitude that are likely unphysical and numerically challenging. This correction is believed to have led to an over-prediction of the 3L mode by the 4-, and 5- mode FTF simulations. A correction of this sort is likely necessary for any spatially resolved FTF simulations with high-frequency modes (which may have pressure nodes in the heat release zone) and needs to be investigated further. Based on the results of all NLE-FTF simulations, it appears that we may have to consider \( N + 1 \) modes FTF for accurate prediction of the \( N \) dominant mode system, where \( N \) is the number of dominant modes expected in the system. For example, if a system exhibits first harmonic at 2000 Hz and if we would like to predict the behavior of the system till the third harmonic, 6000 Hz, then it may be necessary to include modes up to 8000 Hz in the FTF formulation.

A comparison of the pressure mode shapes between the hybrid RANS/LES simulation and the NLE-FTF simulation is shown in Figure 14. All the NLE-FTF simulations with a varying number of modes in the FTF reproduced the mode shape of the first longitudinal mode accurately. The 1-mode FTF simulation failed to reproduce the mode shape of the second longitudinal mode. It was expected since only the information related to the first longitudinal mode was included in the FTF. The 2-, 3-, 4- and 5-mode FTF simulations reproduced the mode shape of the second longitudinal mode well. From the results, it is evident that if a sufficient number of modes are included in the FTF, the NLE-FTF approach can predict accurate limit cycle behavior, mean flow conditions, and mode shapes.

One of the interesting features observed in the reduced-fidelity NLE-FTF simulations is the linear
growth of pressure fluctuations before reaching the limit cycle although the FTF used corresponds to the limit cycle of the original simulations. The flow fluctuations in the NLE-FTF simulation started at a very low level and grew until they reached the limit cycle prescribed by the FTF extracted from the high-fidelity simulation as shown in Figure 7(a). Since the hybrid RANS/LES simulation did not exhibit the growth of modes to limit cycle, the experimental data were used here for the comparison with the NLE-FTF simulations. In the experiments, the growth rate of the first longitudinal mode was found to be approximately 76 s\(^{-1}\). In the 2-, 3-, 4-, and 5-mode FTF simulations the growth rate of the first longitudinal mode was found to be 96 s\(^{-1}\), 116 s\(^{-1}\), 98 s\(^{-1}\), and 95 s\(^{-1}\) respectively, in reasonable agreement with each other and the experiment. The growth rate of the second longitudinal mode in the experiment, 4-mode FTF, and 5-mode FTF simulation was found to be 300 s\(^{-1}\), 270 s\(^{-1}\), and 330 s\(^{-1}\) respectively. This potential ability of the NLE-FTF model to grow to the limit cycle prescribed by the extracted FTF at limit cycle conditions is remarkable and needs to be further explored. For instance, nonlinearities of the heat release field at the conditions of this study may be sufficiently weak such that linear growth to the limit cycle is a good approximation (acoustic nonlinearities are accounted for by the NLE framework). The use of amplitude-dependent FTFs, or flame describing functions, are probably needed for cases where there are strong nonlinear effects of amplitude on the heat release.

**Number of sample points used in unsteady heat release calculation**

In addition to varying the number of modes in the FTF, a sensitivity analysis is also performed by varying the number of sampling points of pressure used in Fourier transform to obtain the unsteady heat release. By varying the number of sample points, we effectively varied the rate at which pressure data is collected in the NLE-FTF simulation to calculate the unsteady heat release. The rate at which pressure data were collected determines the highest frequency resolved. Four cases were simulated with the number of sampling points set to 128, 256, 512, and 1024 points. For this analysis, all the simulations were run using the 3-mode FTF, since that simulation showed better agreement with the hybrid RANS/LES simulation in terms of the limit cycle amplitude. It was found that the NLE-FTF simulation with 128 and 256 sampling points exhibited pressure fluctuations with peak-to-peak amplitudes measured around 14% of the mean pressure. Whereas, the NLE-FTF simulation with 512 and 1024 sampling points exhibited pressure fluctuations with peak-to-peak amplitudes measuring around 13% and 10.8% of the mean pressure respectively. A comparison of PSDs between the FTF-NLE simulations with a varying number of sampling points and hybrid RANS/LES simulations is shown in Figure 15. It can be observed from the PSDs comparison plot that as the number of sampling points was increased the prediction capability of the NLE-FTF simulations seemingly improved. The NLE-FTF simulations with less number of sampling points over estimated the first two longitudinal modes. It is noteworthy that the difference in the limit cycle amplitudes between the hybrid RANS/LES simulations and the NLE-FTF simulation is within 2%.

**Mesh size**

Mesh sensitivity analysis was performed by varying the mesh size from 20,000 nodes to 100,000 nodes. This analysis was performed using the 3-mode FTF, similar to the sampling points analysis. Three simulations were performed by setting mesh size to 20,000, 50,000, and 100,000 nodes corresponding to the coarse, intermediate, and fine mesh sizes respectively. The peak-to-peak limit cycle amplitudes of pressure fluctuations were found to be 4%, 8%, and 10.8% of the mean pressure in the coarse, intermediate, and fine mesh respectively. This deviation of results at lower mesh size is expected possibly due to excessive numerical damping in the coarse mesh. A comparison of the PSDs between the hybrid RANS/LES simulation and the NLE-FTF simulation at various mesh sizes is shown in Figure 16. From the PSDs comparison, it is clear that as the mesh size was increased from coarse to fine, the limit cycle amplitudes of pressure fluctuations converged to

![Figure 15. Comparison of PSDs between the NLE-FTF simulations with a varying number of sampling points and the hybrid RANS/LES simulation.](image-url)
the hybrid RANS/LES simulation results. The fine mesh, which was used for hybrid RANS/LES simulation was used for all the NLE-FTF simulations.

**Two-dimensional reference point-based FTF**

Most previous applications of the FTF use a reference signal, e.g. velocity fluctuations at the combustor inlet, as input. To understand the importance of accounting for local coupling between heat release and pressure fluctuations, further analysis was performed using a two-dimensional point-based distributed FTF. In two-dimensional point-based distributed FTF, instead of calculating the gain and phase of the FTF using local heat release and pressure information, the gain and phase of the FTF were calculated using a reference pressure signal located upstream of the dump plane. For this study, the pressure signal 0.0127 m upstream of the dump plane was used as the reference and only the first three dominant modes, 1700 Hz, 2750 Hz, and 3375 Hz were considered in the extraction of FTF. The gain and phase of the two-dimensional point-based distributed FTF is shown in Figure 17.

One advantage of using FTFs based on the reference signal is that it eliminates the issues related to the presence of pressure nodes in the heat release zone, which were observed in two-dimensional spatially resolved FTFs with 4 and 5 modes. However, the dependency of the heat release fluctuations of the entire combustor on the pressure signal at one particular location makes the approach vulnerable. The obtained FTFs were integrated with the NLE solver in the same way as outlined in section 2. The pressure trace measured in the NLE-FTF simulation, 0.368 m downstream of the dump plane is shown in Figure 18.

From the plot, it can be observed that the pressure fluctuations grew exponentially up to 40% of the mean pressure before the system reached a limit cycle with pressure fluctuations that are 30% of the mean pressure, far off the expected results. In contrast, the NLE-FTF simulation performed using two-dimensional spatially resolved FTF reached a limit cycle with pressure fluctuations 10.8% of the mean pressure, as shown in Figure 8(a), close to the $\rho'$ predicted by reference hybrid RANS/LES simulation. A comparison of the limit cycle amplitudes and PSDs between the two-dimensional point-based FTF and reference hybrid RANS/LES simulation is shown in Figure 19. The PSD and pressure trace comparison show that the NLE-FTF simulation with two-dimensional point-based FTF has resulted in a completely different

![Figure 16. Comparison of PSDs between the NLE-FTF simulations with varying mesh size and the hybrid RANS/LES simulation.](image)

![Figure 17. The gain and gain-weighted phase of the first three modes of two-dimensional point-based FTF.](image)

![Figure 18. The pressure signal measured 0.368 m downstream of the dump plane in the NLE-FTF simulation with two-dimensional point-based FTF.](image)
system behavior in comparison to the reference hybrid RANS/LES simulation. The instantaneous high heat release events in the rocket combustor may affect the local coupling between pressure and heat release fluctuations. Hence, the use of a reference pressure signal may not be able to accurately capture the coupling between pressure and heat release fluctuations, leading to results that are far off from the reference simulation. Hence, it is preferable to use spatially resolved FTFs based on local heat release and pressure for prediction of combustion instabilities in rocket combustors.

One-dimensional spatially resolved FTF

To understand the importance of accounting for two-dimensional effects, further analysis was performed using a one-dimensional spatially distributed FTF. The one-dimensional spatially distributed FTF was obtained by using spatially averaged (in the radial direction) DMD modes of pressure and heat release. The gain and phase of the FTF were then calculated using local pressure and heat release fluctuations. For this study the 3-mode FTF, with the first three dominant modes, 1700 Hz, 2750 Hz, and 3375 Hz were considered. The gain and phase of the one-dimensional spatially distributed FTF are shown in Figure 20. It can be seen that there is no variation of the gain and phase of the FTF in the radial direction for the one-dimensional FTFs. For this study, two-dimensional axisymmetric NLE simulation was performed together with the one-dimensional FTF.

A comparison of the pressure traces and PSDs between the hybrid RANS/LES simulation, the NLE-FTF simulation with two-dimensional spatially resolved FTF (henceforth referred as 2D FTF simulation), and the NLE-FTF simulation with one-dimensional spatially resolved FTF (henceforth referred as 1D FTF simulation) is shown in Figure 21. In 1D FTF simulation, the limit cycle has peak-to-peak pressure fluctuations 14% of the mean pressure, 3% higher than those observed in the 2D FTF simulations. Also, the growth rate of the first longitudinal mode measured in the 1D FTF simulation is 36 s⁻¹, much lower than the growth rate obtained in the 2D FTF simulations. Although no significant difference in the limit cycle amplitudes was observed between the 2D
FTF and 1D FTF simulations, in both the simulations local gain and phase were used to calculate the corresponding heat release fluctuations and the simulations were performed using 2D NLE solver. Since the computational cost is the same for both the 1D FTF and 2D FTF simulations and better agreement with the high-fidelity simulations was observed in the case of 2D FTF simulations, it is preferable to use 2D FTF simulations for the prediction of combustion instabilities in rocket combustors.

6. Summary and conclusions
A hybrid approach for developing flame transfer functions for the prediction of combustion instability was presented. The flame transfer functions are generated from high-fidelity simulations and are incorporated into a nonlinear Euler CFD model. To preserve physical insights from the high-fidelity simulations, multi-mode and spatially distributed transfer functions are used. Dynamic mode decomposition was used to extract the flame transfer functions corresponding to the strongest modes apparent in the pressure and heat release spectra. The unsteady heat response was accounted for as a fluctuating source term that depends on the local pressure data. Accurate mean conditions were maintained in the reduced-fidelity simulation by using the species destruction rates from the simulation combined with a variable gain approach that enforces dependency on local cell constituents. To verify model numerics, a Rijke tube test case was used. The gain of the transfer function extracted from the reference simulation of the test case matched the $n$ of the linear model used and the phase of the transfer function extracted was found to be zero, consistent with the linear model used in the simulation to create the unsteady flame response, confirming the FTF extraction procedure is correct.

The reduced-fidelity approach was then applied to a model rocket combustor that exhibits moderately nonlinear self-excited instability and for which an extensive set of test data and high-fidelity simulations exist. Results from the hybrid model were compared to the experimental and simulation data, namely mean pressure, limit cycle amplitude, frequency and mode shape, and growth rate. The sensitivity of the model to the number of modes used in the FTF, the number of sampling points used in the Fourier transform of the unsteady heat release calculation, and the mesh size were analyzed. It was seen that the agreement between the model and reference results improved with an increase of the number of modes included in the FTF. However, including very high-frequency modes with non-co-located pressure and heat release nodes could lead to very large gradients in the gain of FTF and cause numerical instability. Imposing a limit on the pressure node to condition the very large gradients in the gain of FTF helped stabilize the simulation. The reduced-fidelity approach with $N$ mode FTF reproduced the $N - 1$ dominant modes of the reference simulation reasonably well, and it was concluded that the number of modes included in the FTF should preferably at least one mode more than the expected number of dominant modes of the system under study.

The key phenomena responsible for combustion instability, the accumulation of fuel near the dump plane during high amplitude compression cycle and the flow of fuel into the chamber during expansion.

![Figure 21. A comparison of the (a) PSDs and (b) limit cycle pressure trace between the hybrid RANS/LES simulation, the NLE-FTF simulation with two-dimensional spatially resolved FTF, and the NLE-FTF simulation with one-dimensional spatially resolved FTF.](image-url)
cycle leading to a detached flame was reasonably reproduced by the reduced-fidelity model. However, as expected, the reduced-fidelity model could not reproduce all the details of the high-fidelity simulation. The model with flame transfer functions that depend on the pressure data at specific locations in the chamber instead of local pressure data could lead to different behavior than the reference simulation. Due to the distributed nature of non-premixed flames, local flame transfer functions dependent on the local pressure field are preferred over flame transfer functions dependent on pressure at a single and specific location.

The reduced-fidelity approach described in this paper provided more physical insights into the unstable behavior of the system than the traditional acoustic solvers. It allowed for accurate treatment of boundary conditions similar to high-fidelity simulations and captured nonlinear dynamics and steep-fronted waves. This approach also allowed for accurate modeling of coupling between heat release and pressure fluctuations in rocket combustors. The results suggest the reduced-fidelity model has the potential to predict the growth and behavior of combustion instabilities into the weakly nonlinear regime. For more nonlinear behavior, amplitude-dependent flame describing functions are likely necessary. The motivation of the study is the development of a tool that can predict combustion instabilities in full-scale combustors using data from high-fidelity simulations of a smaller physical regime that contains representative flow physics. Using a rocket combustor, for example, FTFs would be obtained from simulations of a single- or multiple-element set. The FTFs would then be applied in the analysis of the full-scale combustor that has hundreds of injector elements. An underlying assumption is that the geometric influences on heat release in the smaller system are preserved in its full-scale. A key next step would be to model a multi-element combustor by representing all the elements with the FTFs derived from the output of a single- or few-element high-fidelity simulation. The need to re-scale the heat release comes from the fact that local mean conditions are not well preserved to account for the observed combustion efficiency. The proposed correction, therefore, can be easy to invoke even in the absence of high-fidelity simulation for the full scale system. The important next step in proving the generality and utility of this approach is the application to transverse instabilities in a combustor with multiple elements.

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### Appendix I

The hybrid RANS/LES simulations were performed using Generalized Equation and Mesh Solver (GEMS), an in-house Fortran based three-dimensional finite volume compressible flow solver. The reference simulation in the current work is two-dimensional, only the two-dimensional formulation of GEMS is presented here. The partial differential equations that are being solved are

\[
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} - \frac{\partial E_v}{\partial x} - \frac{\partial F_v}{\partial y} = H \tag{11}
\]

where \(Q\) is a vector of conserved variables,

\[
Q = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho u + \rho v + p \\ \rho u Y_l \end{pmatrix} \tag{12}
\]

where \(\rho\) is the density, \(u\) and \(v\) are the velocities in \(x\) and \(y\) directions respectively, \(p\) is the pressure, \(\rho u^2 + p\) is the total energy, \(Y_l\) is the species mass fraction of \(l\)-th species. The inviscid flux vectors \(E\), and \(F\) are given by,

\[
E = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u h_0 \\ \rho u Y_l \end{pmatrix}, \quad F = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v h_0 \\ \rho v Y_l \end{pmatrix} \tag{13}
\]

The viscous flux vectors \(E_v\), and \(F_v\) are given by,

\[
E_v = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \rho \nu \tau_{xx} + \nu \tau_{xy} - q_x \\ -\rho \nu V_{x,l} Y_l \end{pmatrix}, \quad F_v = \begin{pmatrix} 0 \\ \tau_{yy} \\ \tau_{yx} \\ \rho \nu \tau_{xy} + \nu \tau_{yy} - q_y \\ -\rho \nu V_{y,l} Y_l \end{pmatrix} \tag{14}
\]

where \(V_{i,l}\) is the diffusion velocity of species \(l\) in the direction \(i\) and the heat flux term \(q_i\) is

\[
q_i = -K \frac{\partial T}{\partial x_i} + \rho \sum_{j=1}^{N} V_{i,j} h_j + Q \tag{15}
\]

where \(h_j\) is the enthalpy of species \(j\) and the shear stress term \(\tau_{ij}\) is

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_m}{\partial x_m} \delta_{ij} \right) \tag{16}
\]

The source term \(H\) is

\[
H = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \omega_l \end{pmatrix} \tag{17}
\]

where \(\omega_l\) is the chemical source term of species \(l\).

If the chemical mechanism has \(N\) species and \(M\) reactions, the species production rate of species \(l\) is

\[
\dot{\omega}_l = W_l \sum_{m=1}^{M} (v^l_{ln} - v^l_{lm}) r_m \tag{18}
\]

where \(W_l\) is the molecular weight of species \(l\), \(r_m\) is the rate of reaction \(m\),

\[
r_m = k_{f,m} \prod_{l=1}^{N} [X_l]^{v^l_{ln}} - k_{r,m} \prod_{l=1}^{N} [X_l]^{v^l_{lm}} \tag{19}
\]

where \(v^l_{ln}, v^l_{lm}\) are the stoichiometric coefficients of species \(l\) on the right and left side of reaction \(m\),

\[
\sum_{l=1}^{N} v^l_{ln} X_l \leftrightarrow \sum_{l=1}^{N} v^l_{lm} X_l \tag{20}
\]
\( k_{f,m} \) is the rate of forward reaction of reaction \( m \), given in Arrhenius form,

\[
k_{f,m} = AT^b \exp \left( \frac{-E_a}{RT} \right)
\]

(21)

where \( R \) is the universal gas constant, \( E_a \) is the activation energy, \( A \) and \( b \) are the Arrhenius constants of a given reaction. The reverse reaction rate \( k_{r,m} \) is determined using the equilibrium constant

\[
k_{r,m} = \frac{k_{f,m}}{K_{C,m}}
\]

(22)

where the equilibrium constant \( K_{C,m} \) is

\[
K_{C,m} = \left( \frac{1 \text{bar}}{RT} \right) \sum_{i=1}^{N} \frac{w_{m} - v_{m}}{\text{exp} \left( \frac{\Delta h^0}{R} - \frac{\Delta h^0}{RT} \right)}
\]

(23)

where \( h^0 \) is the stagnation enthalpy and \( s^0 \) is the stagnation entropy.

The conservation equations described above when solved on a mesh that meets the scale-resolution requirements constitute a Direct Numerical Simulation (DNS). It is important to note that the above described governing equations must be extended to third-dimension in order to perform DNS. Unfortunately, the computational expense associated with the DNS is too high. Hence, in the current work, a hybrid RANS/LES simulation was performed. In this approach the large scale eddies are resolved where the grid and time scale provides sufficient resolution, operating in LES mode, and where the resolution provided is not sufficient, the eddies are modeled using RANS, operating in RANS mode. So, this model operates in two modes based on the grid resolution to model turbulence.

The hybrid RANS/LES model requires the flow variables be decomposed into mean and fluctuating component in time. This decomposition can be performed in two ways: 1. Reynolds decomposition, where the mean component is time averaged and 2. Favre averaging, where the mean component is density averaged. In the case of compressible flow simulations, Favre averaging offers the advantage of simplified closure terms and eliminates complex nonlinear closure terms involving density and velocity fluctuations. Hence, Favre averaging is followed in GEMS. Favre averaging decomposes a quantity, \( x(\bar{x}, t) \) into the mean, \( x(\bar{x}, t) \) and the fluctuating component (perturbation), \( x'(\bar{x}, t) \) as follows,

\[
x(\bar{x}, t) = x(\bar{x}, t) + x'(\bar{x}, t)
\]

(24)

where \( x(\bar{x}, t) \) is given by

\[
x(\bar{x}, t) = \frac{\int_{t}^{t+\delta t} \rho(\bar{x}, t) x(\bar{x}, t) \, dt}{\int_{t}^{t+\delta t} \rho(\bar{x}, t) \, dt} = \left\langle x(\bar{x}, t) \right\rangle
\]

(25)

In the above equation, \( \left\langle \cdot \right\rangle \) indicates time averaging. Using Favre averaging, the vector of conserved variables is,

\[
\left\langle Q \right\rangle = \begin{pmatrix}
\left\langle \rho \right\rangle \\
\left\langle \rho \bar{u} \right\rangle \\
\left\langle \rho \bar{v} \right\rangle \\
\left\langle \rho \bar{w} \right\rangle \\
\left\langle \rho \bar{Y}_i \right\rangle
\end{pmatrix}
\]

(26)

The inviscid flux vectors \( E \) and \( F \) are given by,

\[
E = \begin{pmatrix}
\left\langle \rho \right\rangle \bar{u} \\
\left\langle \rho \bar{u} \bar{u} \right\rangle \\
\left\langle \rho \bar{u} \bar{v} \right\rangle \\
\left\langle \rho \bar{u} \bar{w} \right\rangle \\
\left\langle \rho \bar{u} \bar{Y}_i \right\rangle
\end{pmatrix},
\]

\[
F = \begin{pmatrix}
\left\langle \rho \right\rangle \bar{v} \\
\left\langle \rho \bar{u} \bar{v} \right\rangle \\
\left\langle \rho \bar{v} \bar{v} \right\rangle \\
\left\langle \rho \bar{v} \bar{w} \right\rangle \\
\left\langle \rho \bar{v} \bar{Y}_i \right\rangle
\end{pmatrix}
\]

(27)

The viscous fluxes \( E_v \) and \( F_v \) are given by,

\[
E_v = \begin{pmatrix}
0 \\
\bar{u} \bar{u} - \left\langle \rho \right\rangle \bar{u}^2 \\
\bar{u} \bar{v} - \left\langle \rho \right\rangle \bar{u} \bar{v} \\
\bar{u} \bar{w} - \left\langle \rho \right\rangle \bar{u} \bar{w} \\
\bar{u} \bar{Y}_i - \left\langle \rho \right\rangle \bar{u} \bar{Y}_i
\end{pmatrix}
\]

\[
F_v = \begin{pmatrix}
0 \\
\bar{v} \bar{u} - \left\langle \rho \right\rangle \bar{v} \bar{u} \\
\bar{v} \bar{v} - \left\langle \rho \right\rangle \bar{v} \bar{v} \\
\bar{v} \bar{w} - \left\langle \rho \right\rangle \bar{v} \bar{w} \\
\bar{v} \bar{Y}_i - \left\langle \rho \right\rangle \bar{v} \bar{Y}_i
\end{pmatrix}
\]

(28)

where the heat flux term \( \bar{q}_i \) is

\[
\bar{q}_i = -K \frac{\partial \bar{T}}{\partial x_i} + \left\langle \rho \right\rangle \sum_{j=1}^{N} (V_{ij}) \bar{Y}_j \bar{q}_j
\]

(29)

The Reynolds stress terms, \( \bar{u}^i_i \bar{u}_j \) are modeled using Boussinesq approximation,

\[
R_{ij} = -\bar{u}^i_i \bar{u}_j = \nu_j \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - 2 \frac{\partial \bar{u}_m}{\partial x_m} \delta_{ij} \right) - \frac{2}{3} \nu \delta_{ij}
\]

(30)
where $\nu_t$ is the turbulent viscosity. The turbulent kinetic energy $k$ is given by,

$$k = \frac{1}{2} \sum_{i=1}^{3} \overline{u_i^2}$$  \hspace{1cm} (31)

The energy equation closure term is given by,

$$\overline{u_i^2} e^\mu = - \nu_t \frac{\partial \hat{h}}{\partial x_i}$$  \hspace{1cm} (32)

where $\nu_t$ is the turbulent Prandtl number and in general is set to be 0.71. The species equation closure term is given by,

$$\overline{u_i Y_i} e^\mu = - \nu_t \frac{\partial \hat{Y}_i}{\partial x_i}$$  \hspace{1cm} (33)

where $S_{c_j}$ is the turbulent Schmidt number and in general is set to be 0.90.

In order to close the above system of equations, Wilcox two-equation $k-\omega$ model\textsuperscript{50} was used. The model solves for $k$ and $\omega$ and the turbulent viscosity $\nu_t$ is calculated as,

$$\nu_t = k \tilde{\omega}$$  \hspace{1cm} (34)

where $\tilde{\omega}$ is the dissipation, given by,

$$\tilde{\omega} = \max \left( \omega, \frac{7}{8} \sqrt{\frac{2 S_{c_j} S_{g_j}}{\beta'}} \right)$$  \hspace{1cm} (35)

The partial differential equations for $k$ and $\omega$ are as follows,

$$\frac{\partial (\rho) k}{\partial t} + \nabla \cdot ((\rho) \bar{u} k) - \frac{\partial}{\partial x_j} \left( \left( \mu + \sigma \frac{\partial (\rho) k}{\partial \omega} \right) \frac{\partial k}{\partial x_j} \right)$$

$$= \langle \rho \rangle \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \beta^* k \omega$$  \hspace{1cm} (36)

where $\Delta$ is the largest grid dimension for the cell and $C_{\text{hybrid}}$ is set to a recommended value of 0.78.\textsuperscript{51}

When Favre averaging is applied, the source term $H$ is given by

$$H = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \tilde{\omega}_f \end{pmatrix}$$  \hspace{1cm} (41)

The modeling parameters for the above turbulence equations is given in Table 3.

| Parameter | Value |
|-----------|-------|
| $\gamma$ | 13/25 |
| $\beta$ | $\beta_0 f_i$ |
| $\beta_0$ | 0.0708 |
| $\beta^*$ | 0.09 |
| $\sigma$ | 0.5 |
| $\sigma^*$ | 3/5 |
| $\sigma_d$ | 0 for $\left( \frac{\partial k}{\partial \omega} \right) \leq 0$, otherwise 1/8 |
| $f_i$ | $(1 + 85 f_{i0})/(1 + 100 f_{i0})$ |
| $x_{\omega}$ | $|\Omega_{i0} S_{i}/(\beta^* \omega)^3|$ |
| $S_{i0}$ | $S_{i0} - 1/2 S_{\omega} \delta_{i0}$ |

When using the hybrid RANS/LES model, appropriate turbulent length scale, $L_T$ defined by the model should be used. In the case of $k - \omega$ model, $L_T$ is given by,

$$L_T = \sqrt{\frac{k}{\omega}}$$  \hspace{1cm} (38)

The effect of $L_T$ can be included in the equation for turbulent kinetic energy $k$ given above through the second source term as,

$$\beta^* k \omega = \frac{k^{3/2}}{L_T}$$  \hspace{1cm} (39)

The hybrid RANS/LES model when operating in LES mode, the length is set to be the grid size and when operating in RANS mode, the length is calculated as per the $k-\omega$ model used which is given in Eq. 38. Mathematically, it is expressed as,

$$L_T = \min(L_T, C_{\text{hybrid}} \Delta)$$  \hspace{1cm} (40)
species production rate, $\bar{\omega}_f$. As per the laminar flame rate model,

$$\bar{\omega}_f \equiv \omega_f(\bar{T}) \quad (42)$$

The above formulation implies that the production rate is only a function of mean quantity. Although this is a poor assumption for a RANS simulation, in the case of a hybrid RANS/LES simulation where the large eddies are resolved, this assumption is more reasonable and becomes exact when very fine grids are used.

The numerical schemes employed were explained in detail by Harvazinski.\textsuperscript{46} The Navier-Stokes equations given in this section were solved in the high-fidelity simulations performed in GEMS following finite volume methodology, employing a second-order implicit scheme in time with dual time method to reduce factorization errors. In GEMS, spatial fluxes were evaluated using a second-order approximate Riemann solver.