



## Full Length Article

## Real-time prediction of lean blowout using chemical reactor network

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## ABSTRACT

Lean blowout (LBO) of combustion systems is a concern that can cause costly and time-intensive reignition of land-based gas turbines and can affect the rate of descent for aircraft and the maneuverability of military jets. This work explores the feasibility of model-based combustor monitoring and real-time prediction of combustion system proximity to LBO. The approach makes use of (1) real-time temperature measurements, coupled with (2) the use of a real-time chemical reactor network (CRN) model to interpret the data as it is collected. The approach is tested using a laboratory jet-stirred reactor (JSR), operating premixed on methane at near atmospheric pressure. The CRN represents the combustion reactor as three perfectly stirred reactors (PSRs) in series with a recirculation pathway; the model inputs include real-time temperature measurements and mass flow rates of fuel and air. The goal of the CRN is to provide a computationally fast means of interpreting measurements in real time regarding proximity to LBO. The CRN-predicted free radical concentrations and their trends and ratios are studied in each combustion zone. The results indicate that the hydroxyl radical maximum concentration moves downstream as the combustion reactor approaches LBO. The ratio of hydroxyl radical concentrations in the flame zone versus the recirculation zone is proposed as a criterion for the LBO proximity. The model-based process monitoring approach sheds insight into combustion processes in aerodynamically stabilized combustors as they approach LBO.

## 1. Introduction

## 1.1. Overview and motivation

It is well established that oxides of nitrogen ( $\text{NO}_x = \text{NO} + \text{NO}_2$ ) emissions can be controlled by lowering the flame temperature through leaning of the flame fuel-air equivalence ratio ( $\Phi$ ). Today, most land-based, gas-fired, gas turbine engines for power generation and mechanical drive use dedicated premixing chambers to fully pre-mix the fuel with air prior to the combustor, with some engines offering single-digit  $\text{NO}_x$  emissions. However, by operating very lean to reach low  $\text{NO}_x$  and particulate matter emission, the combustors have limited margins between stable combustion and lean-flame instabilities and lean blowout. In recent years, lean burn concepts such as rich burn - quick quench lean burn combustors, double annular combustors, axial staging, lean direct injection and lean-premixed and pre-vaporized concepts have been investigated by several aircraft engines developers, e.g., NASA, GE, Pratt and Whitney, Rolls Royce [1]. Many of these engines employ combustion staging that may cause flame fluctuations due to local fuel-air ratio variance that may result in flame instabilities and extinction. While improving pollution and efficiency

characteristics, the combustion instabilities in these engines present significant challenges. Experimental studies of aero-engine instabilities employ flow visualization of species distribution in different combustor geometries, injector designs and fuel compositions (both gaseous and liquid), e.g., [2–6]. CFD modeling of these thermo-acoustic instability mechanisms is an active area of the research, e.g., [7–9] however these models are computationally intensive and are not conducive for large parametric studies. Recently, hybrid models such as CFD-CRN approach [10] semi-empirical model [11] for prediction of blowout in lean-premixed aero-engine has been proposed, however, these model often lack physical insights related to the LBO phenomenon.

For land-based applications, fluctuations in power demand during low power operation may cause blowout resulting in an expensive and time-consuming shutdown, purge, and restart procedures, and these steps can create frequency stability issues [12]. The diffusion-flame combustors of aircraft gas turbines provide superior stability, though there are areas of concern, as discussed as follows, and  $\text{NO}_x$  emissions are significantly higher than for lean-premixed engines. During throttling of aircraft gas turbine engines, control over the air flow rate can be challenging because of the inertia of the compressor [13], causing a critical undershoot of the fuel-air equivalence ratio leading possibly to a

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flame blowout. Therefore, a wide safety margin is generally maintained in aero-engines, to remain within a safe operating envelope, by restricting the rate of power change in the engine, by constraining the maneuverability of military jets, and by increasing the time of descent for the aircraft. Reducing the NO<sub>x</sub> emissions of jet aircraft, as well as the carbon soot formation, by lean combustion is of significant interest. By lean direct injection (LDI), the objective is to rapidly mix the liquid fuel spray with air prior to ignition, thereby leading to a leaner, lower temperature flame. The success of premixing methods for aircraft engines will depend on the ability to control LBO [14]. Current blowout monitoring approaches are based on the sensing of the low-frequency combustion oscillations that precede the blowout event. This approach requires expensive equipment and modifications to the combustors. The objective of the present study is to develop a real-time modeling and analytical tool to assess the system proximity to blowout using real-time chemical kinetic modeling. This approach has the potential to significantly reduce the cost and hardware needed for an active blowout detection and control.

### 1.2. Blowout phenomenon

The lean flame blowout condition is associated with the lowest equivalence ratio that can sustain a flame within a specific combustion geometry [15]. The LBO process depends both on the rate of chemistry and the gas residence time in the flame stabilization region. Early research was primarily based on correlating the blowout based on experimental results to Damkohler number (*Da*). The Damkohler number is defined as the ratio of mixing time to the chemical time ( $\tau_{mix}/\tau_{chem}$ ). Longwell et al. [16] proposed that blowout occurs when the rate of entrainment of reactants into the recirculation zone cannot be balanced by the rate of burning of those gases. Recently, the effect of local *Da* non-uniformity in the reactor on LBO has been investigated [17] suggesting that *Da* gradients in the reactor can lead to local flame extinction, on-set of flow instabilities resulting in LBO. Zukoski and Marble [18] observed that at blowout, the free-stream combustible mixture has a contact time with the wake behind the stabilizer equal to the ignition time of the mixture. Yamaguchi et al. [19] proposed a flamelet description based on local extinction due to flame stretch. Geikie and Ahmed [20] used a Lagrangian Flame Vortex method to study blowout caused due to local flame extinctions. Chauduri [21] discussed the behavior of the flame near blowout in terms of flame shape, velocity, and local extinguishing and re-ignition events. Spalding [22] and Kundu et al. [23] studied the role of the recirculation zone on blowout criteria. Nicholson and Field [24] and Chao et al. [25] reported increased flame detachment and reattachment events near blowout. King [26] investigated the effect of parameters such as inlet temperature, pressure and velocity on afterburner lean blowout.

Of particular relevance to this work are the studies focused on identifying parameters associated with LBO proximity and LBO prevention related to local flame extinction and reignition phenomena. Nair and Lieuwen [27] studied changes in the low-frequency acoustic spectrum, the authors describe an increased presence of time-localized and intermittent events in acoustic data approaching blowout for three different combustors. The events were correlated to local flame extinction, and re-ignition events in a swirl-stabilized burner or flame detachment and reattachment in a bluff body stabilized combustor. Li et al. [28] studied early blowout detection in a partially premixed, swirl-stabilized dump combustor by analyzing low-frequency temperature fluctuations caused by local extinction and reignition events using FFT power spectrum analysis. Mukhopadhyay et al. [29] used a symbolic non-linear time series analysis for the chemiluminescence signal of the CH\* radical for partially and fully premixed flames. The CH\* emissions were used to identify the heat release rate in the combustor. Yi and Gutmaek [30] observed intensified low-frequency oscillations in OH\* measurements near LBO and used two indices: normalized chemiluminescence root mean square and normalized

cumulative duration of LBO precursors to characterize the approach of a blowout. Again, they observed intensified low-frequency oscillations near lean blowout corresponding to large-scale flame extinction and reignition events in swirling shear layer. Muruganandam et al. [31,32] investigated LBO precursors based on OH\* chemiluminescence as well as the acoustic disturbances near LBO. These current methods can be used for active prediction and control of LBO require engine hardware modifications, such as optical access, which can be expensive and require maintenance and frequent calibrations.

### 1.3. Chemical reactor network

The concept of combustor modeling using a CRN was introduced by Bragg [33]. By Bragg's approach, a perfectly stirred reactor (PSR) is used for the primary combustion zone, and a plug flow reactor (PFR) is used for the secondary (post-flame) zone. Various CRN models, involving arrangements of PSR and PFR elements, have been used to study pollutant formation in laboratory reactors and gas turbine engines, e.g. [10,34–39]. Sigfrid et al. [40] employed a two-element reactor to study the influence of lean blowout limit of an industrial gas turbine. Lefebvre [41] established a quantitative relationship between blowout equivalence ratio and physical properties of the combustor, such as velocity, temperature, pressure, and dimensions of the flame holder, based on the well-stirred reactor concept. Karalus [42] used a two element CRN to study the behavior of OH in hydrogen and methane flames, based on the convective time scale as the reacting gases flowed through a jet-stirred reactor. Other CRNs for industrial swirl-stabilized combustors have been reported in the literature [34,37,43].

In current work, in-house UW CRN code was used [44–47]. The PSR reactor concept is implemented by balancing the Arrhenius source terms of net production of each species by convective removal of that species from the PSR control volume. The PFR concept is modeled by a series of PSRs. One of the major advantages of the current code is in the implementation of the fast convergence algorithm, which enables near-real-time chemical kinetic calculations in complex CRN arrangements [46,48].

The chemical kinetic mechanism used in the present CRN modeling is GRI 3.0, an optimized chemical kinetic mechanism to model natural gas combustion [37]. It contains 325 reaction steps and 52 species. The GRI 3.0 mechanism has been validated using experimental data for methane, ethane, hydrogen and carbon monoxide. For example, Hu et al. found good agreement between the laminar burning velocities calculated experimentally and computationally using the GRI 3.0 mechanism for the methane-hydrogen-air flame [38]. Flame speed validation [49–52] and ignition delay comparison with experimental data [53,54] have been reported for GRI 3.0.

In this work, we demonstrate a simple, computationally efficient chemical reactor network model tuned for a range of the combustor operational envelope. With this CRN, we compute non-measurable combustion variables in real-time and use these to predict proximity to lean blowout. In order to investigate this approach, a laboratory jet-stirred reactor (JSR) is used to conduct experiments. A CRN comprising of three PSR elements and real-time temperature input was developed to model the JSR. The model monitors the combustor free radical species and reports the results in real time estimating reactor proximity to blowout. In the sections that follow we describe: 1) the experimental setup and methodology, 2) the CRN development and its evaluation using steady-state operating conditions of the JSR, and 3) the blowout experiments and the RT-CRN application describing the combustor transient behavior.

## 2. Experimental methods

### 2.1. Experimental setup

The experimental study focuses on characterizing lean blowout of

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