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CHEMICAL REACTOR NETWORK APPLICATION TO EMISSIONS PREDICTION FOR INDUSTIAL DLE GAS TURBINE

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ABSTRACT

A chemical reactor network (CRN) is developed and applied to a dry low emissions (DLE) industrial gas turbine combustor with the purpose of predicting exhaust emissions. The development of the CRN model is guided by reacting flow computational fluid dynamics (CFD) using the University of Washington (UW) eight-step global mechanism. The network consists of 31 chemical reactor elements representing the different flow and reaction zones of the combustor. The CRN is exercised for full load operating conditions with variable pilot flows ranging from 35% to 200% of the neutral pilot. The NO_X and the CO emissions are predicted using the full GRI 3.0 chemical kinetic mechanism in the CRN. The CRN results closely match the actual engine test rig emissions output. Additional work is ongoing and the results from this ongoing research will be presented in future publications.

INTRODUCTION

Detailed knowledge of NO_X formation in the flame is required for the development of sub-10 ppm lean premixed combustors. Relatively small changes in the premixer (injector) exit profiles of velocity and fuel concentration, the interaction of the pilot flame with the main recirculation zone and main flame,

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and the interaction of the dome air and gas from neighboring injectors with the main flame can significantly change the NO_X emission. An intelligently designed chemical reactor network, guided by CFD results of the flow field and reaction space, and used interactively during the combustor rig testing, can provide answers regarding the quantitative NO_X behavior of the combustor. Further, as experience is gained, two opportunities arise: 1) upgrades can be made to the CRN so that it can be made sufficiently robust to handle a range of combustion liners and injectors without the need for further structural changes to the network of reactor elements and linkages, and 2) a CFD-to-CRN translational software tool can be developed that permits the essential CFD results to be used to build the CRN for individual combustors. In this paper, our initial work with the CRN is presented. Results obtained with the CRN for NO_X and CO are compared to the engine test rig emissions data. The CRN is run with full chemical kinetics. Additionally, it is run with global kinetics, verifying that the global kinetics used to obtain the CFD results are valid.

Starting in the nineteen fifties, engineers began to use chemical reactor models to understand the combustion process. The concept of modeling the combustor by a perfectly stirred reactor (PSR) followed by a plug flow reactor (PFR) was introduced by S.L. Bragg (1953). Experimental use of the concept was shown by Longwell and Weiss (1955) in their back-mixed well stirred reactor at near blow-out conditions, where the back-mixing of recirculating gas was assumed fast compared to the controlling chemical reaction rate. Zonal combustion modeling was proposed by Swithenbank (1970) as an improvement for combustor design via correlation parameters, and followed experimental testing. In the zonal modeling, the combustor volume is divided into zones represented by idealized reactor elements, such as PSR, PFR, and MIX.

Chemical reactor modeling of combustion systems is not necessarily limited to the use of extensive chemical reactor networks. Simple two/three reactor models were found useful in modeling research combustion reactors. Recently, Rutar et al. (2000) and Rutar and Malte (2002) showed the methodology for modeling the NO_X emissions of the experimental jet stirred reactor with a simple two or three idealized reactors scheme. There are a number of investigations using simple chemical reactor models to evaluate the emission trends for gas turbine combustor applications (e.g., Schlegel et al., 1996, and Feitelberg et al., 2001). This approach provides a quick and useful way to evaluate the emission trends and the effects of parameters of interest using detailed chemical kinetic mechanisms. However, to go beyond the trend evaluations of the industrial systems, more complicated models are required due to the complexities of the flow field and the boundary conditions.

The development and application of the zonal model for emission control in gas turbine combustion was described by Rubins and Pratt (1991). The authors tested several possible configurations for the annular ALF-502 GT combustor with the purpose of CO and NO_X reduction. Their model included several MIX,

PSR, and PFR elements in series, including air injection from the wall. In order to evaluate the flow field in the combustor, the combustion geometry was evaluated in a water tunnel, then the combustor was divided into the zones corresponding to the flow patterns.

Lean blowout modeling for an aircraft engine application using zonal modeling was investigated by Sturgess et al. (1991) and Ballal et al. (1993). Later, a hybrid CFD-CRN model for gas turbine combustors was proposed by Sturgess and Shouse (1996). The development of their model employed the post-processing of CFD simulations. Sturgess (1997), using the same approach, developed a chemical reactor network for evaluation of an abbreviated chemical kinetic mechanism for Jet-A/JP-5/JP-8 fuels by comparing CRN predictions with experimental emissions data.

The injector boundary conditions play a significant role in the levels of nitrogen oxide emission. The effect of fuel-air unmixedness in the chemical reactor model was investigated by Nicol et al. (1997) and Rutar et al. (1997). The model of Nicol et al. divided the fuel-air stream into 5 parallel flow paths with the discrete fuel-air equivalence ratio obtained from a Gaussian distribution function. A finite-rate mixing model was used to incorporate the effects of large and small scale mixing into the chemical reactor scheme in the work of Tonouchi and Pratt (1995) and Tonouchi (1996).

Roby et al. (2003) modeled the experimental results of Mellor (1996) using a chemical reactor network with the premixer outlet flow split into two streams to account for imperfect premixing. The authors also discussed the ability of the network to predict non-linear emission trends for high fuel–air ratio combustors. Novosselov (2002) also employed a chemical reactor network for NO_X and CO emissions prediction of the lean premixed gas turbine combustor of Mellor (1996). The CRN development was based on the CFD solution of the combustor using eight-step global chemistry.

Chemical reactor modeling is found to be a valuable tool in the evaluation of pollutant formation and blowout performance of combustion systems. The methodologies of the development vary between the authors. While most authors address the modeling of the combustion processes in the flame and the post-flame regions, only a few investigators have looked at the possible effects of the fuel-air mixture non-uniformities. Thus, the need exists for models that can account not only for the detailed flame chemistry but also for the interactions between chemistry, mixing, and complex boundary conditions.

ENGINE TEST RIG

The experimental hardware consists of a DLE engine test rig rated at 15 khp driving a water brake. The combustion system is lean premixed and the flame is swirl stabilized at the dump plane. An annular augmented backside cooled

(ABC) combustor is used. The premixing and swirl stabilization are provided by fourteen fuel injectors. Each injector consists of the typical Solar SoLoNO$_X$ "main" and "pilot" circuits.

The engine test rig is operated on natural gas at several low emissions load conditions. The primary focus for this study is emissions prediction at full load operating conditions.

CFD ANALYSIS

Despite the tremendous advancement in computational hardware and software technologies, performing detailed chemistry with CFD remains a daunting task for most users today. One simple way to incorporate detailed chemistry (such as the full GRI 3.0 mechanism) is to use a combined CFD and CRN approach.

Three dimensional (3D) CFD modeling provides basic insight to the flow, temperature and species fields/profiles in the combustor. These fields/profiles aid the visualization and interpretation of the combustor flow and reaction space and are necessary for constructing an accurate CRN.

In the current exercise, the test rig combustion system is modeled using Star-CD Version 3.24. A five million cell, sector geometry (one complete injector and sector of the annular combustor) with periodic boundary condition is used. Actual engine test rig pressure, temperature and flow rates are simulated. The K-epsilon turbulence closure model is used. The rate limiting approach is used in determining the effective reaction rate; that is, the smaller of the turbulent mixing reaction rate and the chemical kinetic rate is selected. The turbulent mixing reaction rate is computed based on the eddy break-up (EBU) model of Magnussen and Hjertager (1976). The chemical kinetic rate is calculated using the University of Washington eight-step, pressure-sensitive, global kinetic mechanism (Novosselov and Malte, 2005). The fuel used in the CFD modeling is methane diluted with 2.35% by volume of nitrogen, providing the same adiabatic equilibrium flame temperature as the actual natural gas used in the engine rig testing. The flow, temperature, and species fields from the CFD simulations provide insight for the CRN development. A representative temperature field in the combustor is shown in Figure 1.

CHEMICAL REACTOR NETWORK FOR GAS TURBINE COMBUSTOR

The University of Washington chemical reactor code, which is based on the original CREK code of Pratt and Wormeck (1976) and the later work of Nicol (1996), is used in the development of the CRN. The development uses insights gained from 3D CFD modeling of the engine test rig combustor.   The basic

methodology for using CFD to guide the development of the CRN is discussed in the MSME and PhD theses of Novosselov (2002 and 2006, respectively).
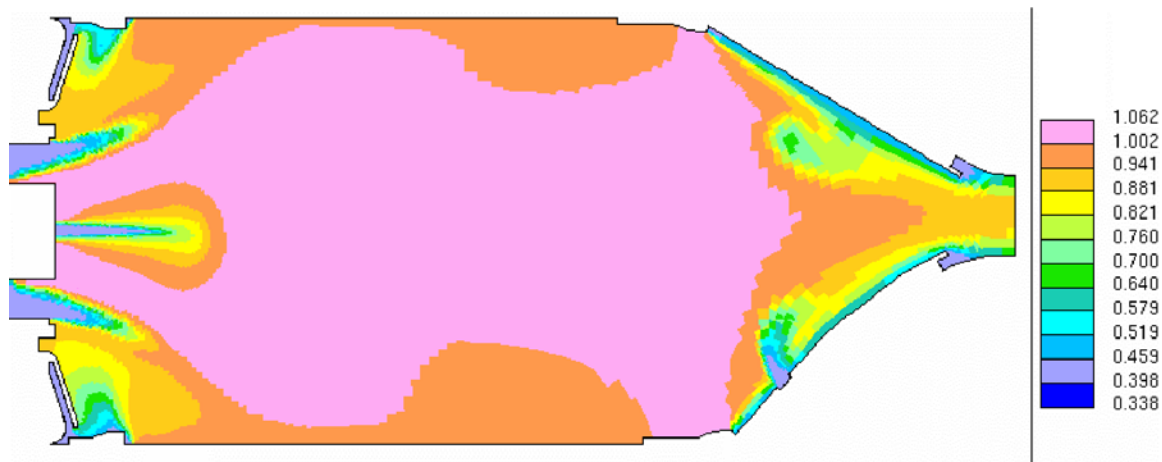
Figure 1. Engine test rig combustor configuration and typical CFD predicted temperature profile plot at full load condition. The temperature is normalized by the adiabatic equilibrium temperature calculated for the mean fuel-air ratio of the premixer.

The combustor CRN is constructed based on CFD-predicted flame behavior and combustor boundary conditions. The eight critical factors required to build the CRN are as follows:

- Fuel-air distribution in the premixer/injector main circuit.
- Velocity profile in the premixer/injector main circuit.
- Rate of entrainment of the main recirculation zone and dome recirculation zone gases into the main flame.
- Cross-flow turbulent mixing within the injector main circuit outlet stream and the resultant main flame.
- Interaction and mixing of the pilot gas with the main recirculation zone and the main flame.
- Mixing of gas from neighboring injectors/flames into the main flame.
- Temperatures, fuel-air ratios, and volumes of the main regions of the burning flow field.
- Fluctuations in flame temperature.

The flow and flame patterns are CRN-modeled by adjusting the volumes and input flow rates of the reactor elements of the network and the flow splits between the elements. The network consists of 31 PSR, PFR, and MIX elements. Each element type is described below:

- PSR stands for perfectly stirred reactor (i.e., a continuously stirred tank reactor), in which mixing to the molecular scale is assumed to happen instantaneously compared to chemical reaction. The chemical reaction occurs homogeneously in the reactor. The flow conditions corresponding

to the PSR can be calculated based on the dissipation gradient method; that is, when the pressure drop and the volumetric flow rate meet a critical condition, the reactor element is treated as perfectly stirred (Swithenbank, 1970).

- PFR stands for plug flow reactor, in which the flow is assumed to move as a plug and the chemical reaction proceeds one-dimensionally, longitudinal mixing in the reactor is assumed to be zero.

- MIX stands for an element in which the entering streams are uniformly mixed without chemical reaction.

Figure 2 shows the CRN layout with the flow splits between the reactors. Some MIX elements are not shown on the figure in order to avoid clutter. The 31-element CRN is exercised for full load operating conditions with variable pilot flows ranging from 35% to 200% of the neutral pilot.

The 31 element CRN includes several distinct regions:

- Main flame zone (MFZ) consisting of the inner, center, and outer fuel-air input streams as provided by the premixer/injector main circuit.
- Pilot flame zone (PZ) consisting of the pilot flow input stream as provided by the injector pilot circuit.
- Center (main) recirculation zone (CRZ) consisting of the back-mixed hot product gas flow.
- Dome recirculation zone (DRZ) consisting of the combustor dome air input stream.
- Post-flame zone (PFZ) consisting of the CO burnout zones and secondary dilution input stream.

The flow parameters in each of the regions are determined based on the CFD flow, temperature and species fields, and the design/experimental boundary conditions.

The premixer outlet stream and resultant main flame is divided into three streams: outer, center, and inner. Combustion is initiated in the center stream by using a single PSR element. The inner and outer flame streams are ignited due to the entrainment of small amounts of hot gas. Each flame stream is modeled by using a few PSRs in series.

The PFRs are used to model those parts of the flow that do not satisfy the condition required for a PSR, and those parts that are used to complete the combustion process in post-flame zones, allowing the carbon monoxide concentration to relax and reach the local equilibrium value. As the secondary dilution air enters the combustor, the CO chemistry is quenched. This brings CO close to the engine emission.
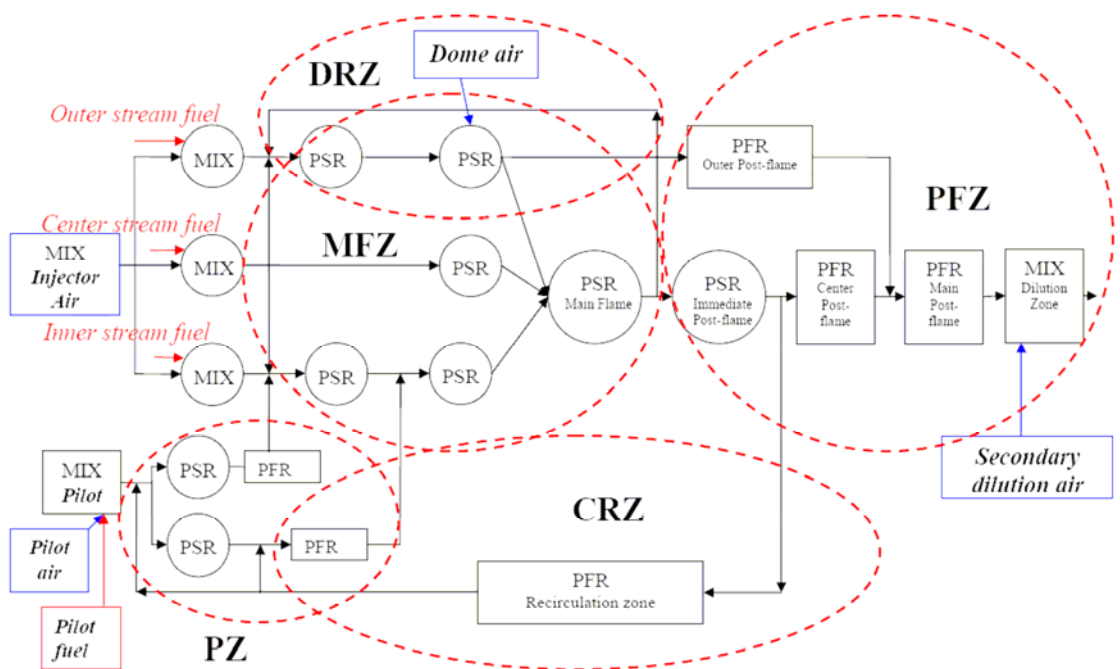
**Figure 2. 31-element CRN for evaluating the NO$_x$ and CO emissions of the engine test rig combustor.**

The fuel used in the CRN modeling is natural gas, of the same composition as that of the natural gas burned in the engine test rig, except for the substitution of the small amount of butane in the natural gas with propane in the modeling.

The CRN-modeling of the main features of the flow are discussed in the following sections.

Injector Mixing Profiles

One of the key areas of the CRN development is the flow mapping of the premixer. The premixer flow is critical and determines the basis of the flame and reaction zone structure. Figure 3 represents a radial fuel-air ratio profile used in the current study.

Radial Profile: The radial fuel-air ratio profile of the injector is mapped into the CRN as three separate streams with their unique values of mass flow and fuel mass fraction. This approach allows the existence of locally high fuel-air ratios (though lean) and variable velocities in the flame. Introduction of cross-mixing between the streams in the CRN model helps in maintaining the local flame temperatures in the range as predicted by the CFD modeling. The inner stream has the main recirculating gas mixing into it; while the outer stream is diluted by the dome cooling air and the hot gases from the neighboring injectors.
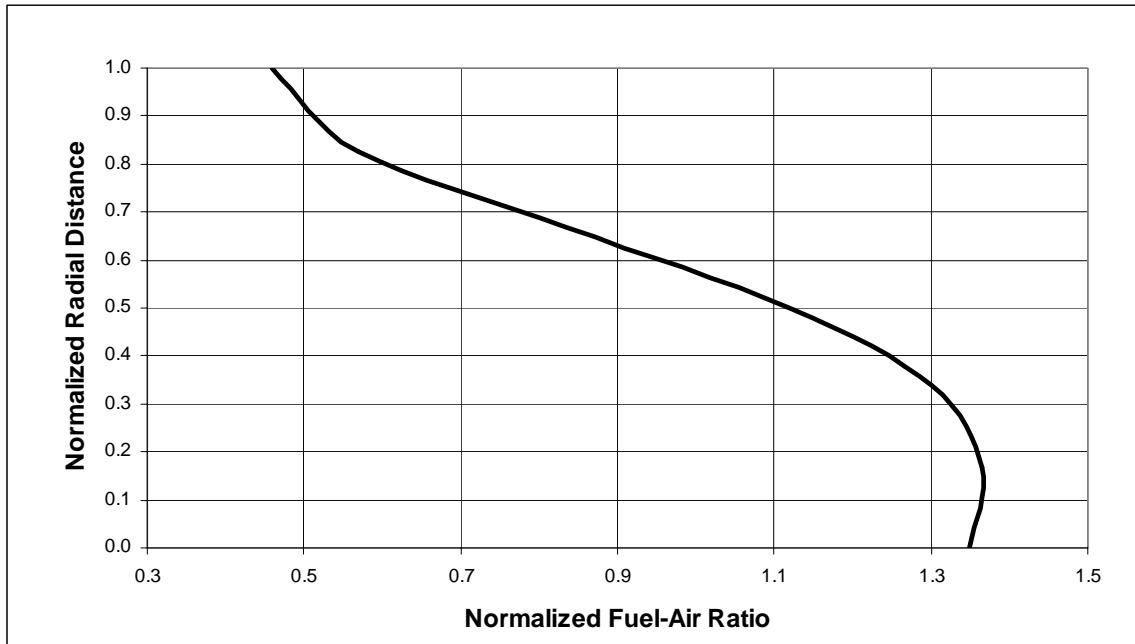
Figure 3. Example of the fuel-air ratio profile at the premixer outlet. The fuel-air ratio is normalized by its mean value. The radial distance shown is the distance outward from the inner radius of premixer divided by the outer to inner radius difference.

Circumferential Profile: The injector also exhibits a circumferential variability in fuel-air ratio. In order to find the effect of the circumferential fuel-air variations, NO_X emissions are evaluated in the CRN for several radial profiles corresponding to the different angle positions (i.e., circumferential positions) of the injector. The NO_X predictions for the angular locations are divided by the mean value. This yields a correction factor that accounts for the circumferential non-uniformity of the fuel-air ratio. This correction is a function of the pilot fuel flow rate and is equal to a 10-20% increase of the NO_X predicted emission. The 10 percent correction corresponds to the high pilot cases, since in these cases the pilot flame produces relatively higher levels of NO_X and the emissions are not affected as much by the circumferential injector non-uniformity.

Flat or Uniform Profile: If a radially and circumferentially uniform fuel-air ratio injector profile is assumed, the predicted NO_X emissions are a factor of three

lower than the experimental emission levels. It is clear that the degree of uniformity has significant impact on the NO_X emissions output.

Flame Modeling

In the early literature, a single PSR was used to represent the flame. However, the use of several PSRs-in-series spreads out the flame, that is, it permits the flame to progress and produce intermediates and incomplete products of combustion, and then to consume these species and produce more heat as the final state of the flame is reached. Thus, in our CRN, PSRs-in-series are used to model the flame. [Of interest in this regard is the theory described in the chemical reaction engineering text by Levenspiel (1972), which shows that the use of multiple PSRs-in-series yields a residence time distribution similar to that of a one-dimensional chemical reactor with longitudinal diffusion.]

Cross-mixing between the streams of different fuel-air ratio is used to smooth out the fuel-air ratio, as predicted by the 3D CFD analysis. The fuel-air ratio in the premixer outlet stream becomes more uniform due to the effects of turbulent mixing and pressure gradients acting on the stream. The CFD results also give information about the fuel-air ratio levels in the different parts of the flame.

The pilot flame is modeled as two PSRs in parallel, each followed by a PFR with the addition of the hot main recirculation zone gas. The ignition of the pilot happens upon mixing with a small amount of hot recirculation zone gas. The pilot flame has a significant effect on the nitrogen oxide emissions. As a relatively rich pilot mixes with the recirculation gas and ignites, it creates a hot zone with relatively long residence time. The increase in temperature triggers the thermal Zeldovich NO_X pathway and roughly doubles the NO_X emission compared to the neutral pilot case.

Recirculation Zones Modeling

The two major parameters of the recirculation zones that require modeling are: mass flow rate (entrainment) and temperature. Both the flow rate and the temperature are readily available from the analysis of the 3D CFD solution. The mass flow rate can be found by the integration over the zero axial velocity iso-surface. The temperature of the main recirculation zone can be matched in the CRN by allowing some of the dome cooling air to mix into the main flame and eventually enter the center recirculation zone.

The dome recirculation zone brings cool air into the flame. The mixture in the outer part of the stream/flame mixes with gas from the neighboring injectors and burns at the relatively low temperature due to the lower fuel-air ratio of the outside fuel-air stream diluted by the dome cooling air.

Effect of Temperature Fluctuations on NO$_X$ Formation

In order to incorporate the effect of temperature fluctuations on the NO$_X$ formation into the CRN, a simplified single-injector combustor model is used. The model consists of a single ABC can-type combustor with assumed injector fuel-air ratio profile. The simplified system is modeled with Fluent 6.2 using the limiting reaction rate approach as discussed above.

Nitrogen oxides emissions are calculated using the Fluent NO$_X$ post-processor chemistry in the time-averaged simulation. A joint fuel-temperature probability density function (PDF) is added to the model to predict NO$_X$ emissions. The turbulent fluctuation correction is calculated as a ratio of NO$_{x\ PDF}$ /NO$_{x\ time\ averaged}$. This correction accounts for a 10-25 percent increase in NO$_X$ formation depending on the fuel-air ratio. The higher value corresponds to leaner cases and the cases with low pilot fuel flow rates. In the cases where the combustor temperature is above 1800K, the effect of the temperature fluctuations on the nitrogen oxides formation diminishes due to the increased contribution of post-flame thermal NO$_X$. The likelihood of temperature fluctuations is less in the post-flame zones than in the flame zones.

RESULTS AND DISCUSSION

In this study, a combined CFD and CRN approach for emissions prediction has been attempted showing very promising results. The CFD is used for detailed flow analysis and the CRN is used for detailed chemical kinetic analysis. The combined approach provides an approximate, but fairly accurate prediction of actual engine test rig results. Furthermore, the combined approach aids the analyst with the detailed interpretation of both the flow and chemistry as discussed in the following sections.

Engine Test Rig and CRN Prediction

The full GRI 3.0 mechanism (GRI MECH 3.0, 2005) is used for CRN model development and validation. Figure 4 shows NO$_X$ predictions with variable pilot and for natural gas as the fuel. The emission results presented are normalized and compared to the engine test rig data. Also shown in Figure 4 are calculated NO$_X$ emissions based on the work of Leonard and Stegmaier (L&S), 1994. The higher value represents a "no cross-mixing scenario" or worst-case condition where the injector flow is split into three distinct segments without any cross-mixing and, thus, no fuel-air ratio or temperature smoothing effects. The calculated NO$_X$ emission is performed for each stream separately and then weighted according to the mass flow for each stream. The L&S calculation is also performed for a uniform premixer, at the mean fuel-air ratio, leading to the lower L&S curve. The L&S calculations do not treat the pilot.
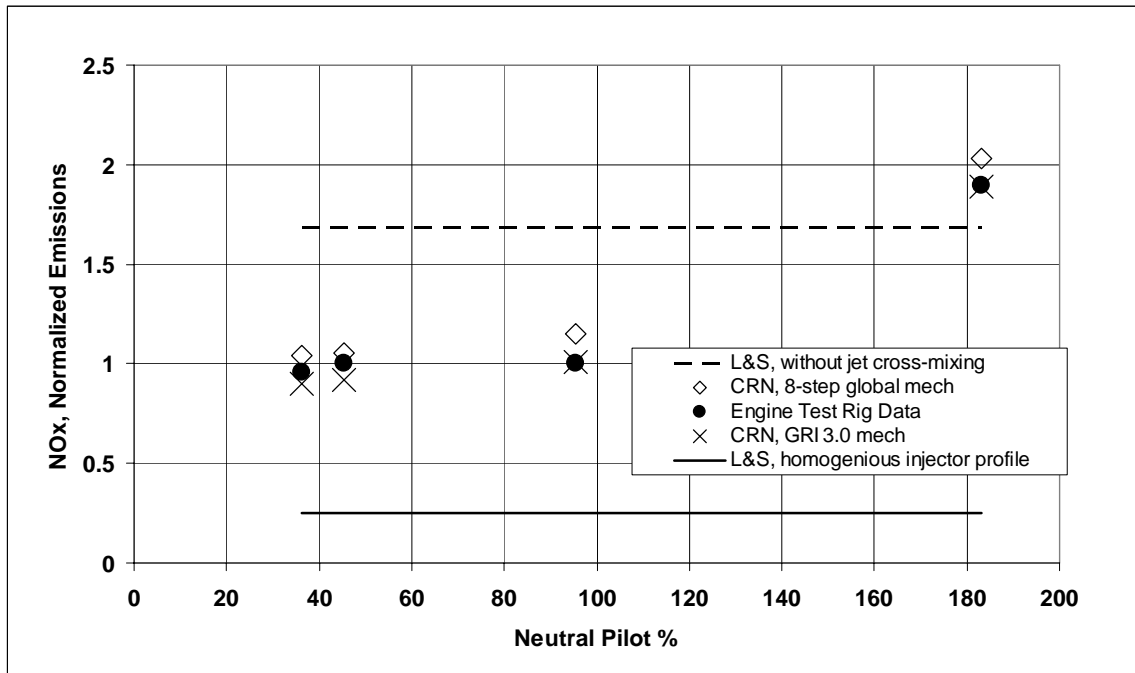
Figure 4. Comparison of measured and predicted NO$_X$ emissions. Normalization is based on the engine test rig NO$_X$ emission for 95% pilot, which is very close to the 100% neutral pilot condition.

As seen in Figure 4, very close agreement is obtained between the CRN predictions and the engine test rig NO$_X$ data. The experimental data and the CRN prediction of nitrogen oxides emissions fall in between the two Leonard and Stegmaier curves showing both the impact of radial fuel-air non-uniformities and the turbulent mixing. Namely, a skewed radial fuel-air distribution creates the hot local zones in the combustor and, thus, keeps the NO$_x$ levels above the lower L&S line. On the other hand, the cross-mixing prevents the NO$_x$ emission from rising above the higher L&S curve. The rise of nitrogen oxides emissions at the high pilot case is attributed to the increase of the local temperature in the PZ (see Figure 2) and, consequently, to the thermal NO$_x$ formation rate in that region. The calculations for the sub-neutral pilot cases agree with the experimental data and do not show any significant change in the NO$_X$ emissions with respect to the pilot fuel flow rate.

The full GRI 3.0 mechanism is used for model development and validation. A companion set of calculations is performed using the UW eight-step global mechanism. The results obtained with the UW eight-step global mechanism generally show an increase of about 5-10% in NO$_X$ when compared with the full GRI 3.0 mechanism. The CRN computations using the global mechanism predict temperatures in the flame zone that are slightly higher (by 3 to 8°C) than GRI 3.0. This is due to the lack of endothermic reactions that produce radical species in the flame, and explains the higher level of NO$_X$ output. Post-flame temperatures for both mechanisms are in agreement.

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The CO emissions stay relatively flat for all of the modeled cases (see Table 1). This agrees with the experimental data as well. The predicted CO emissions for both the eight-step global mechanism and full GRI 3.0 are about 2 ppm. The level of CO is at the chemical equilibrium condition before the injection of the secondary cooling air into the combustor. The difference between the experimental and predicted values is small and can be attributed to the measurement instrument resolution or to a slight CO wall quenching effect, which is not modeled in this CRN.

Table 1. CO predictions in the CRN

% of Neutral Pilot	35%	45%	95%	185%
GRI 3.0, CO ppmvd, 15%O_2	1.79	1.83	1.82	1.84
UW 8-Step, CO ppmvd, 15%O_2	1.93	1.99	1.97	1.99

NO_X Formation Mechanisms and Zones of Formation

CRN modeling helps to understand the zones and pathways that contribute to the NO_X emissions in the lean-premixed gas turbine combustor. Both zonal and mechanism pathway contributions may change with modifications to the combustor setup (liner, injector) or boundary conditions (fuel-air ratio, pressure, load).

Table 2 shows relative contributions of the different NO_X formation mechanisms for the modeled combustor using the NO_X chemistry of GRI 3.0. The cases with the pilot at less than neutral (not listed) are very similar to the neutral pilot case.

The five pathways are:
1. Fenimore or prompt NO_X
2. NNH chemistry
3. N_2O pathway
4. Flame Zeldovich chemistry influenced by super-equilibrium O-atom
5. Thermal Zeldovich chemistry influenced by equilibrium O-atom

Prompt and NNH nitrogen oxide form in the early part of the flame and then their rates fall off quickly as the flame continues to completion. The N_2O and flame Zeldovich routes are very active in the heart of the flame and persist into the near post-flame zone. Thermal Zeldovich is primarily a post-flame zone effect. [The relatively low contributions of the prompt and NNH pathways are a result in part of the pressure assumed, which is engine pressure. High pressure tends to diminish these pathways.]

Table 2. NO$_X$ Formation Pathway Contributions

Pilot Level	Prompt	NNH	N$_2$O	Flame Zeldovich	Thermal Zeldovich
Neutral Pilot	8%	4%	45%	19%	25%
High Pilot	5%	2%	33%	18%	42%

Table 3 shows the contributions of the different combustion zones to the NO$_X$ emissions. As noted, most of the NO$_X$ is formed in the main flame or in both the main and pilot flames.

Table 3. NO$_X$ Formation Zones

Pilot Level	Main flame	Pilot flame	Recirculation zone	Post flame
Neutral pilot	72%	2%	9%	17%
High pilot	37%	46%	6%	11%

CONCLUSIONS

The current combined CFD and CRN approach shows the ability to accurately predict NO$_X$ (and CO) emissions for industrial DLE combustors. The combined approach maximizes the strengths of each tool used with flow information provided by CFD and reaction and pollutant information provided by CRN.

The CRN tool provides significant insight to the pollutant formation chemistry and behavior. It also may be used as a means for parametric analyses and for design, since its turnaround time is typically several orders of magnitude less than the simplest CFD analysis.

Ongoing CRN work includes model enhancement (for robustness) and evaluation of the following:
- Other combustion test rigs and systems.
- Other fuel types.
- Intelligent tools to link the CFD and CRN analyses.

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