GT 2007-27990

Development and Application of an 8-Step Global Mechanism for CFD and CRN Simulations of Lean-Premixed Combustors

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ASME Turbo Expo
Montreal
May 14-17, 2007

Outline

- Purpose of 8-step mechanism:
  - CFD and CRN predictions of NOx and CO for natural gas-fired lean-premixed combustion turbines.
- Development of 8-step mechanism:
  - Foundation in high-pressure JSR measurements.
  - Chemical reactor modeling with GRI 3.0 used to develop the “database.”
  - Regression analysis used to obtain the 8 global steps.
- Application and verification of 8-step mechanism:
  - 15 atm bluff body combustor.
  - Gas turbine engine test rig.
  - CFD model of generic can-type combustor.

The 8-Steps

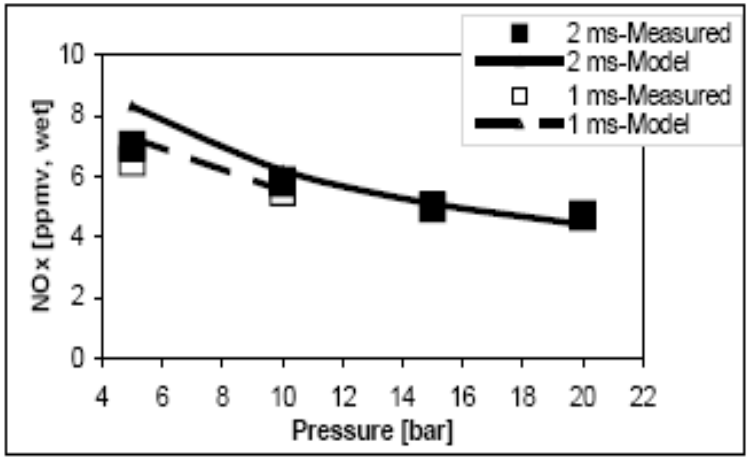
$CH_4 + 3/2O_2 \Rightarrow CO + 2H_2O$
$R_1=10^{13.354-0.004628P}[CH_4]^{1.3-0.01148P}[O_2]^{0.01426}[CO]^{0.1987}\exp\{-(21932+269.4P)/T\}$
$CO + 1/2O_2 \Rightarrow CO_2$
$R_2=10^{14.338+0.1091P}[CO]^{1.359-0.0109P}[H_2O]^{0.0912+0.0909P}[O_2]^{0.891+0.0127P}\exp\{-(22398+75.1P)/T\}$
$CO_2 \Rightarrow CO + 1/2O_2$
$R_3=10^{15.8144-0.07163P}[CO_2]\exp\{-(64925.8-334.31P)/T\}$
$N_2 + O_2 \Rightarrow 2NO$ (flame-NO by Zeldovich and nitrous oxide mechanisms)
$R_4=10^{14.122+0.0376P}[CO]^{0.8888-0.0006P}[O_2]^{1.1805+0.0344P}\exp\{-(46748+126.6P)/T\}$
$N_2 + O_2 \Rightarrow 2NO$ (flame-NO by prompt and NNH mechanisms)
$R_5=10^{29.8327-4.7822\log(P)}[CO]^{2.7911-0.04880P}[O_2]^{2.4613}\exp\{-(61265+704.7P)/T\}$ §
$N_2 + O_2 \Rightarrow 2NO$ (thermal-NO by H-atom attack on N_2O)
$R_6=10^{14.592}[N_2][H_2O]^{0.5}[O_2]^{0.25}T^{-0.7}\exp(-69158/T)$
$N_2 + O_2 \Rightarrow 2NO$ (thermal-NO by O-atom attack on N_2O)
$R_7=10^{10.317}[N_2][O_2]\exp(-52861/T)$
$N_2 + O_2 \Rightarrow 2NO$ (thermal-NO by O-atom attack on N_2)
$R_8=10^{14.967}[N_2][O_2]^{0.5}T^{-0.5}\exp(-68899/T)$

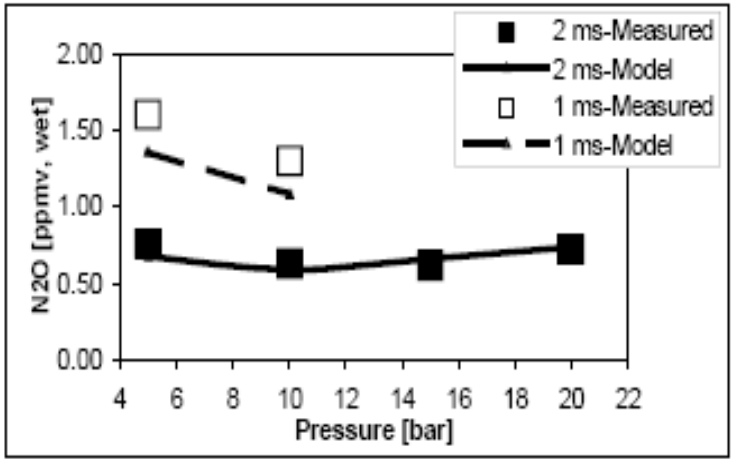
Nitric Oxide Reaction Chemistry for Lean-Premixed Combustion

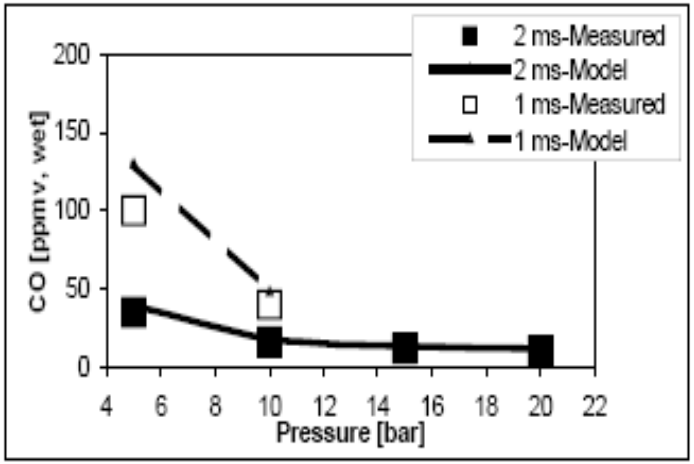
Zeldovich mechanism	
Rxn 1	$N_2 + O \Rightarrow NO + N$
Rxn 2	$N + O_2 \Rightarrow NO + O$
Rxn 3	$N + OH \Rightarrow NO + H$
Rate	$d[NO]/dt = 2k_1[N_2][O]$
Nitrous oxide mechanism	
Rxn 4	$N_2 + O + M \Rightarrow N_2O + M$
Rxn 5	$N_2O + O \Rightarrow NO + NO$
Rxn 6	$N_2O + H \Rightarrow NO + NH$
Note	Under lean-premixed combustion, quantitative oxidation of NH to NO is assumed.
Note	Several reactions [6], not shown here, convert N_2O back to N_2.
Rate	$d[NO]/dt = 2k_5[N_2O][O] + 2k_6[N_2O][H]$

Prompt NO	
Rxn 7	$N_2 + CH \Rightarrow HCN + N$
Note	Under lean-premixed combustion, quantitative oxidation of HCN and N to NO is assumed.
Note	N reacts to NO by Rxn's 2 and 3.
Rate	$d[NO]/dt = 2k_7[N_2][CH]$
NNH mechanism	
Rxn 8	$N_2 + H \Rightarrow NNH + H$
Rxn 9	$N_2 + H + M \Rightarrow NNH + M$
Rxn 10	$NNH + O \Rightarrow NO + NH$
Rxn 11	$NNH + O \Rightarrow N_2O + OH$
Note	As noted above, the oxidation of NH to NO is assumed quantitative
Note	Several reactions [6], not shown here, convert NNH back to N_2.
Note	The NO rate for the NNH chemistry does not include reaction 11.
Rate	$d[NO]/dt = 2k_{10}[NNH][O]$

Foundation in High-Pressure Jet-Stirred Reactor Measurements:
Modeling of data of Bengtsson by Rutar and Malte
(phi = 0.55, T = 1828K, 88% PSR/ 12% PFR).







Chemical reactor schemes used in developing the "database" – pressure 5-20 atm, inlet air temperature corresponding to 85% efficient compression from 288K, phi 0.45-0.75

Reactor Schemes (adiabatic)	CH_4 Oxidation	CO Oxidation	CO_2 Dissociation	Flame NO by Zeld & N_2O	Flame NO by Prompt & NNH
PSR: blowout to 3 millisec (ms)	X	X	X	X	X
PSR at blowout + PSR to 3 ms	X	X		X	X
PSR from blowout to 3 ms + PFR to 3 ms				X	
PSR from blowout to 3 ms + PFR approaching CO⇔CO_2 equilibrium		X	X		
PSR from blowout to 3 ms + PFR with air addition approaching CO⇔CO_2 equil.		X	X		

"Data" provided

- Temperature
- Major species concentrations: CH_4, CO, CO_2, O_2, H_2O, N_2, and OH.
- Species involved in NO formation: CH, N_2O, NNH, O, and H.
- Rates of CH_4 and CO oxidation and CO_2 dissociation.
- Rates of NO formation by the Zeldovich, nitrous oxide, prompt, and NNH mechanisms.

Global Rate Expression

The general equation used for the global reaction rates, R_1-R_5, is:

$$R = 10^{n+mP}\,[A]^{a+xP}\,[B]^{b+yP}\,[C]^{c+zP}\,\exp\{-(T_a+T_{a1}P)/T\}$$

where:

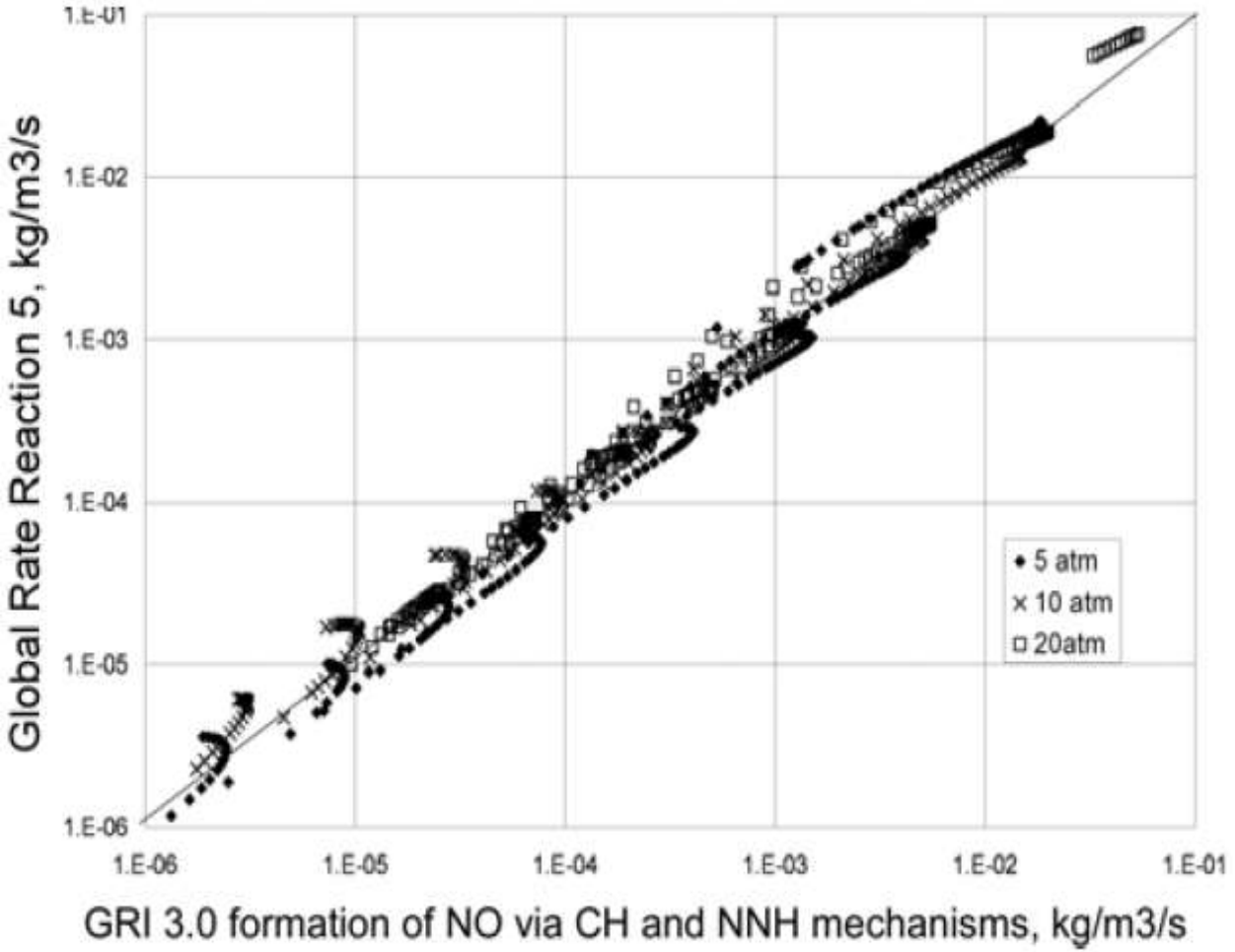
$T_a+T_{a1}P$ is the activation temperature (K)
T is the combustion temperature (K)
[ ] is the species concentration ($kmol/m^3$)
P is pressure (atm)
R is reaction rate ($kmol/m^3$-s)
n, m, a, b, c, x, y, z, T_a, and T_{a1} are coefficients and parameters to be determined

Obtaining the Global Rates

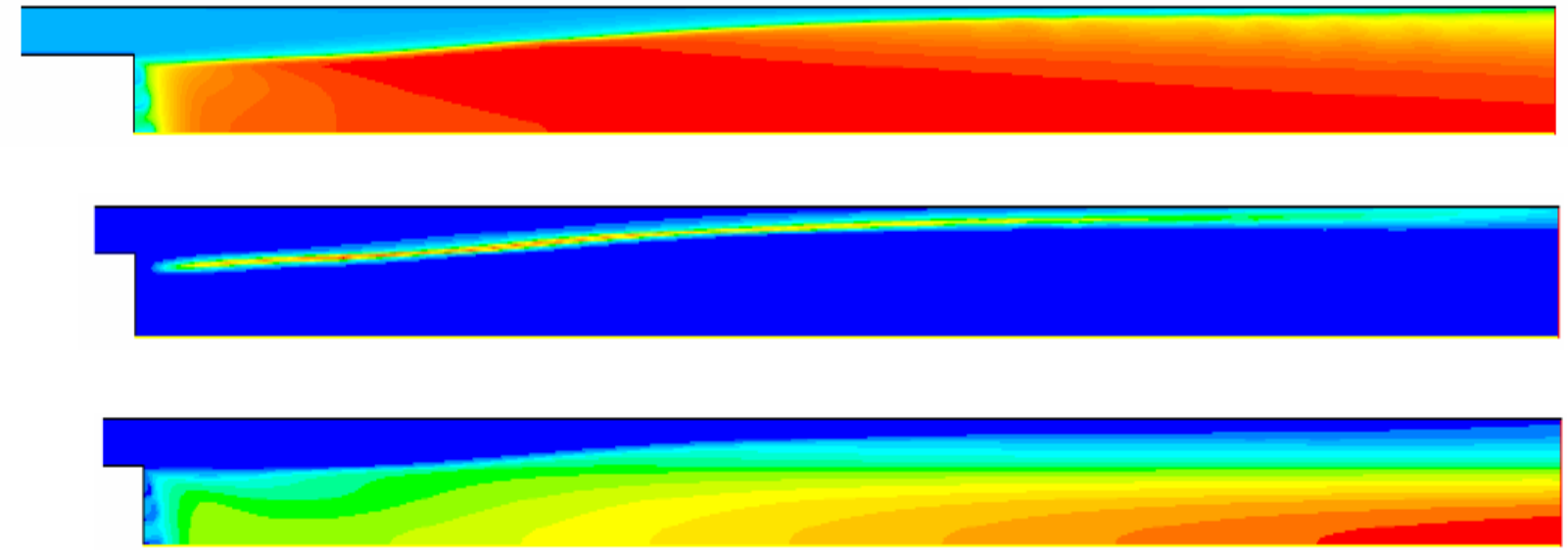
Regression analysis on the CRN database is performed to obtain the global rate expressions for R_1-R_5. Following selection of the species dependences for each global rate, the natural logarithm of the global rate expression is written and then least squares analysis is conducted to obtain the coefficients and parameters. The global rate expressions that give the best agreement to the CRN database are listed in Table 3 below. As a surrogate for the flame free radicals, CO is used

The remaining steps (6-8) cover thermal NO formation; thus, they depend on equilibrium thermo-chemistry. These steps only involve the Zeldovich and nitrous oxide mechanisms, since only these survive into the post-flame zone.

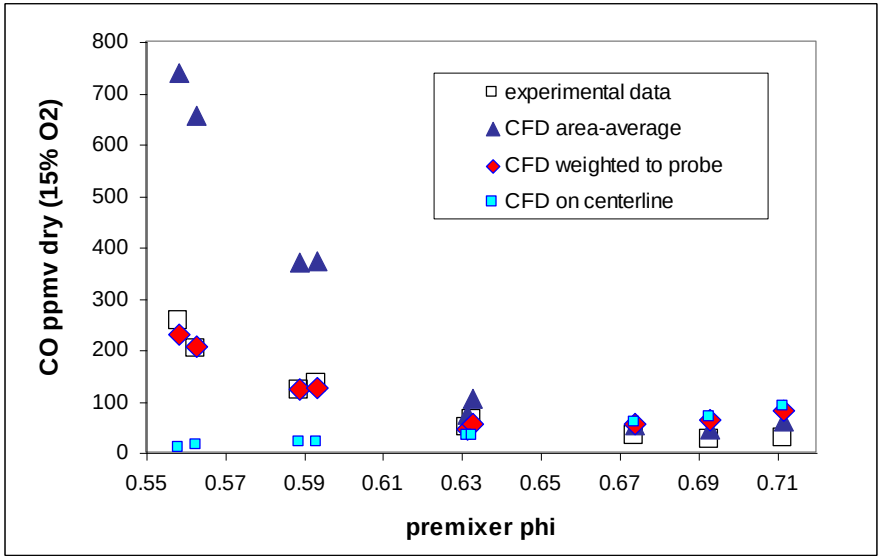
Example: Global Rate vs Rate by Elemental Chemistry

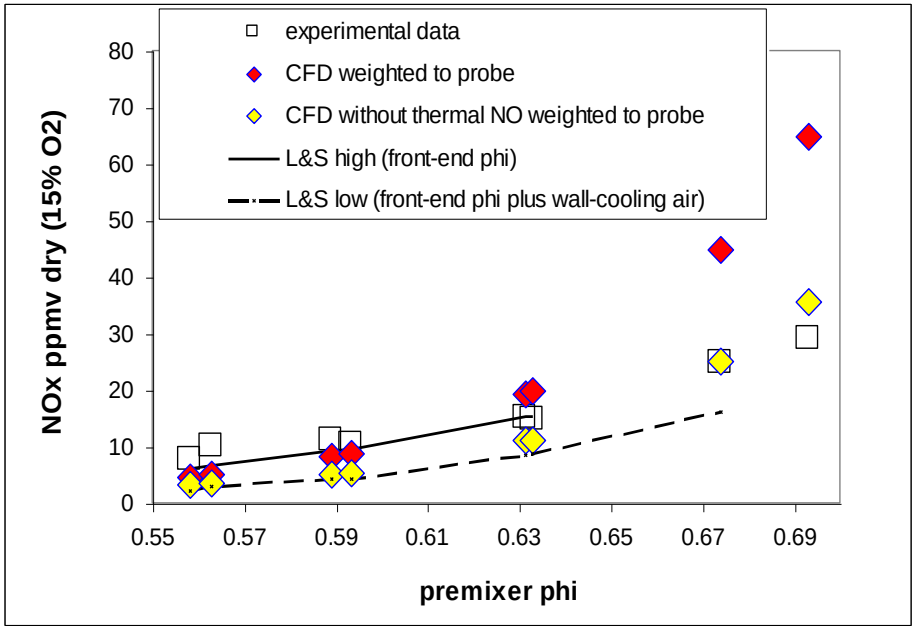


Bluff body combustor (Bucher et al.): methane, 680K inlet T, 14.3 atm, 1.1 kg/s air, 0.63 blockage ratio, effusion cooled.
Temperature field by 2-D CFD shown top plot: 1930K peak.
(flow from left to right)
Predicted CO (2.2% peak) and NO (14 ppm peak) also shown.
(phi = 0.59)



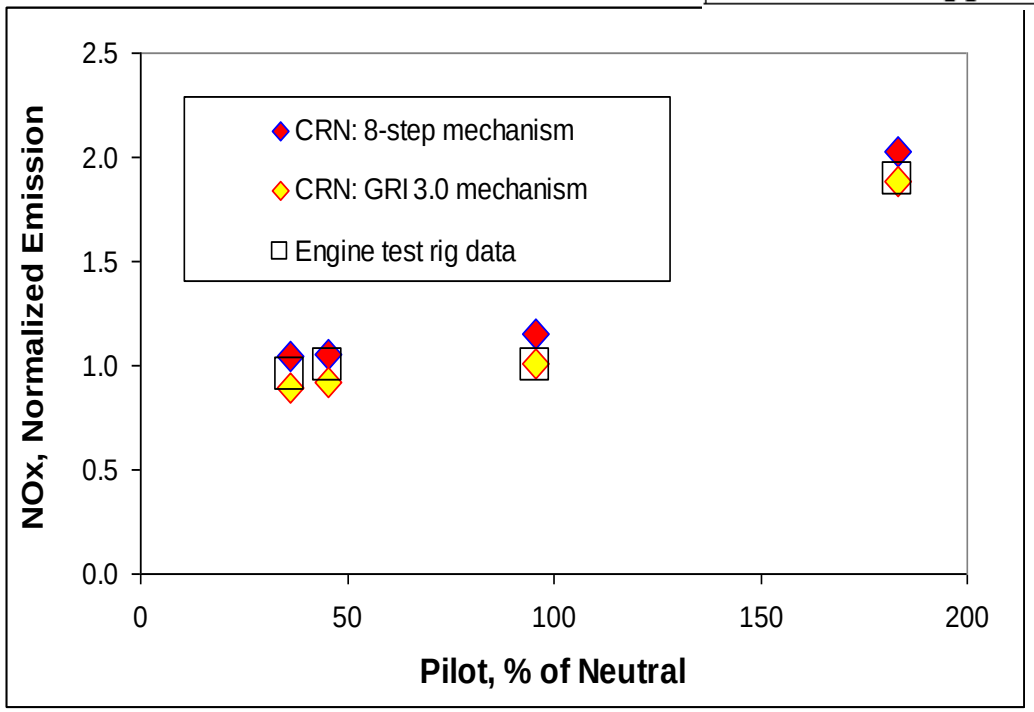
Bluff body: comparison of modeling results to measurements



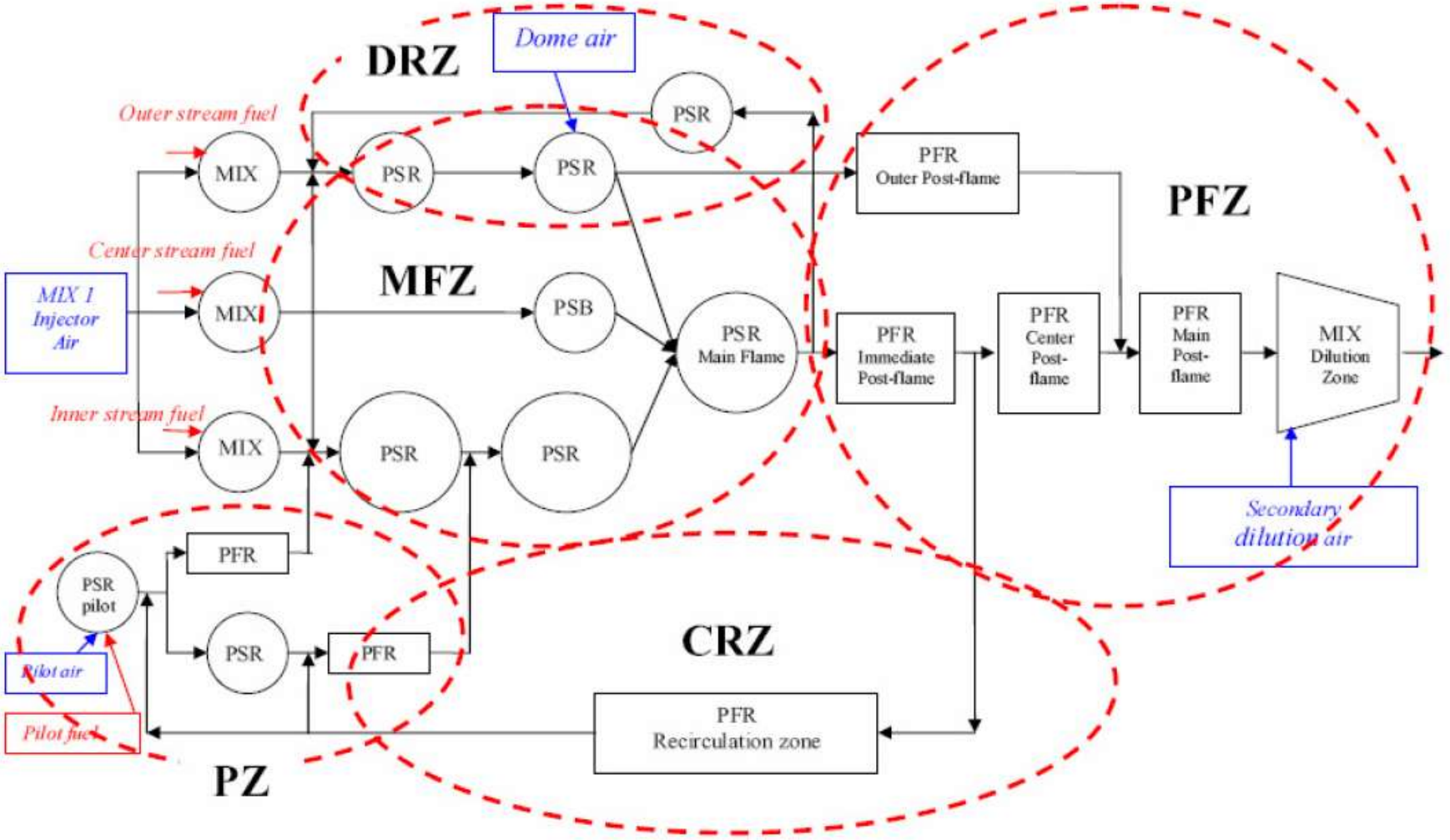


Gas Turbine Engine Test Rig Data (Novosselov et al.): Comparison between data and 31-element CRN predictions using full mechanism and 8-step mechanism.

Pilot Level	35-185% of neutral
GRI 3.0 in CRN	1.82 ± 0.03 ppmv (dry 15% O_2)
8-step in CRN	1.96 ± 0.03 ppmv (dry 15% O_2)
The CO emissions measured for the engine test rig are within a few ppmv of the CRN calculations.	



31-Element CRN for Lean-Premixed GT Combustor (Novosselov)



Application of 8-Step Mechanism in Modeling Generic Lean-Premixed Gas Turbine Combustor (phi = 0.475, 50% pilot, 16 atm)

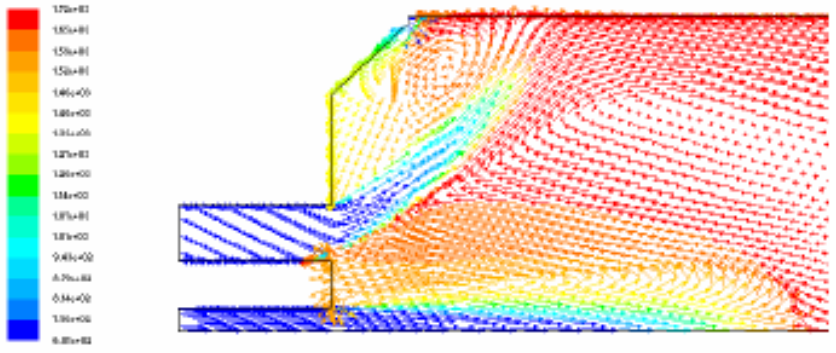


Figure 1. Vectors of velocity colored by temperature.

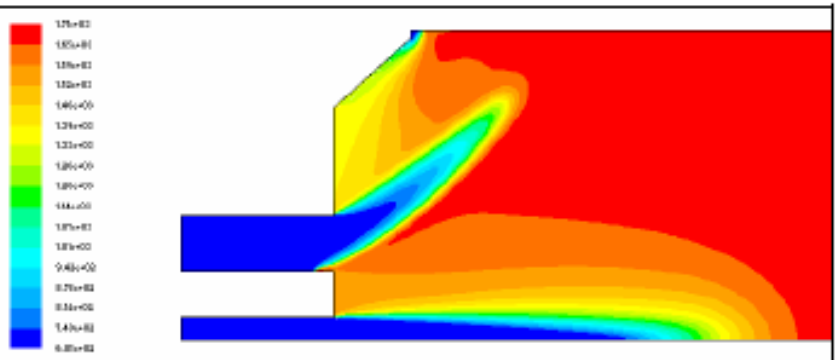


Figure 2. Temperature contour plot. Maximum is 1710 K.

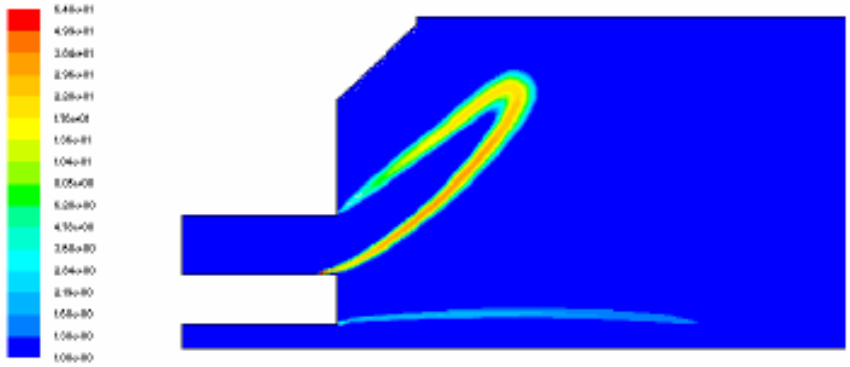


Figure 3. Rate of methane destruction reaction. Maximum rate is 65 kmol/m^3/s.

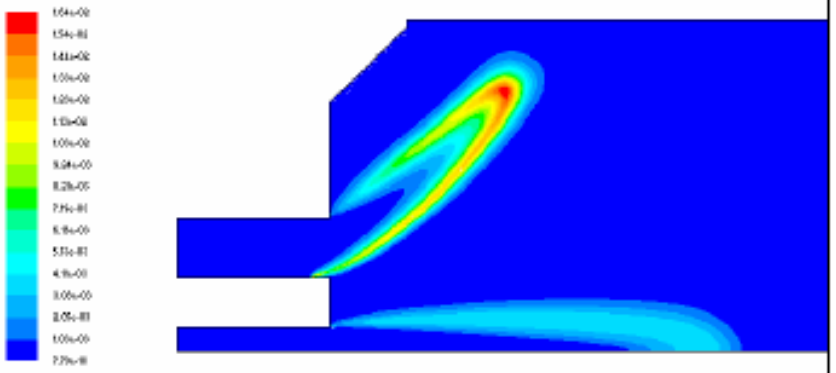


Figure 4. Mole fraction of CO. Maximum is 0.016 kmolCO/kmol total.

Application of 8-Step Mechanism in Modeling Generic Lean-Premixed Gas Turbine Combustor (rates)

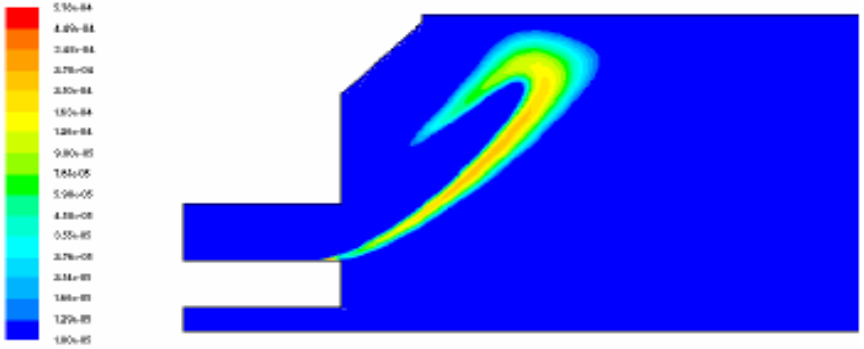


Figure 5. Rate of NO formation via non-thermal Zeldovich and nitrous oxide mechanisms (global step 4). Maximum rate is 5.78e-4 kmol/m^3/s.

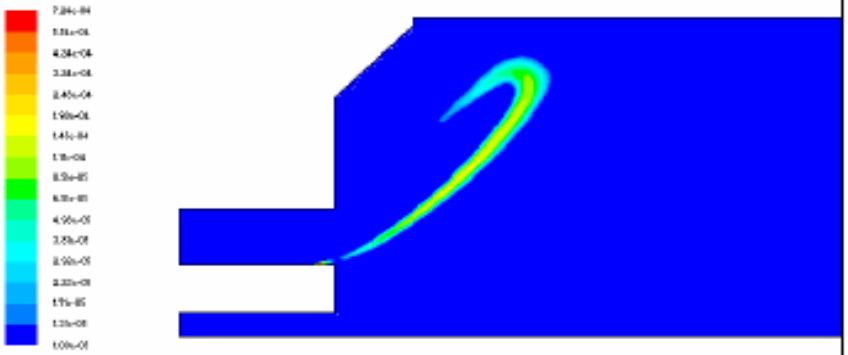


Figure 6. Rate of NO formation via prompt and NNH mechanisms (global step 5). Maximum rate is 7.25e-4 kmol/m^3/s.

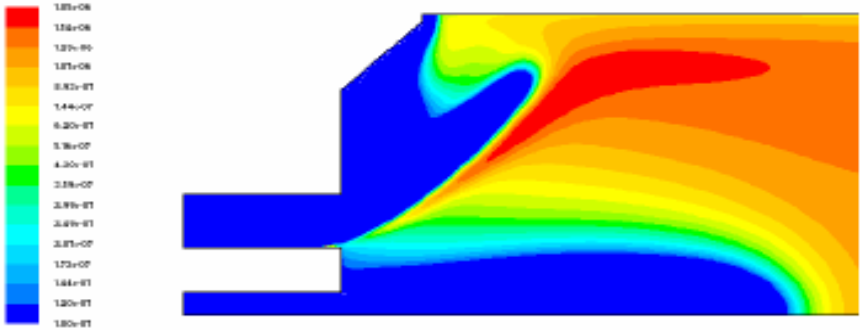


Figure 7. Rate of NO formation via thermal nitrous oxide mechanism assuming O-atom and N_2O equilibrium (global step 7). Maximum rate is 1.85e-6 kmol/m^3/s.

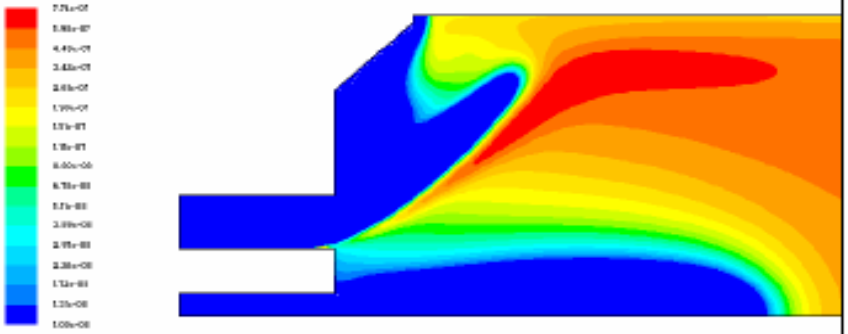


Figure 8. Rate of NO formation via thermal Zeldovich mechanism assuming equilibrium O-atom (global step 8). Maximum rate is 7.74e-7 kmol/m^3/s.

CFD Modeling Assumptions and Boundary Conditions

(bluff body at left, generic GT combustor at right)

Computational domain	2-D unstructured grid with 110,000 cells
Solver	Segregated RANS with species transport and volumetric reactions
Turbulence closure	Reynolds stress model
Convergence scheme	Second order (QUICK)
Pressure velocity coupling	Pressure implicit splitting of operators (PISO)
Wall treatment	Standard wall function
Heat loss	Convection and radiation heat transfer for top wall
Radiation heat transfer	Discrete ordinates (DO) model
Chemical kinetic rates	Eight-step mechanism
Chemical mixing rates	Eddy breakup rates

Computational domain	2D structured grid, 31, 000 cells
Solver	Segregated RANS with species transport and volumetric reactions
Turbulence closure model	Reynolds stress with quadratic pressure strain
Convergence scheme	Second order (QUICK)
Wall treatment	Standard wall function
Heat loss	Convective and radiative heat transfer
Radiative heat transfer	Discrete Ordinates (DO) Model
Chemical kinetic rates	UW eight-step global mechanism
Chemical mixing rates	Eddy break-up (EBU) model

END