Perfectly Stirred Reactor Network Modeling of NOx and CO Emissions from a Gas Turbine Combustor with Water Addition

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Outline

- Objectives
- Methodology
- Overview of major accomplishments
- Combustor description
- Final model performance
- NOx and CO emissions along the network
- Effect of pressure on NOx emissions
- Summary and conclusions
- Acknowledgements
Objectives

• Primary Objective: model effect of water addition on CO emissions
• Secondary Objectives:
  • Explain NOx and CO emissions trends versus FAR
  • Explain NOx emissions trends versus WFR
  • Determine NOx dependence on pressure
  • Understand the physics that govern net emissions output from combustor
  • Understand how combustor design changes might effect emissions
Methodology

• FLUENT CFD solution used to set up network:
  • PSR cell sizes selected such that gradients in temperature, FAR, velocity, and CO2 concentration are low in each cell
  • Network tuned such that each reactor cell matches CFD estimates of
    • Temperature
    • Velocity
    • CO2 Concentration
    • FAR
• Tuning parameters include mass transfer between cells, front end radial fuel distribution, and radial resolution in the lean section
• Lean section then readjusted to match experimentally measured temperature and CO profile at combustor exit
• Careful attention necessary to ensure all parameters of interest are met, which are often coupled
• Emissions trends as functions of FAR coincide well with experimental results without artificial network tuning to improve NOx and CO emissions
• NOx emissions trends as a function of WFR coincide well with experimental results
• Improved understanding of effect of water mixing on NOx emissions gained
• Effect of water on CO emissions understanding improved, but still needs work
• NOx pressure exponent estimation looks promising
Gas Turbine Combustor Schematic

Source: http://en.wikipedia.org/wiki/File:Combustor_diagram_componentsPNG.png
• Front end core is divided into 3 regions: a region representing a jet of fuel and air, a region representing a recirculation zone, and the rest of the rich core
• The quench zone and the set of reactors just downstream is modeled 3-dimensionally to capture gradients in the circumferential direction
• The rest of the network is 1-dimensional
• A collector volume is placed at the end of the network so that average emissions values may be determined
• Red arrows: fuel air and water inputs
• Blue arrows: mass transfer between parallel volumes
• Green arrows: mass transfer downstream
• Yellow arrows: air entering from walls
Quench Zone Architecture

- Blue arrows: mass transfer between parallel volumes
- Green arrows: mass transfer downstream
- Yellow arrows: air entering from walls

Quench Zone Repeated a total of 15 times
1st Part of Lean Section Architecture

- Blue arrows: mass transfer between parallel volumes
- Green arrows: mass transfer downstream
- Yellow arrows: air entering from walls
Last Part of Lean Section Architecture

- Blue arrows: mass transfer between parallel volumes
- Green arrows: mass transfer downstream
- Yellow arrows: air entering from walls
Comparison Between Corrected CO and NOx Measurements and PSR Results Versus FAR

- Agreement achieved without artificial model tuning
- Each data point has same model architecture; pressure, temperature, and FAR are only the parameters adjusted to coincide with experimental conditions
Experimental and PSR Radial CO\textsubscript{2} Exit Concentration Profile

- PSR CO\textsubscript{2} radial variation in core is not dramatic
- Fair agreement achieved with experimental results
PSR and Experimental CO Mole Fraction at Combustor Exit

- PSR CO radial variation in core is more significant than CO\(_2\) variation
- Middle volume peak is attributed to reduced residence time there, which reduces the time available for CO to CO\(_2\) oxidation
Comparison Between Corrected NOx Measurements and PSR Results Versus WFR

- Distributing the water in the front end according to the bulk flow mass distribution rather than the fuel flow mass distribution results in better agreement with experimental results.
Comparison Between NOx Progress Variable Along Combustor for Dry and Wet Cases

• NOx is produced almost entirely in the quench zone for both wet and dry conditions
• At high watering, NOx formation ceases halfway through the network
Comparison Between NOx in the Front End for Dry and Wet Cases

• Very little NOx is produced in the front end at high watering
Comparison Between NOx Formation Along Combustor For Ideal Water Mixing and Bulk Flow Mixing Assumptions

• When water is distributed according to the bulk flow rather than the fuel flow, most of the NOx is still produced in the quench zone.
• Result indicates that non-ideal water distribution results in non-uniform stoichiometric flame temperature reduction which leads to NOx increases.
Comparison Between Corrected CO Measurements and PSR Results Versus WFR

- Wet CO trend with WFR is not captured accurately with PSR network
Comparison Between CO along Combustor for Dry and Wet Cases

- CO decrease is attributed to reduced formation rates in front end due to kinetic rate reduction
- Kinetic rate reduction for CO to CO$_2$ oxidation is not enough to replicate the experimental trends observed
Comparison Between CO in The Lean Section for Dry and Wet Cases

- Wet CO predictions in the lean section show reduced oxidation, but not enough to cause a net increase in CO with water addition
Redistribution of the Water Downstream Doesn’t Help
When NOx Emissions are Kept Near Experimentally Measured Values

- Redist1: 30% Panel 1, 50% Panel 2, 20% Panel 3; distributed by volume
- Redist2: 30% Panel 1, 50% Panel 2, 20% Panel 3; distributed by fuel flow rate
- Redist3: Water placed at beginning of quench zone; distributed by fuel flow rate
- Redist4: Water placed at second set of quench zone volumes; distributed by fuel flow rate
- Redist6: Water placed as late as possible to keep NOx at reasonably low levels, consistent with experimental data, and only in volumes which need NOx emissions help; distributed by fuel flow rate

- Redistributing the water downstream of the front end, even to the point where CO formation ceases and oxidation begins does not fix the problem
Redistribution of the Water Downstream Doesn’t Help
When NOx Emissions are Kept Near Experimentally Measured Values

- Redist1: 30% Panel 1, 50% Panel 2, 20% Panel 3; distributed by volume
- Redist2: 30% Panel 1, 50% Panel 2, 20% Panel 3; distributed by fuel flow rate
- Redist3: Water placed at beginning of quench zone; distributed by fuel flow rate
- Redist4: Water placed at second set of quench zone volumes; distributed by fuel flow rate
- Redist6: Water placed as late as possible to keep NOx at reasonably low levels, consistent with experimental data, and only in volumes which need NOx emissions help; distributed by fuel flow rate

- Dry CO emissions predictions are low than wet cases regardless of where the water is placed
### Effect of Water on CO Production/Depletion For Various Mechanisms

X’s denote cases that were not run, and DNC denotes cases that did not converge.

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- Equilibrium calculations suggest that with high residence times, water addition always reduces CO.
- At finite residence times, water addition increases CO for lean conditions, and reduces CO for rich conditions.
Residence Time Effect + Network Results Versus Single Volume Results

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- When residence time is varied, increases in CO with water addition for slightly rich conditions are now observed, but not for equivalence ratios of 2 or higher.
- PSRnet cases represent actual volumes within the network, which paradoxically exhibit CO reduction with water addition for slightly rich conditions.
- When these actual volumes are simulated with the inputs being CO, CO₂, N₂, and H₂O, increases in CO with water addition are still observed.
PSR Network Predicts a Reduction in the NOx Pressure Exponent with Increases in WFR

- Dry point coincides well with data available for similar combustors
- Wet pressure exponent calculation trends with WF ratio seem reasonable
PSR Network Development Summary and Conclusions

- PSR network is capable of reproducing emissions trends and values as a function of FAR without any tuning to improve NOx and CO emissions predictions when the selected parameters agree with the CFD solution.
- PSR network is capable of reproducing NOx emissions trends and values as a function of WFR.
- PSR network currently does not trend with experimental results for CO emissions as a function of WFR.
- For the dry conditions results indicate that the perfectly stirred assumption is adequate to capture experimental dry NOx and CO emissions trends.
- Wet NOx emissions predictions suggest that water may not follow the fuel in an ideal manner, and quench zone NOx production suffers from water mixing according to the bulk flow mass flux rather than the fuel flow mass flux.
- PSR network is a suitable tool for estimating NOx pressure exponents for the combustor investigated under dry and wet conditions. Confidence gained in this use of the PSR tool from the fact that the dry pressure exponent compares well with exponents measured for similar combustors.