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## Analysis of Lean Premixed/Prevaporized Combustion with KIVA-II

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## Abstract

Requirements to reduce the emissions of pollutants from gas turbines used in aircraft propulsion and ground based power generation have led to consideration of lean premixed/prevaporized (LPP) combustion concepts. This paper describes some of the LPP flame tube analyses performed at the NASA Lewis Research Center with KIVA-II, a well-known multi-dimensional CFD code for problems including sprays, turbulence, and combustion. Modifications to KIVA-II's boundary condition and chemistry treatments have been made to meet the needs of the present study. The study itself focuses on two key aspects of the LPP concept, low emissions and flame stability (including flashback and lean blowoff).

## Background

Nitrogen oxides ( $\text{NO}_x$ ) are serious components of air pollution, and considerable effort is being expended to reduce their emission from stationary and mobile combustion

devices. As  $\text{NO}_x$  formation is reduced substantially at lower equivalence ratios ( $\phi$ ), there is a great deal of interest in lean combustion. An LPP system (Fig. 1) separates the fuel injection and combustion processes to vaporize the fuel and mix it completely with air before it burns, avoiding hot spots to further minimize  $\text{NO}_x$  emissions. Unfortunately, lean combustion also leads to increased problems with flame stability.<sup>1</sup>

Numerical studies of an LPP flame tube are being conducted at Lewis to examine both emissions and stability, with the geometry used by Anderson adopted to permit comparisons to be made with his experimental data. This flame tube was circular in cross section with a diameter of 10.25 cm. Propane was introduced 260 cm upstream of the flameholder into an air stream with a flow velocity of 2500 cm/sec and an inlet pressure of 5.5 atmospheres. Although tests were run with inlet temperatures of 600 and 800 K, the calculations being reported here consider only the latter value. The water-cooled flameholder (Fig. 2) was 1.92 cm thick and pierced with 61 circular holes of 0.635 cm diameter, yielding an open area of 25 percent.  $\text{NO}_x$  and CO were measured 10, 20, and 30 cm downstream of the flameholder.<sup>1</sup>

## Numerical Method

The calculations are being performed with KIVA-II, a program developed originally to study the in-cylinder combustion dynamics of internal combustion engines. However, because the code can treat problems combining sprays, turbulence, and combustion, it can also be employed in the analysis of gas turbine combustors, as well as their laboratory analogues, e.g., the LPP flame tube examined in this study.<sup>2,3</sup>

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However, as originally released, KIVA-II cannot treat the flameholder's complicated geometry. To rectify this, the program's boundary condition treatment has been revised to allow an arbitrary obstacle geometry to be incorporated within the mesh. To reduce computational costs, the three-dimensional flameholder geometry has been simplified to allow a two-dimensional axisymmetric analysis to be performed. Two alternative geometries (Fig. 2) have been considered, leading to the two 35x120 grids (Fig. 3) used in this study.

The original KIVA-II is also restricted to laminar kinetics. For this study, a mixing controlled combustion model (that of Magnussen and Hjertager<sup>4</sup>) has been added. Calculations have been performed with both chemistry treatments utilizing two simplified reaction schemes, that of Ying and Nguyen<sup>5</sup> and that of Kundu and Deur<sup>6</sup>. Although both include NO<sub>x</sub> formation, the first mechanism (11 steps) considers thermal NO<sub>x</sub> alone, while the latter (23 steps) models both thermal and prompt NO<sub>x</sub>.

## Results

To date, 24 analyses have been completed, yielding flowfield and emissions information over a range of conditions.

In the first series of calculations, the Ying and Nguyen reaction mechanism was coupled with the mixing controlled combustion model and the 51 percent open area flameholder grid (Fig. 4). Lean blowoff was found to occur at equivalence ratios below 0.6, while flashback took place at ratios greater than 0.9. By comparison, Anderson found that blowoff occurred at equivalence ratios below approximately 0.4, and as data was recorded at equivalence ratios up to 1.01, it can be assumed that flashback took place only at higher ratios. Finally, the calculated NO<sub>x</sub> levels were substantially less than those measured, e.g., approximately 25 percent low for the 0.9 equivalence ratio case shown in the figure.<sup>1,7</sup>

In the next series, the chemistry treatment was the same, but the revised grid reducing the flow area to 35 percent was employed. Blowoff now took place at an equivalence ratio between 0.4 and 0.5, and flashback did not occur until the equivalence ratio exceeded 1.0 (Fig. 5). NO<sub>x</sub> predictions did not change appreciably.

To this point, the surfaces of the flameholder had been treated as adiabatic. If the flameholder was water-cooled, it might better be modeled as having a constant temperature. Two cases, with 800 and 400 K flameholder temperatures respectively, were run at an equivalence ratio of 1.0, utilizing the above chemistry treatment and the original 51 percent open area grid. At the higher temperature, there was no apparent effect, but some minor changes were noted with the 400 K flameholder (Fig. 6).

In the final series of calculations, the Kundu and Deur mechanism was employed with the adiabatic, 51 percent open area flameholder. The mixing controlled combustion model was not utilized. Blowoff occurred at an equivalence ratio of 0.4, but flashback was observed at ratios above 0.7, requiring the use of a setup which artificially eliminates the phenomenon to evaluate emissions at the higher ratios. The calculated NO<sub>x</sub> levels more closely followed the experimental values (Fig. 7).

## Future Work

Work continues to explore the limits of stable combustion demonstrated in the above analyses, while maintaining the quality of the NO<sub>x</sub> predictions obtained with the larger mechanism. Mechanism development has been hampered by a lack of experimental data providing flame propagation speeds at higher equivalence ratios. (It is not surprising that flashback began at ratios greater than 0.7, since that is where the available data stopped.) Work also continues to develop a full three-dimensional analysis, to incorporate a scalar PDF combustion/turbulence model, and to study acoustic effects on flashback.

## References

- <sup>1</sup>Anderson, D. N., "Effect of Equivalence Ratio and Dwell Time on Exhaust Emissions from an Experimental Premixing/Prevaporizing Burner," NASA Lewis Research Center, NASA-TM-X-71592, Cleveland, Ohio, March 1975.
- <sup>2</sup>Amsden, A. A., O'Rourke, P. J., Butler, T. D., "KIVA-II: A Computer Program for Chemically Reacting Sprays with Sprays," LA-11560-MS, Los Alamos National Laboratory, Los Alamos, New Mexico, May 1989.
- <sup>3</sup>Cline, M. C., Deur, J. M., Micklow, G. J., Harper, M. R., and Kundu, K. P., "Computation of the Flowfield in an Annular Gas Turbine Combustor," AIAA Paper 93-2074, June 1993.
- <sup>4</sup>Magnussen, B. F., and Hjertager, B. H., "On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion," *Proceedings of the 16th Symposium on Combustion*, The Combustion Institute, Pittsburgh, Pennsylvania, 1977, pp. 719-729.
- <sup>5</sup>Ying, S. L., and Nguyen, H. L., "Numerical Simulation of Jet-A Combustion Approximated by Improved Propane Chemical Kinetics," AIAA Paper 91-1859, June 1991.
- <sup>6</sup>Kundu, K. P., and Deur, J. M., "A Simplified NO<sub>x</sub> Formation Mechanism for CFD Use," AIAA Paper 94-2905, June 1994.
- <sup>7</sup>Anderson, D. N., private communications, NASA Lewis Research Center, Cleveland, Ohio, May 1994.

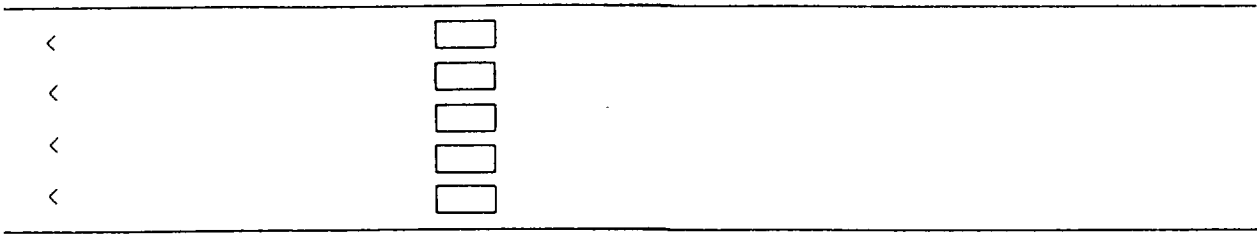
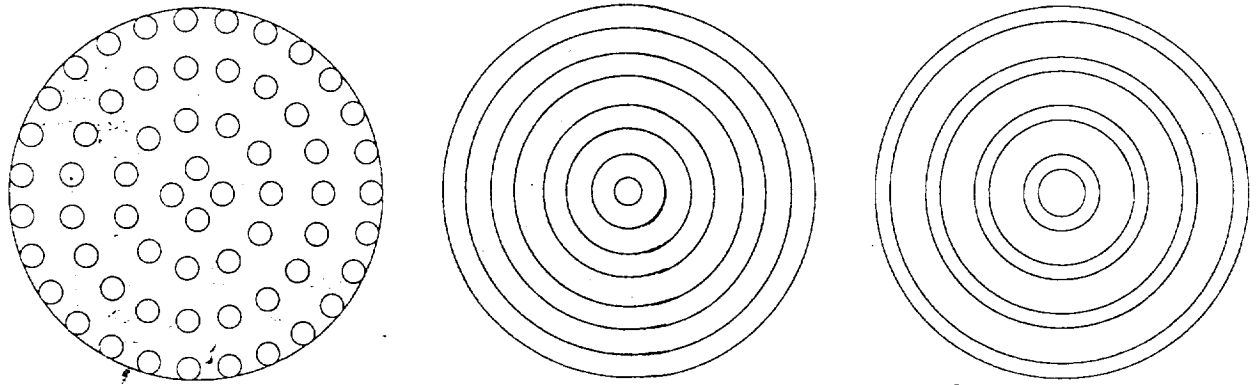
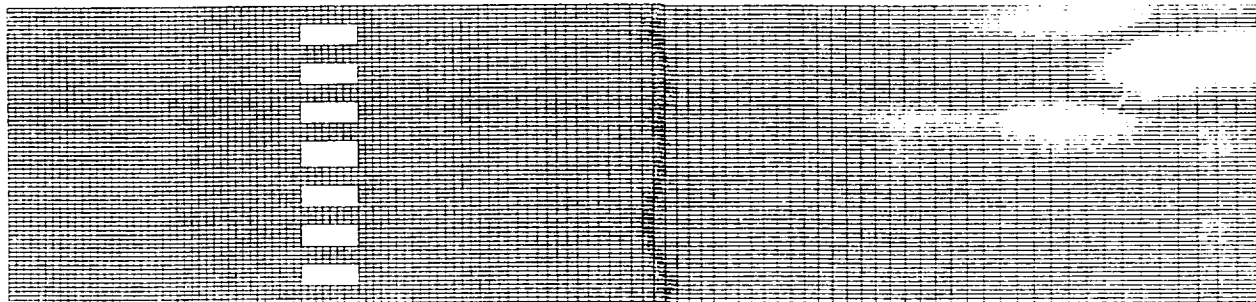


Figure 1. Schematic of a Generic LPP Flame Tube.

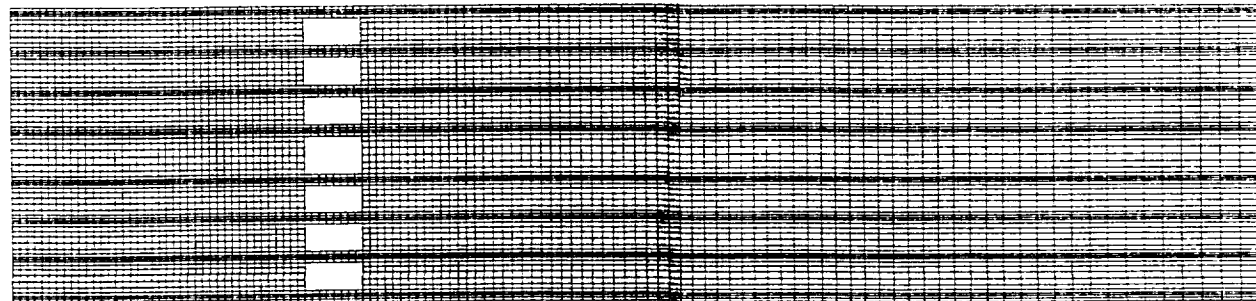


A. Experiment (25% Open Area). B. Preliminary Analyses (51% Open Area). C. Revised Analyses (35% Open Area).

Figure 2. Experimental and Analytical Flameholder Geometries for Anderson LPP Flame Tube.

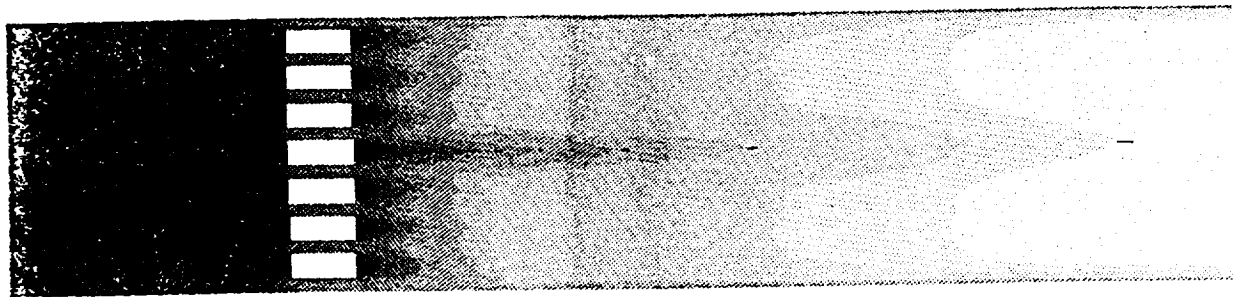


A. Preliminary Analyses (51% Open Area Flameholder Geometry).

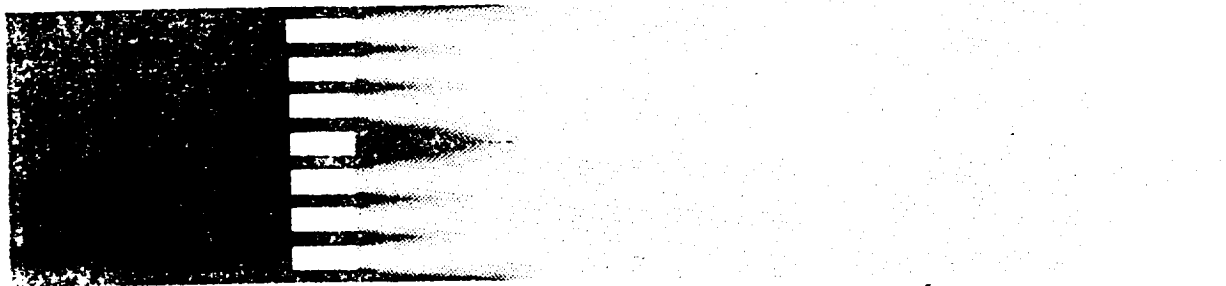


B. Revised Analyses (35% Open Area Flameholder Geometry).

Figure 3. Axisymmetric KIVA-II Grids for Anderson LPP Flame Tube Analyses.



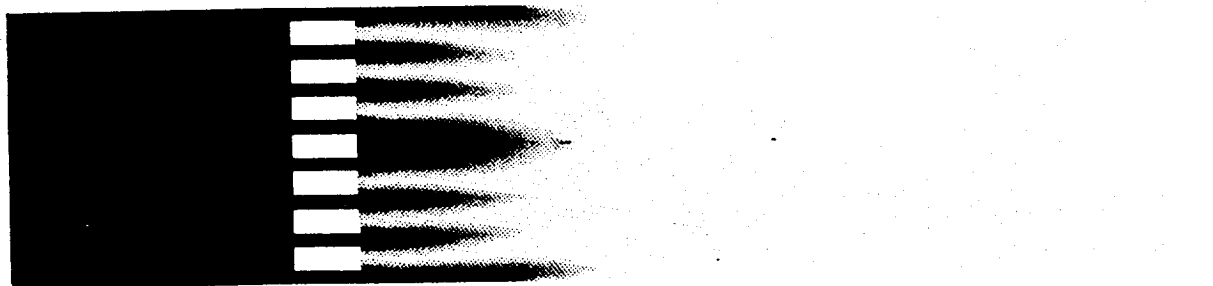
A. Axial Velocity (0 - 11000 cm/sec).



B. Temperature (700 - 2600 K).



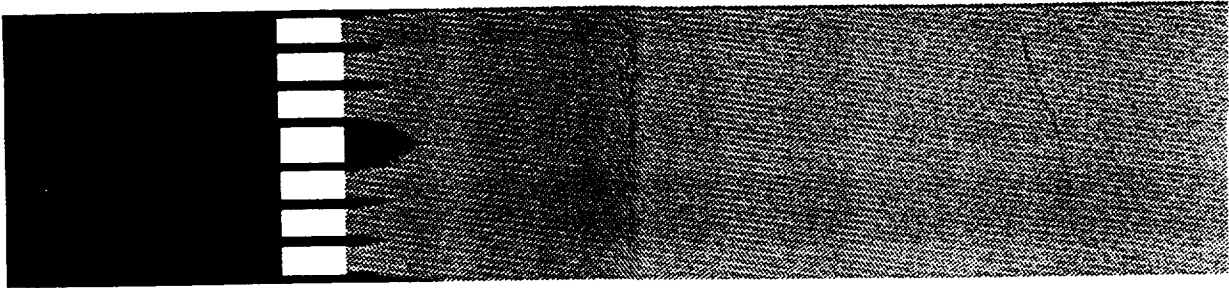
C. NO<sub>x</sub> Emission Index (0 - 60 g/kg).



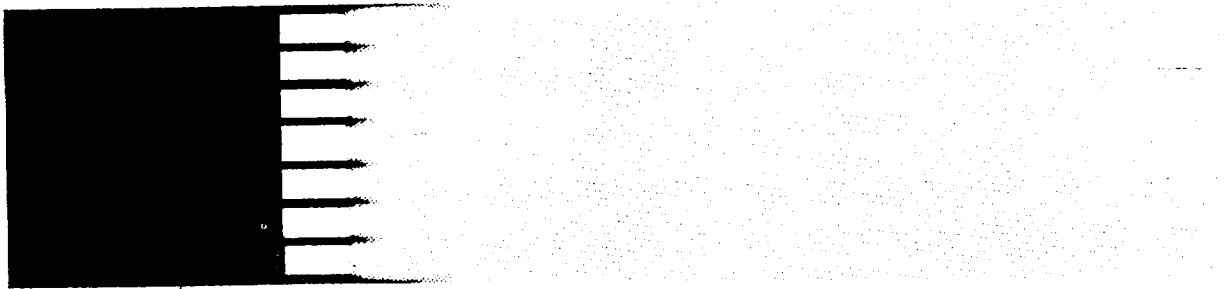
D. CO Emission Index (0 - 230 g/kg).



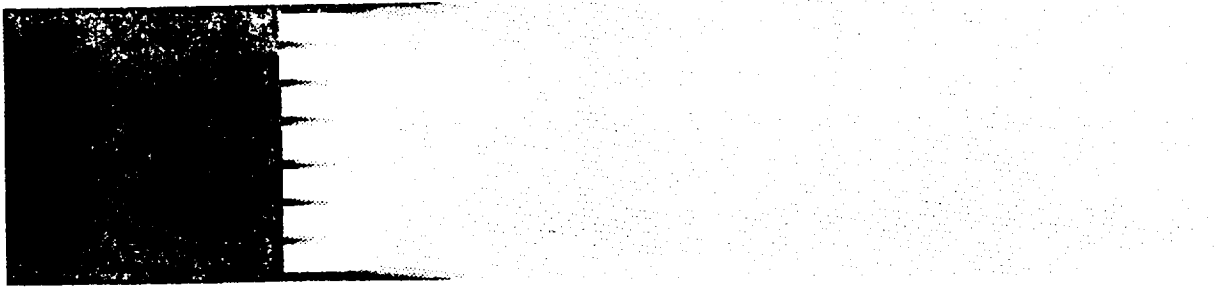
Figure 4. Typical KIVA-II Results for Anderson LPP Flame Tube Analysis ( $\phi = 0.9$ ).



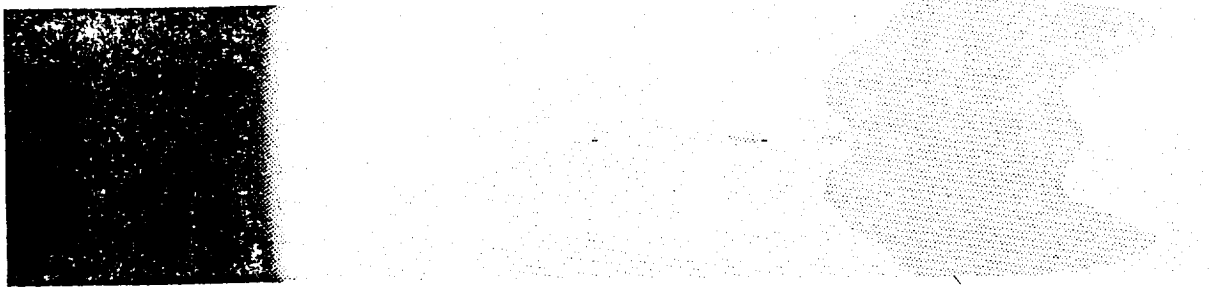
A.  $\phi = 0.5$ .



B.  $\phi = 1.0$ .



C.  $\phi = 1.2$ .

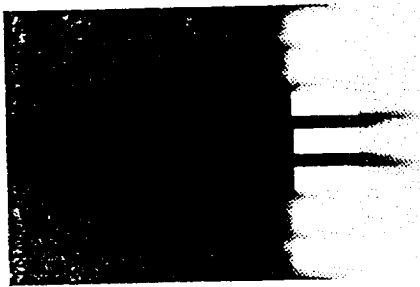


D.  $\phi = 1.5$ .

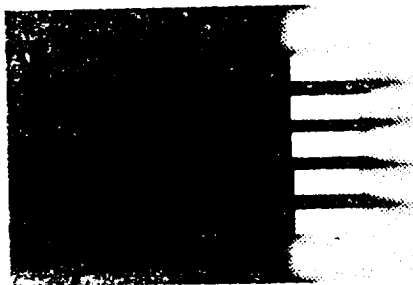
700 K

2600 K

Figure 5. Equivalence Ratio Effects on Temperature Distribution in Anderson LPP Flame Tube (Revised Grid Geometry).



A. Adiabatic Flameholder.



B. Fixed Flameholder Temperature (400 K).

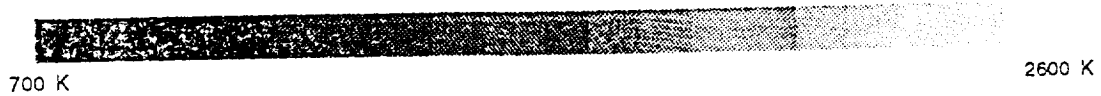


Figure 6. Effects of Flameholder Heat Transfer Model on Temperature Distribution in Anderson LPP Flame Tube ( $\varnothing = 1.0$ ).

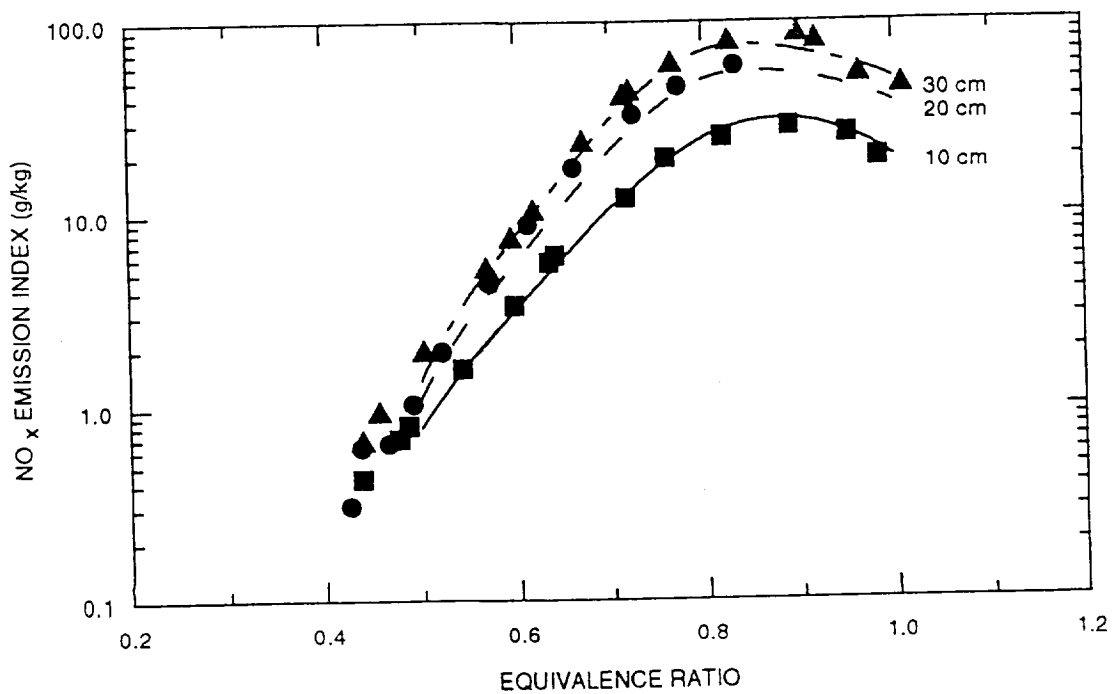


Figure 7. Comparison of KIVA-II Analysis Results (curves) with Anderson LPP Flame Tube Data.<sup>1</sup>

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