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HSR COMBUSTION ANALYTICAL RESEARCH

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HSR COMBUSTION ANALYTICAL RESEARCH

Program Objectives and Approaches

Increasing the pressure and temperature of the engines of a new generation of supersonic airliners increases the emissions of nitrogen oxides (NO_x) to a level that would have an adverse impact on the Earth's protective ozone layer. In the process of evolving and implementing low emissions combustor technologies, NASA Lewis has pursued a combustion analysis code program to guide combustor design processes, to identify potential concepts of greatest promise, and to optimize them at low cost, with short turnaround time. The computational analyses are evaluated at actual engine operating conditions. The approach is to upgrade and apply advanced computer programs for gas turbine applications. Efforts have been made in further improving the code capabilities for modeling the physics and the numerical method of solution. Then test cases and measurements from experiments are used for code validation.

HSR Combustion Analytical Research

Objective:

- **Use advanced computer models to analyze and design combustor components and subcomponents, understand the physics, and determine how to optimize the design to improve the performance**

Approach:

- **Emphasis on applying and upgrading existing codes – KIVA-II, LERC3D for gas turbine combustor applications**
  - **Improve codes capabilities**
  - **Codes validation**

Figure 1

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Lewis Key Milestones

Due to schedule constraints, the analytical research program is being conducted over a period of 5 years as shown in figure 2 and involves three major milestones. The first milestone was accomplished with the development and use of two-dimensional and three-dimensional codes, KIVA-II and LeRC3D, to guide low emissions combustion concept experiments. These codes will be updated based on results obtained from combustion concept experiments by the end of FY93. These codes will then be used as predictive design tools for low emissions combustors by the end of FY95.

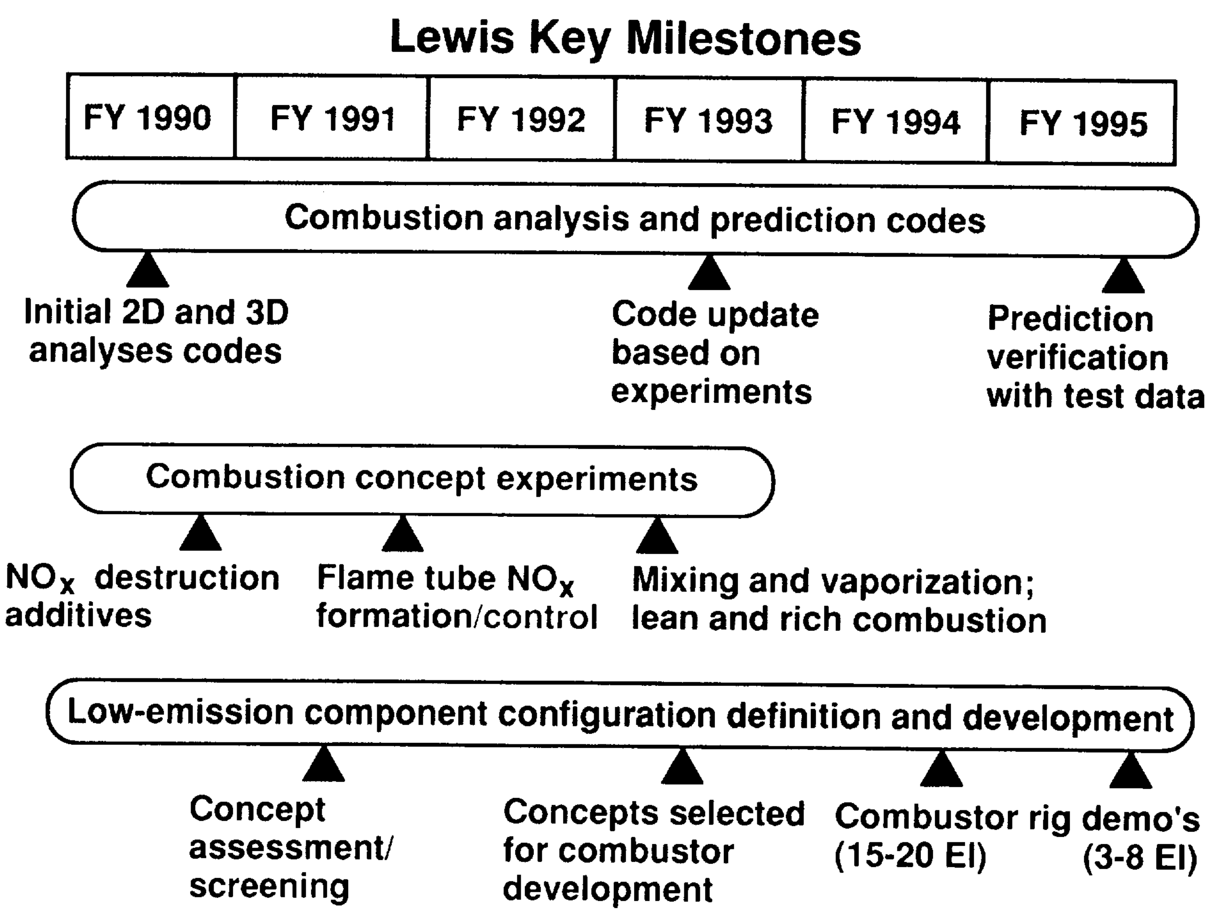

Figure 2

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Organization and Activities Listing

The overall combustion analytical codes evolution plan involves in-house research and contracts and grants; and it provides strong collaborative relationships and technology transfer between industry, universities, and government agencies. Figure 3 lists the activities for the HSR Combustion Analytical Research Program.

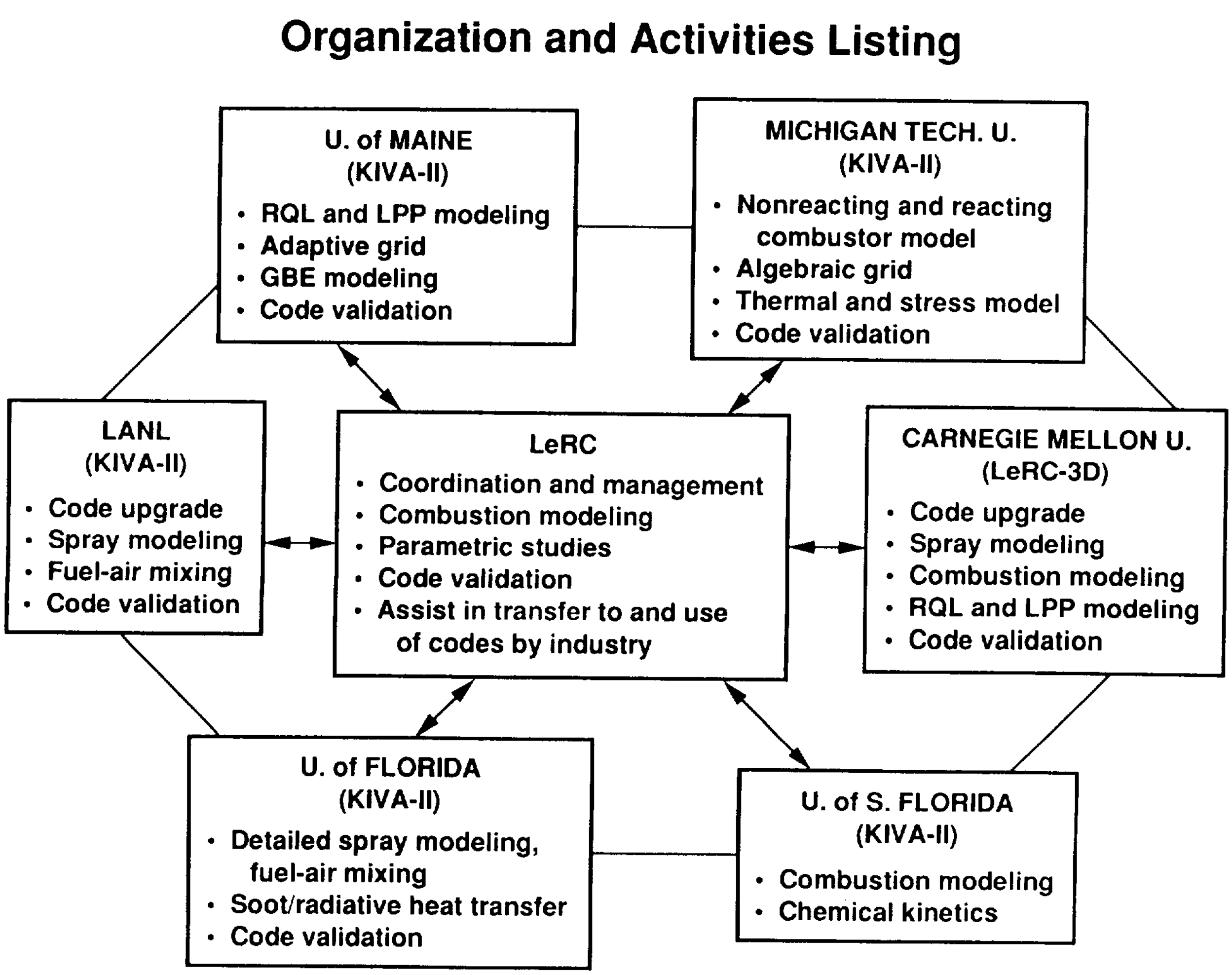

Figure 3

HSR COMBUSTION ANALYTICAL RESEARCH

Description of Computer Code KIVA-II

To provide insight into the combustion process and combustor design, KIVA-II and LeRC3D have been used. These codes are operational and calculations have been performed to guide low emissions combustion experiments. KIVA-II (ref. 1), developed by Los Alamos National Laboratory, is one of the most developed and validated codes of the available multi-dimensional computer programs for prediction of the in-cylinder combustion dynamics in internal combustion engines. There are features of KIVA-II that make it well suited for other applications, so KIVA-II has been adapted for gas turbine combustor applications.

In terms of modeling the physics, the major features of KIVA-II are as follows:

- KIVA-II is a two- and three-dimensional turbulent compressible flow solver of reacting multicomponent gas mixture with liquid spray using an Eulerian-Lagrangian approach.
- Turbulence is modeled using the k-ε model.
- Combustion is modeled by a chemical-kinetics-controlled model using global or detailed chemical reactions (ref. 2) or by a mixing-controlled model (ref. 3). The user can conveniently provide a chemical kinetics mechanism by making appropriate modification to the input data file (ref. 2).
- The extended Zeldovich NO_x mechanism is included.
- Stochastic particle spray model includes vaporization, coalescence, and breakup.
- A soot formation/oxidation and a radiative heat transfer model are also included.

In terms of numerics, KIVA-II is based on the following:

- Time-dependent finite-difference code with arbitrary mesh capability, using an implicit-continuous Eulerian technique with conjugate residual iteration for the flow solver.

Key Features of KIVA-II

Description of Computer Code KIVA-II

Physics

Turbulent compressible flow of reacting multicomponent gas mixture with liquid spray

κ-ε turbulence model with wall functions

Combustion models:
Chemical kinetics controlled, mixing controlled model

NO_x formation model:
Extended Zeldovich mechanism

Spray model:
Stochastic model, vaporization, coalescence, breakup

Soot formation/oxidation

Radiation heat transfer

Numerical method

2D or 3D time-dependent finite difference code

Arbitrary mesh

ICE method with conjugate residual iteration

Optimal quasi-second-order upwind convection

Figure 4

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Description of Computer Code LeRC3D

LeRC3D is a highly advanced code for gas turbine combustor applications. LeRC3D was developed by Carnegie Mellon University with the collaboration/sponsorship of Lewis. In terms of modeling the physics, the major capabilities of LeRC3D (ref. 4) are as follows:

- LeRC3D is a two- and three-dimensional code that solves the N-S equations for turbulent compressible flow of reacting multicomponent gas mixture with liquid spray using an Eulerian-Lagrangian approach.
- The turbulence is modeled by using a k-ε turbulence model with wall functions, or by using a low Reynolds number k-ε model of Chen and Patel, or by using a RNG-based k-ε model.
- Modeling of combustion is done by two different models: the chemical-kinetics-controlled model governed by global or detailed chemical kinetics mechanisms of hydrocarbon combustion, and the mixing-controlled model of Magnussen and Hjertager. The user can conveniently provide a chemical kinetics mechanism by making appropriate modification to the input data file.
- The chemical kinetics model used to study NO_x is the Zeldovich mechanism.
- The spray model includes the fuel vaporization model of Raju and Sirignano.

In terms of the numerical method of solution, LeRC3D is based on the following:

- The flow algorithm is a finite-volume, LU algorithm utilizing van Leer flux-vector splitting with the HOPE algorithm of Liou and Steffan. Source terms are treated implicitly using Shih and Chyu method, diffusion terms are treated implicitly using the procedure of Shih and Steinthorsson.
- A grid system is generated by using an algebraic grid generation method based on transfinite interpolation.

Key Features of LeRC3D

Description of Computer Code LeRC3D

Physics

Turbulent compressible flow of reacting multicomponent gas mixture with liquid spray

Turbulence models:
- κ-ε turbulence model with wall functions
- Low Reynolds no. κ-ε model (Chen & Patel)
- RNG-based κ-ε model

Combustion models:
- Chemical kinetics controlled
- Mixing controlled

NO_x formation model:
- Zeldovich mechanism

Spray model:
- Lagrangian model of Raju & Sirignano

Numerical method

Grid generation:
- Algebraic method using transfinite interpolation

Flow algorithm:
- Finite-volume, LU, implicit

Code:
- Efficient and robust

Figure 5

VERIFICATION OF KIVA-II CODE PREDICTIONS

Fuel Spray - Air Interaction

Figure 6 shows the prediction of a swirling fuel spray in a nonreacting airstream using the KIVA-II code and a comparison with the experimental results (ref. 5). The model air-assist atomizer embodies a nonswirl inner airstream and a swirling outer airstream which help to atomize and distribute fuel injected from a core tube. Predicted and measured air azimuthal velocity profiles are in good agreement. Fuel injection and mixing become increasingly important as more air is used for the combustion process. Detailed models of the interaction of the swirling air and the fuel spray can provide valuable insight into the effect of different variables that presently can only be evaluated experimentally on a global scale at laboratory test conditions.

Verification of KIVA-II Code Predictions

Fuel Spray-Air Interaction

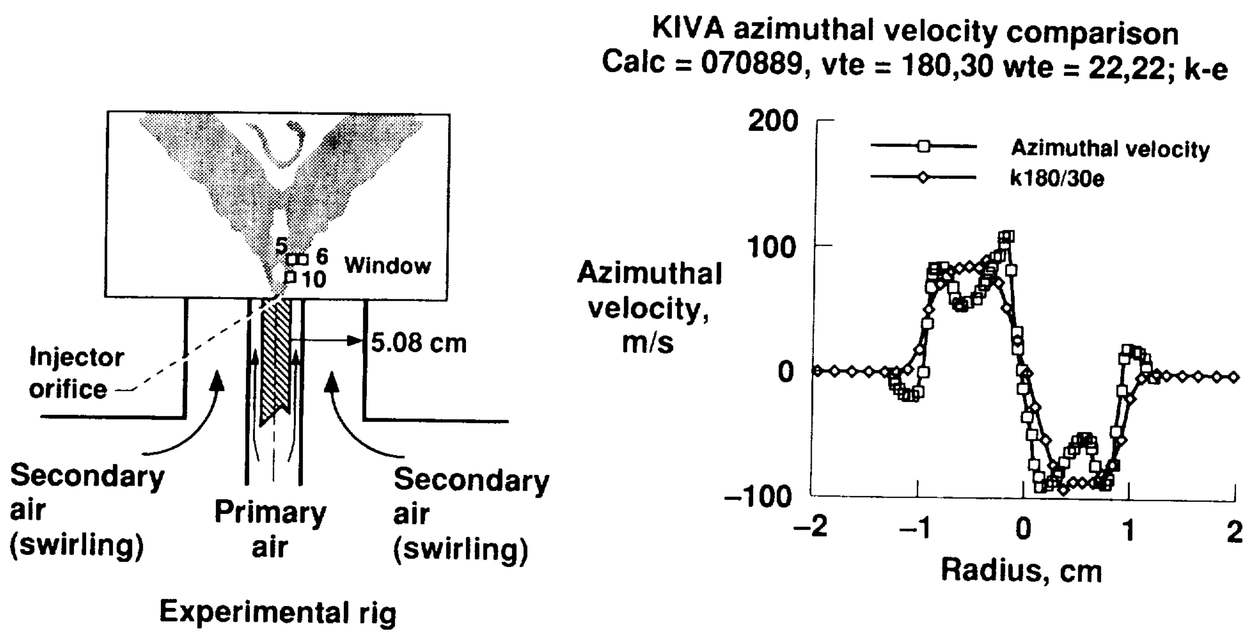

Figure 6

VERIFICATION OF KIVA-II CODE PREDICTIONS

Low NO_x Combustor Emissions

Figure 7 summarizes the comparison of experimental NO_x and CO emission index of a lean premixed prevaporized (LPP) burner (ref. 6) with KIVA-II code predictions. The simplified kinetics mechanism (ref. 2) was used. The predictions agree very well with the test data over the range of equivalence ratio and residence time reported. Calculations using KIVA-II have been performed to guide current low NO_x combustion experiments.

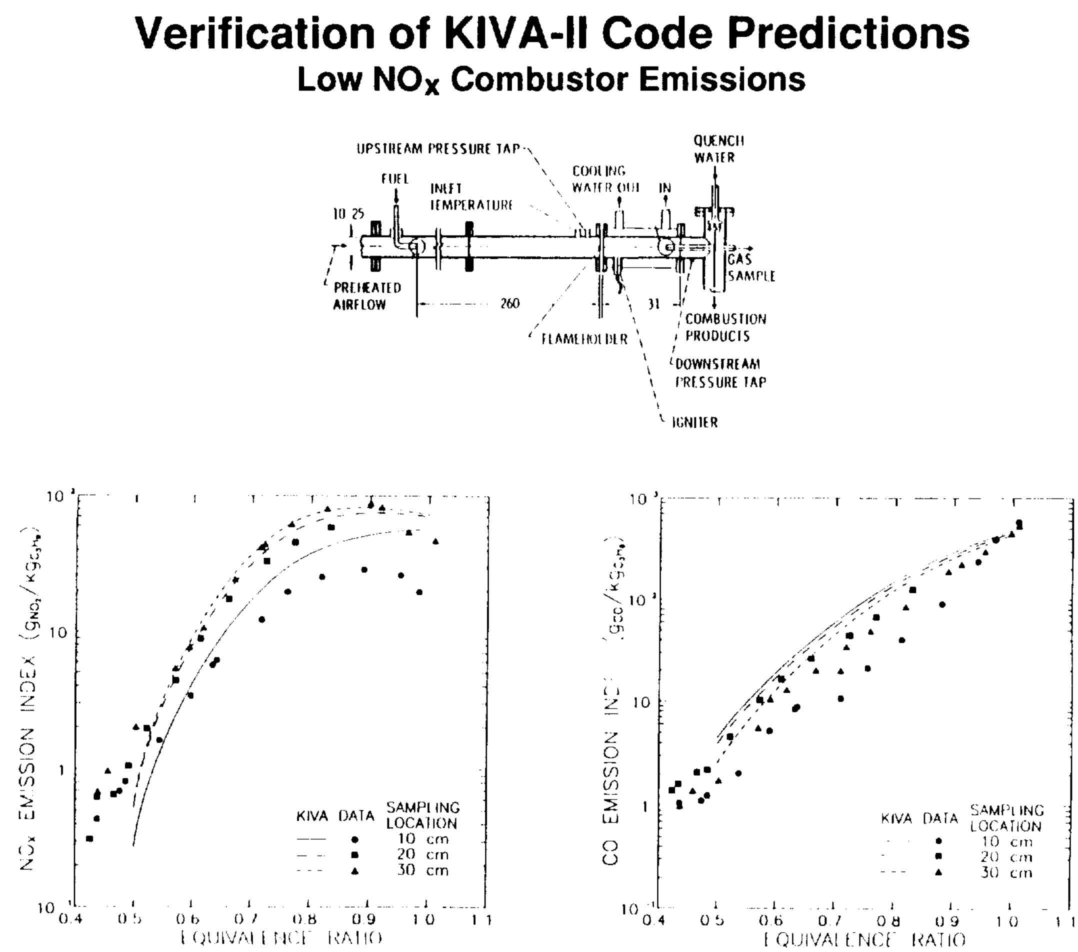

Figure 7

LOW NO_x COMBUSTOR ANALYSIS

(KIVA-II Analysis)

KIVA-II was used to perform two-dimensional analysis of the Rich Burn/Quick Quench/ Lean Burn (RQL) combustor to provide detailed information on the combustor internal flow fields, fuel-air mixing, combustor emissions, gas temperature distribution, and pattern factor. A two-dimensional axisymmetric model was used with propane and primary air injected at the inlet of the rich burn section and quick quench air supplied to the two-dimensional slot in the quick quench section. The upper half above the combustor centerline showing the gas temperature profile is shown in figure 8. The rich zone and lean zone equivalence ratios were set at 1.4 and 0.65, respectively. The gas temperature contours show core hot gas regions that occur in the rich zone and lean zone flame fronts. This figure also indicates that the penetration of the two-dimensional jet reaches near the combustor centerline and that thermal quenching occurs in the quick quench section.

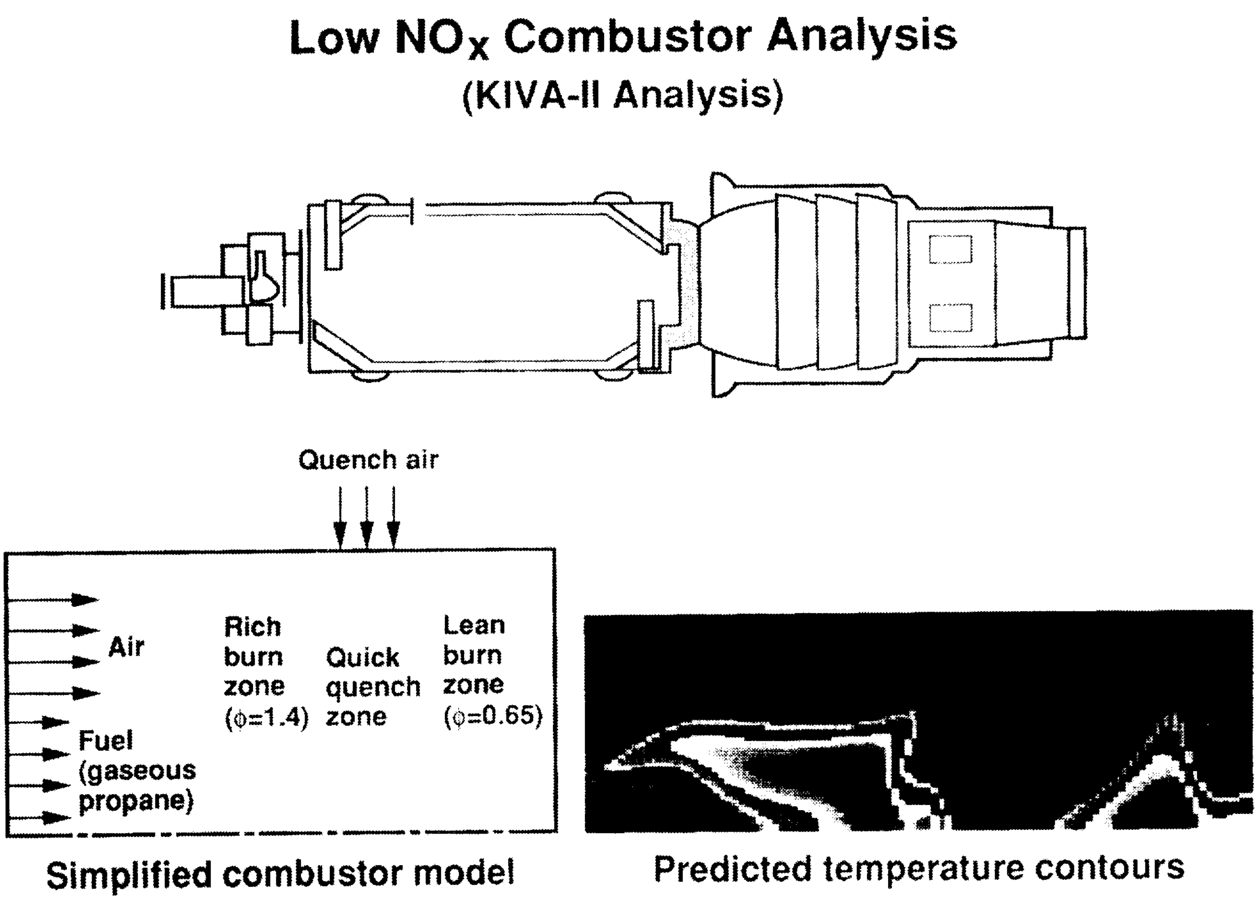

Figure 8

LOW NO_x COMBUSTOR ANALYSIS

(LeRC3D Analysis)

Figure 9 shows the flow field characteristics of the rich burn section of the RQL combustor. As an integral part of the fuel nozzle calculations, two-dimensional analyses (ref. 7) were done to provide the swirling air profiles through the swirlers of the airblast fuel nozzle. The swirlvane cascade analysis provides inlet air profiles to the rich burner analysis. The velocity vectors show a strong central recirculation zone downstream of the airblast fuel nozzle. Calculations using LeRC3D have been performed to guide current low NO_x combustion experiments.

LeRC3D Analysis

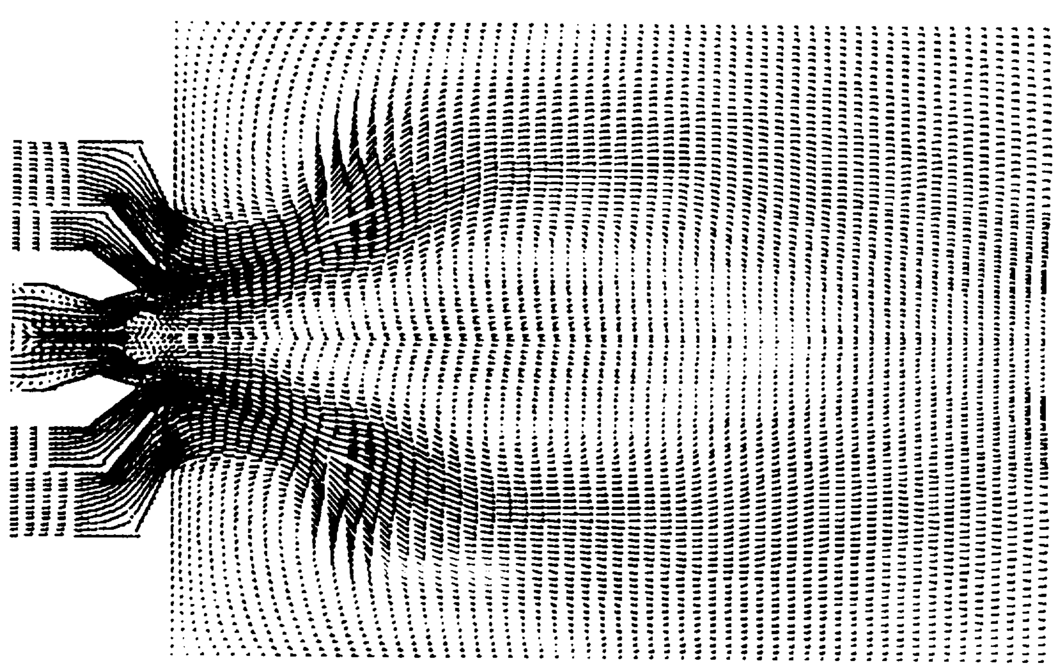

Figure 9

REFERENCES

1. Amsden, A.A., O'Rourke, P.J., and Butler, T.D., "KIVA-II: A Computer Program for Chemically Reactive Flows With Sprays," Los Alamos National Laboratory, LA-11560-MS, May 1989.

2. Nguyen, H.L., and Ying, S.J., "Critical Evaluation of Jet-A Spray Combustion Using Propane Chemical Kinetics in Gas Turbine Combustion Simulated by KIVA-II," AIAA Paper No. 90-2439, NASA TM-103173.

3. Nguyen, H.L., and Wey, M.-J., "Evaluation of a Hybrid Kinetics/Mixing-Controlled Combustion Model for Turbulent Premixed and Diffusion Combustion Using KIVA-II," AIAA Paper No. 90-2450, NASA TM-103196.

4. Nguyen, H.L., Li, Z., Howe, G.W., and Shih, T.I-P., "Calculations of the Three-Dimensional Flow and Combustion in a Staged Gas Turbine Combustor," accepted for presentation at the AIAA/SAE/ASME/ASEE 26th Joint Propulsion Conference, June 24-26, 1991.

5. Butler, T.D., "Analysis of an Air Assist Atomizer," Los Alamos National Laboratory, private communication, May 1990.

6. Anderson, D., "Effect of Equivalence Ratios and Dwell Time on Exhaust Emissions From an Experimental Premixed Prevaporizing Burner," NASA TM X-71592.

7. Micklow, G.J., and Nguyen, H.L., "Effect of Vane Twist on Performance of Dome Swirlers for Gas Turbine Airblast Atomizers," AIAA Paper No. 90-1955, NASA TM-103195.