FACT SHEET
LES Software for the Design of Low Emission Combustion Systems for Vision 21 Plants

I. Project Participants

CFD Research Corporation (Prime)
Georgia Institute of Technology
University of California, Berkeley
Virginia Tech
Rolls-Royce
Solar Turbines
Coen Company
McDermott Technologies
Air Force Research Laboratory
Siemens-Westinghouse
Pratt&Whitney
Woodward FST
Parker Hannifin
GE Power Systems
John Zink Company
Vapor Power
RamGen Power
NASA Glenn Research

II. Project Description

Objectives:
In this three-year project, an advanced computational software tool based on Large Eddy Simulation (LES) methods is being developed for the design of low emission combustion systems required for Vision 21 clean energy plants.

Background:
LES uses Computational Fluid Dynamics (CFD) methods to more accurately simulate turbulent-combustion than previous steady-state CFD methods. LES solves the well-known Navier Stokes equations that describe fluid motion, in such a way that large-scale turbulent eddies are calculated by directly solving the time-dependent Navier-Stokes equations on a computational grid, and modeling only the small-scale (sub-grid) quantities such as turbulence and combustion. This is in contrast to current CFD methods that solve only the steady-state (time independent) Navier-Stokes equations, and must model all scales of turbulence. These steady-state CFD analyses are able to provide qualitative predictions of emissions (e.g. NOx, CO, etc.) in turbulent-combustion flowfields, but cannot provide quantitative predictions. Plus, only the time-dependent methods of LES can provide predictions of unsteady combustion phenomena, such as pressure oscillations in the combustor, flame blowout, flame ignition, etc.

Relevancy:
Steady-state CFD analysis is used to help in the design of combustion systems. However, because it cannot accurately predict emissions, and because it cannot predict time-dependent combustion phenomena, steady-state CFD analysis has only limited value. Excessive hardware tests are still required to develop a new combustion system. With combustion LES software, the combustor designer can make more accurate predictions, and assess certain aspects of combustion that have been impossible to assess until now. This will greatly reduce the number of high cost experiments, as well as reduce the time needed to develop a new combustion system.

Period of Performance: 9/29/2000 – 9/30/2003

Project Summary:
The project was divided into three main tasks. In year 1, various sub-grid turbulence and combustion models were implemented into an existing commercial CFD code. In year 2, the code was further improved and validated against existing experimental data to show the improved accuracy obtained by LES, and its ability to capture time-dependent phenomena. Three validation cases were completed by the prime contractor (CFDRC) as part of alpha testing of the code. In year 3, the software will be given to project participants to beta test the code. Each beta tester will run up to three cases and compare predictions with existing experimental data. At the end of the project, the commercial software will be made available and licensed to all interested parties.

III. Project Costs

DOE costs are $1.6M, with $400K being cost-shared by CFD Research Corporation ($340K), Georgia Tech ($50K), and University of California, Berkeley ($10K).

IV. Major Accomplishments Since the Beginning of the Project

1. Establishment of Combustion LES Consortium 10/00. Approximately 22 people representing 18 organizations attended the consortium meetings. The consortium members served to help guide and direct the software development, plus helped in the selection of validation cases.

2. Simplified Chemical Mechanisms Developed and Implemented (6/01). Simplified chemical mechanisms were developed from full chemical mechanisms (in order to reduce the chemical computational time in the LES calculation), and implemented into the code. These simplified chemical mechanisms were developed for various gaseous fuels reacting with air, such as natural gas, hydrogen, syngas, propane, etc. By being able to model various fuels, the combustor designer can assess the effects of alternate fuels on combustor system performance.
3. Implementation of an Advanced Combustion Model Into Code (3/02). A combustion model named the Linear Eddy Mixing (LEM) model was integrated into the code and validated. LEM accurately models the chemical reactions, mixing, and stirring that occurs at the sub-grid level.
4. Validation Case #3 (P&W Humid Air Turbine, HAT, Combustor) Completed (10/02). The P&W HAT combustor case was an important validation case since it represented a practical combustor configuration running at realistic gas turbine conditions. Measurements were recorded at the DOE-NETL test facilities, under a CRADA between DOE and Pratt & Whitney. Comparisons were made to NOx and CO emission measurements, and good agreement was obtained.

V. Major Accomplishments Planned for the Remaining 12 Months

1. Consortium Participants Will Complete Their Beta Testing (6/03). The beta testers will make predictions with the combustion LES software and compare the predictions to existing experimental data. They will document their results and make recommendations for code improvement.
2. Complete Validation of the DOE Simulation Validation (SimVal) Experiment (6/03). DOE is currently testing combustor configurations for the sole purpose of providing measurements for CFD validation. CFDRC will make predictions and compare them to the measurements.
3. Complete Code Improvements and Release Final Version of Code (9/03).

VI. Issues

No major issues have been identified worthy of upper management attention