EFFICIENT COMBUSTION CHEMISTRY ALGORITHM FOR GAS TURBINE SIMULATIONS

Stephen B. Pope & Jun Xu

Cornell University

Ithaca, NY 14853

M.S. Anand & Sunil James

Rolls-Royce Allison

Indianapolis, IN 46206

RESEARCH AREA: COMBUSTION

Contract:	DE-FC21-92MC29061
DOE COR:	William F. Geer, Jr.
Subcontract:	96-01-SR049
Program Manager:	Larry Golan
Contractor:	Cornell University
Subcontractor:	Rolls-Royce Allison
Period:	6/9/97-6/12/00

OBJECTIVES

Context

- Advanced Turbine System performance depends crucially on the combustor performance
- Computational tools play a central role in the design of combustors
- Detailed chemistry computations---essential for modelling pollutants (e.g., NO_x and CO) extinction etc.---are prohibitively expensive using existing approaches

OBJECTIVES

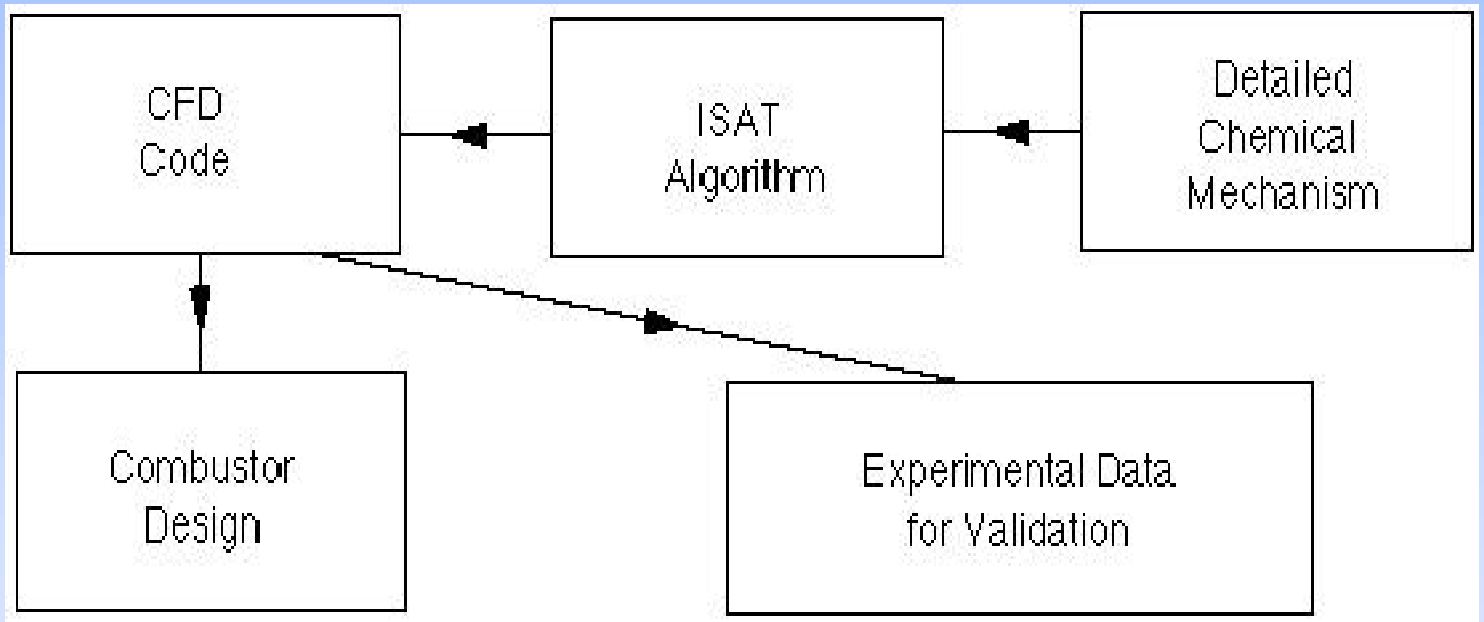
- To develop a methodology for the efficient implementation of detailed combustion chemistry which
  - can be applied to any detailed mechanism
  - is efficient with controlled accuracy
  - requires minimal human effort to apply
- To test thoroughly the methodology with different mechanisms for simple flows under different thermodynamic conditions
- To use the methodology in existing PDF codes for lean premixed combustion in combustor geometries for which there are benchmark quality experimental data

OBJECTIVES

The research will aid the development of efficient combustor design tools. The new methodology addresses the following ATS industry needs:

- Reliable prediction of performance parameters for combustors, e.g.,
  - efficiency
  - exit and wall temperature
  - ignition, lean blow out and stability
- Accurate predictions of the generation of pollutants such as NO_x, CO and UHC

METHODOLOGY: OVERVIEW



METHODOLOGY: ISAT/ILDM

- ISAT does not provide dimension reduction
- Work and storage proportional to N_S^2 (where N_S is the number of species)
- Combine ISAT with ILDM (intrinsic low-dimensional manifolds) to reduce number of degrees of freedom to $N_R < N_S$
- Example: GRI 2, $N_S = 49$

  ISAT/ILDM with $N_R = 10$

  Work and storage reduced by factor of 25

RESULTS

- Piloted Jet Methane Flames (Barlow & Frank 1998)
- Velocity-frequency-composition PDF method
- Augmented Reduced Mechanism
  - 16-species w/o NO_x
  - 19-species w/ NO_x
  - (Sung, Law & Chen 1998)
- ISAT Algorithm
- Mean profiles, scatter plots, burning index (B.I.)

COMPUTATIONAL DETAILS

- 60 x 60 grid
- 100 particles/cell
- 2,000 time steps
- 0.7×10^9 particle steps
- CPU time: 6 days on 5 Intels (Pentium II)
- ISAT speed-up: x 40 (est.)

REFERENCES

- S. James, M.S. Anand, M.K. Razdan and S.B. Pope (1999). "In situ detailed chemistry calculations in combustor flow analyses." In Proceedings of 44th ASME Gas Turbine and AeroEngine Technical Congress, Indianapolis, IN.
- U.A. Maas and S.B. Pope (1992) "Simplifying Chemical Kinetics: Intrinsic Low-Dimensional Manifolds in Composition Space," Combustion and Flame, **88**, 239-264.
- S.B. Pope (1997) "Computationally Efficient Implementation of Combustion Chemistry using In Situ Adaptive Tabulation," Combustion Theory and Modelling, **1**, 41-63.
- V. Saxena and S.B. Pope (1998) "PDF Calculations of Major and Minor Species in a Turbulent Piloted Jet Flame," Twenty-seventh Symposium (Int'l) on Combustion, 1081-1086.
- C.J. Sung, C.K. Law and J.-Y. Chen (1998) "An augmented reduced mechanism for methane oxidation with comprehensive global parametric validation," Twenty-seventh Symposium (Int'l) on Combustion, 295-304.
- Q. Tang and S.B. Pope (1999) "Implementation of radiation in ISAT." Cornell University report FDA 99-05.
- J. Xu and S.B. Pope (1999) "PDF calculations of piloted-jet turbulent flames of methane with local extinction." Cornell University FDA 99-06.

CONCLUSIONS

- PDF/ISAT methodology provides accurate calculations, including minor species and local extinction.
- ISAT methodology refined, tested and demonstrated at Cornell
- ISAT code combined with PDF combustor code at Rolls-Royce Allison
- Algorithm for ISAT/ILDM developed
- University/industry collaboration through research and summer interns