COMPUTATIONS OF EMISSIONS USING A 3-D COMBUSTOR PROGRAM

S. K. Srivatsa
Garrett Turbine Engine Company
Phoenix, Arizona 85010

Objective: Extend a 3-D combustor program:

- To predict pollutant emissions of soot and NO_x
- To include the influence of soot, CO_2, and H_2O on radiation heat transfer
- To extend the two-step hydrocarbon oxidation mechanism to a more detailed four-step scheme

Background: EPA regulations for aircraft gas turbines make it imperative that soot and NO_x emissions be controlled. The use of alternative synthetic fuels, recently being considered, results in significant increases in soot production. Thus, an improved understanding of the physical and chemical processes governing soot production is necessary. Since these processes are not well understood, only an approximate modeling of soot production is currently possible. Lack of general 3-D computer codes has also hindered research in this area. In the present program, soot and NO_x emissions were computed by using an existing general 3-D computer program. This will significantly aid in the development of soot and NO_x production models in practical systems.

Approach: A general 3-D combustor performance program developed by Garrett was extended to predict soot and NO_x emissions. The soot formation and oxidation rates were computed by quasi-global models, taking into account the influence of turbulence. Radiation heat transfer was computed by the six-flux radiation mode. The radiation properties include the influence of CO_2 and H_2O in addition to soot. NO_x emissions were computed from a global four-step hydrocarbon oxidation scheme and a set of rate-controlled reactions involving radicals and nitrogen oxides.

Results: Computations performed for a plug flow reactor show the four-step scheme to be far superior to the two-step scheme in predicting temperature and species concentrations.

- Computations were performed for idle, cruise, and takeoff conditions of a JT8D combustor. These showed that the present model is capable of producing reasonable predictions of smoke and NO_x emissions and of the wall radiation flux.

COMPUTATIONS OF EMISSIONS USING A 3-D COMBUSTOR PROGRAM

SOOT EMISSIONS MODEL

- QUASI-GLOBAL MODELS PARTIALLY VALIDATED WITH WELL-STIRRED REACTOR DATA
- TURBULENCE EFFECTS ACCOUNTED FOR
- TRANSPORT EQUATIONS FOR NUCLEI AND SOOT PARTICLE CONCENTRATIONS
- SOOT PARTICLES OF TWO SIZES

NO_X EMISSIONS MODEL

- C_XH_Y OXIDATION BY A FOUR-STEP SCHEME ($C_XH_Y \rightarrow C_XH_{Y-2}$; $C_XH_{Y-2} \rightarrow CO + H_2$; $CO \rightarrow CO_2$; $H_2 \rightarrow H_2O$)
- SET OF ELEMENTARY REACTIONS INVOLVING N, NO, NO_2, H, H_2, O, O_2, N_2.
- INFLUENCE OF TURBULENCE ON REACTION RATES AS PER EDDY-BREAK-UP MODEL
- RATE-CONTROLLED SPECIES EQUATIONS SOLVED BY ALGORITHM FOR STIFF EQUATIONS

RADIATION MODEL

- SIX-FLUX RADIATION MODEL
- RADIATION PROPERTIES DEPENDENT ON SOOT, CO_2, H_2O CONCENTRATIONS
- RADIATION PROPERTIES INTEGRATED OVER WAVE LENGTH
- EMISSION/ABSORPTION BY SOOT, CO_2, AND H_2O
- CO_2 - H_2O EMISSIVITY CORRELATIONS INCLUDING OVERLAP AND PRESSURE CORRECTION FACTORS

3-D COMBUSTOR MODEL FEATURES

- TURBULENT, RECIRCULATING, REACTING, SWIRLING FLOW
- LIQUID/GASEOUS FUEL
- HEAT TRANSFER
- SOOT AND NO_X MODELS

PROGRAM OUTPUTS

- SOOT AND NO_X EMISSIONS
- RADIANT HEAT TRANSFER TO WALLS
- VELOCITY, TURBULENCE, TEMPERATURE AND CONCENTRATION FIELDS

BENEFITS

- PROVIDES A GENERAL 3-D PROGRAM FOR PREDICTING EMMISSIONS FROM GAS TURBINE COMBUSTORS
- PROVIDES AN ANALYTICAL COMBUSTOR DESIGN TOOL
- PROVIDES A BETTER UNDERSTANDING OF COMBUSTION PROCESSES

COMPUTATIONS OF EMISSIONS USING A 3-D COMBUSTOR PROGRAM

OBJECTIVE:

EXTEND AN EXISTING 3-D COMBUSTOR PROGRAM:

- TO PREDICT POLLUTANT EMISSIONS OF SMOKE AND NO_X:
- TO INCLUDE THE INFLUENCE OF SOOT, CO_2, AND H_2O ON RADIATION HEAT TRANSFER; AND
- TO EXTEND THE TWO-STEP HYDROCARBON OXIDATION MECHANISM TO A MORE DETAILED FOUR-STEP SCHEME

APPROACH

PROGRAM INVOLVED FOUR TASKS

- TASK I — FORMULATION OF THE METHOD
- TASK II — COMPUTER CODING
- TASK III — COMPUTATION OF TEST CASES
  - IDLE, CRUISE, AND TAKE-OFF CONDITIONS FOR A JT8D COMBUSTOR
- TASK IV — REPORTING AND DOCUMENTATION

EXISTING 3-D COMBUSTOR PROGRAM

- GENERAL PROGRAM FOR
  - RECIRCULATING, SWIRLING, TURBULENT, REACTING FLOW
  - GASEOUS AND/OR LIQUID FUEL COMBUSTION
  - RADIATION HEAT TRANSFER
- GENERAL TRANSPORT EQUATION

$$\text{div}\,\left(\rho\overrightarrow{U\phi} - \frac{\mu_t}{\sigma\phi}\,\text{GRAD}\,\phi\right) = S\phi$$

- VARIABLES: $\overrightarrow{U}$, P, k, ε, f, M_{fu}, M_{co} (M_{O_2}, M_{CO_2}, M_{H_2O}), h (T, ρ), R_x, R_y, R_z SPRAY DYNAMICS/COMBUSTION
- PHYSICAL MODELS:
  - TURBULENCE: k-ε MODEL
  - CHEMISTRY: 2-STEP REACTION SCHEME
  - CHEMICAL REACTION RATE: MODIFIED EBU MODEL
  - RADIATION: SIX-FLUX MODEL
- NUMERICAL:
  - FINITE-DIFFERENCE ITERATIVE METHOD
  - SUITABLE FOR COMPLEX GEOMETRIES
  - SUITABLE FOR NON-UNIFORM GRID SPACING

FOUR-STEP HYDROCARBON OXIDATION MECHANISM

- TWO-STEP SCHEME IN ORIGINAL 3D PROGRAM:
  $CxHy + O_2 \rightarrow CO + H_2O$
  $CO + O_2 \rightarrow CO_2$
- FOUR-STEP SCHEME:
  $C_xH_y \rightarrow C_xH_{y-2} + H_2$
  $C_xH_{y-2} + O_2 \rightarrow CO + H_2$
  $CO + O_2 \rightarrow CO_2$
  $H_2 + O_2 \rightarrow H_2O$
- FOUR-STEP SCHEME DESCRIBES THE FOLLOWING BASIC STEPS OF HYDROCARBON OXIDATION
  - TRANSFORMATION OF HYDROCARBON FUEL INTO INTERMEDIATE HYDROCARBONS AND HYDROGEN WITH LITTLE RELEASE OF ENERGY
  - OXIDATION OF INTERMEDIATES TO CO AND H_2
  - OXIDATION OF CO TO CO_2
  - OXIDATION OF H_2 TO H_2O
- TWO ADDITIONAL EQUATIONS FOR: C_xH_{y-2} AND H_2

NO_X EMISSIONS

- SPECIES CONSIDERED: C_xH_y, C_xH_{y-2}, CO, N, NO, NO_2, H, H_2, OH, O, CO_2, H_2O, O_2, N_2
- TRANSPORT EQUATIONS FOR: C_xH_y, CO, C_xH_{y-2}, N, NO, NO_2, H, H_2, OH, O
- CO_2, H_2O, O_2 FROM C, H, O ELEMENT CONSERVATION
- $M_{N2} = 1 - \Sigma M$
- SOURCES OF SPECIES COMPUTED FROM MODIFIED EBU MODEL
- C_xH_y, C_xH_{y-2}, H_2, AND CO SOURCES FROM 4-STEP REACTION SCHEME

NO_X EMISSIONS

- SOURCES OF N, NO, NO_2, H, H_2, OH, O FROM REACTION MECHANISM:

$O + N_2 = N + NO$	$H + NO_2 = NO + OH$
$NO + O = O_2 + N$	$H_2 + O_2 = OH + OH$
$N + OH = NO + H$	$OH + H_2 = H_2O + H$
$N_2 + O_2 = N + NO_2$	$OH + OH = O + H_2O$
$N_2 + O_2 = NO + NO$	$O + H_2 = H + OH$
$NO + NO = N + NO_2$	$H + O_2 = O + OH$
$M + NO = M + N + O$	$M + O + H = OH + M$
$M + NO_2 = M + O + NO$	$M + O + O = O_2 + M$
$M + NO_2 = O_2 + N + M$	$M + H + H = H_2 + M$
$NO + O_2 = NO_2 + O$	$M + H + OH = H_2O + M$

- STRONGLY COUPLED NONLINEAR STIFF EQUATIONS
- PRATT'S CREK PROGRAM FOR STIFF EQUATIONS ADAPTED TO 3-D COMBUSTOR PROGRAM

SOOT EMISSIONS

- VARIOUS STEPS INVOLVED IN SOOT FORMATION/OXIDATION NOT QUANTIFIED
- HENCE QUASI-GLOBAL MODELS CONSISTING OF THREE STEPS
  - *SOOT NUCLEI FORMATION*
  - SOOT PARTICLE FORMATION
  - SOOT PARTICLE OXIDATION
- TRANSPORT EQUATIONS FOR NUCLEI AND SOOT CONCENTRATIONS WITH SOURCES CONTAINING REACTION RATES
- REACTION RATES CONTAIN FORMATION AND OXIDATION RATES DEPENDENT ON:
  - UNBURNT FUEL AND O_2 CONCENTRATION
  - TEMPERATURE
  - TURBULENCE PARAMETERS ε/k (SIMILAR TO EDDY-BREAK-UP MODEL)
- TWO SIZES OF SOOT PARTICLES CONSIDERED: ONE EQUATION FOR EACH SIZE

RADIATION HEAT TRANSFER

- SIX-FLUX RADIATION MODEL — SCHUSTER AND HAMAKER
- MAJOR CONTRIBUTORS TO RADIATION = SOOT, CO_2, H_2O
- RADIATION PROPERTIES DEPENDENT ON SOOT, CO_2, H_2O CONCENTRATIONS
- TOTAL PROPERTIES (INTEGRATED OVER WAVELENGTH)
- CO_2 — H_2O EMISSIVITY CORRELATIONS INCLUDING OVERLAP AND PRESSURE CORRECTION FACTORS

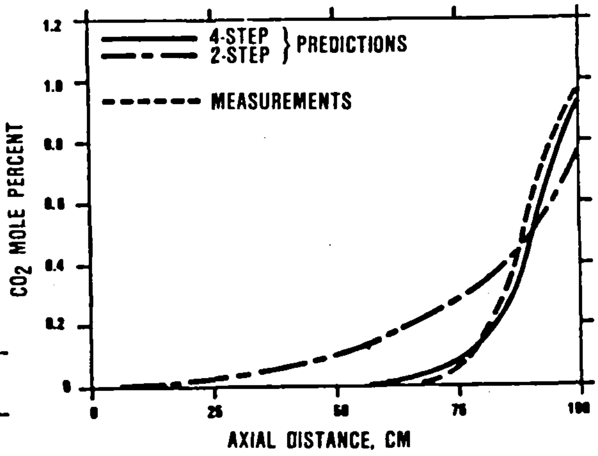
  $$\varepsilon_{C+W} = \varepsilon_C + \varepsilon_W C_W - C_W \Delta\varepsilon$$

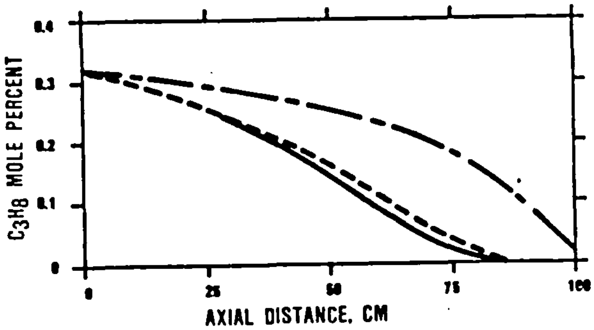
  $$a_{C+W} = Ln(1 - \varepsilon_{C+W}) / S$$
- SOOT RADIATION PROPERTIES
  - ABSORPTION COEFFICIENT COMPUTED FOR BOTH PARTICLE SIZES AND ADDED TOGETHER
- GAS-SOOT MIXTURE
  - ABSORPTION COEFFICIENTS OF GAS AND SOOT ADDED

RESULTS

- FOUR-STEP SCHEME
  - PLUG FLOW REACTOR FOR LEAN, STOICHIOMETRIC, AND RICH PROPANE FLAMES
  - CONSIDERABLE DEVIATIONS OF TWO-STEP PREDICTIONS FROM MEASUREMENTS
  - FOUR-STEP PREDICTIONS AGREE CLOSELY WITH MEASUREMENTS
  - SOME DISCREPANCY IN FOUR-STEP H_2 PREDICTIONS AT HIGHER EQUIVALENCE RATIOS

LEAN C_3H_8 FLAME (ϕ = 0.12)





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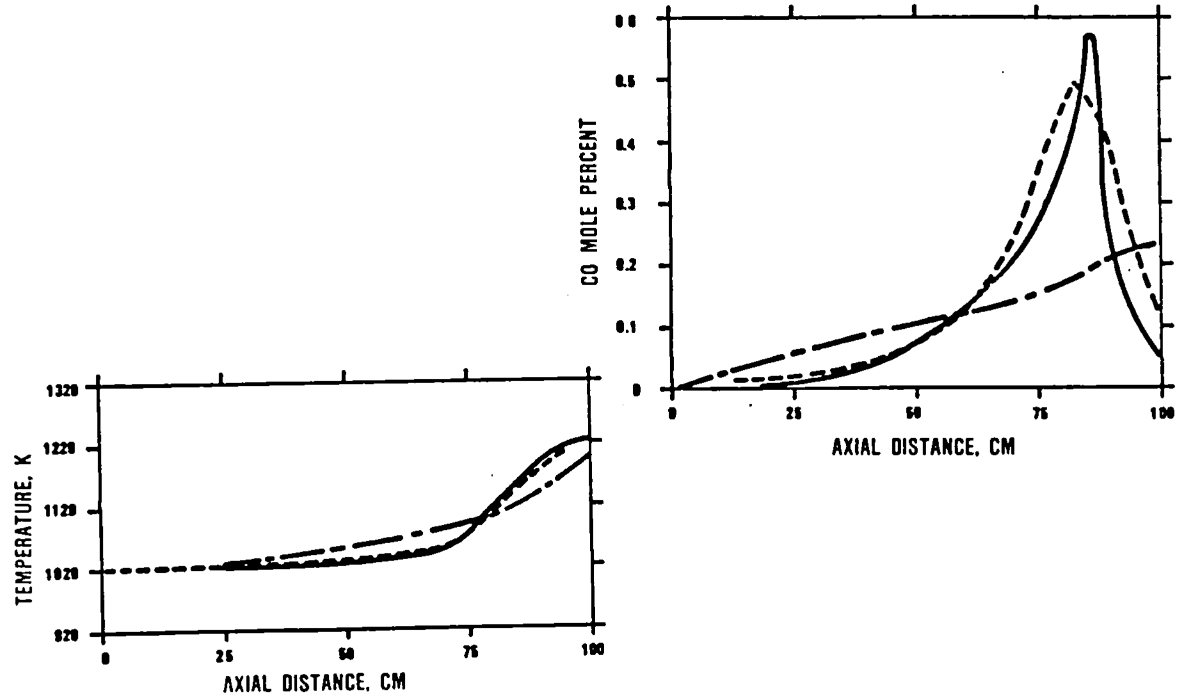
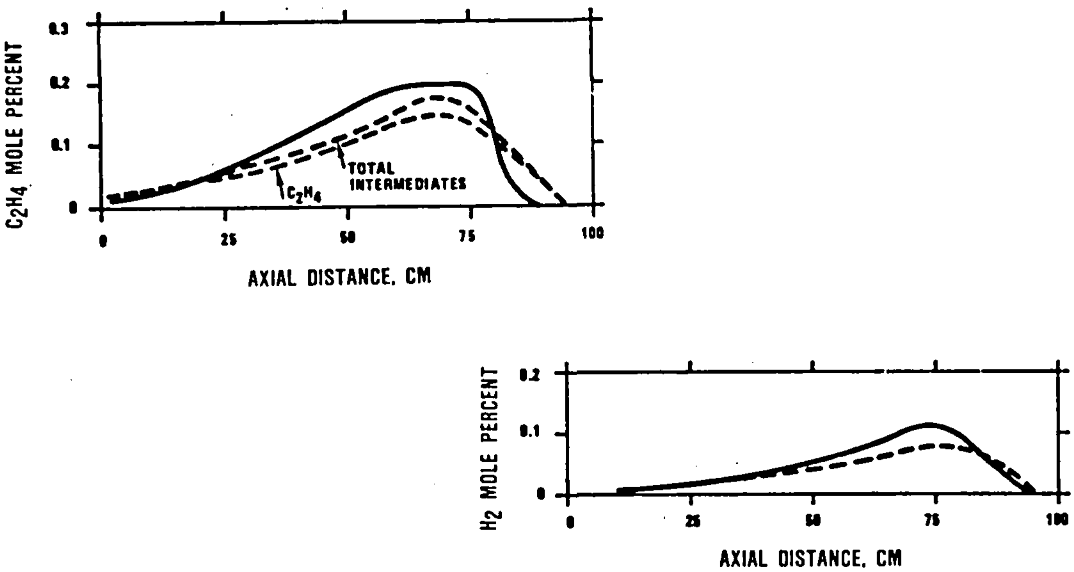
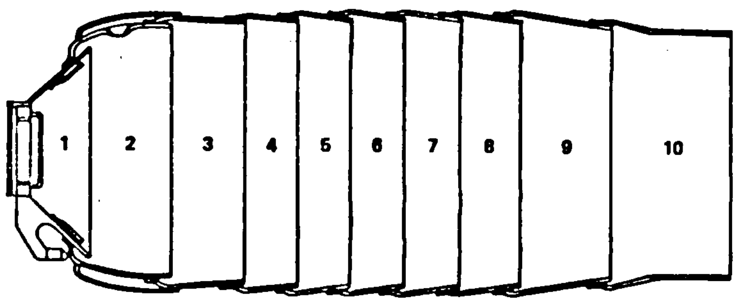


LEAN C_3H_8 FLAME (ϕ = 0.12)



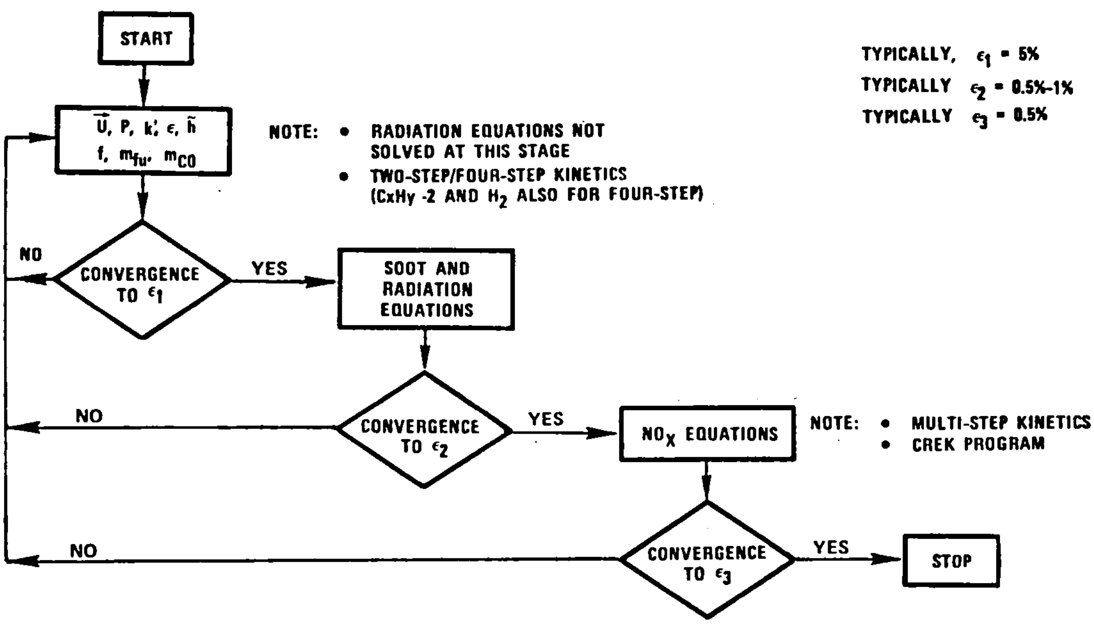
JT8D-17 COMBUSTOR



CASES COMPUTED:

CONDITION	AIRFLOW LBS/SEC	PRESSURE PSIA	TEMPERATURE °F	FUEL/AIR RATIO
IDLE	4.06	39.6	260	0.0074
CRUISE	7.87	103.0	657	0.0138
TAKE-OFF	16.45	256.0	825	0.0182

FLOWCHART OF OVERALL SOLUTION PROCEDURE



PREDICTED EMISSIONS INDEX WITH FOUR-STEP HYDROCARBON OXIDATION SCHEME

	EMISSION INDEX Gm OF EMISSIONS/Kg OF FUEL	
CONDITION	SMOKE	NO_X
IDLE	0.056 (0.6)	≈0
CRUISE	1.3	13
TAKEOFF	1.2 (2.8)	27 (24.4)

NOTE: VALUES IN PARENTHESES ARE EXPERIMENTAL MEASUREMENTS

- PREDICTED RADIATION FLUXES IN THE SAME RANGE AS MEASUREMENTS FOR SLIGHTLY DIFFERENT OPERATING CONDITIONS

CONCLUSIONS

- MODEL PRODUCES REASONABLE RESULTS FOR EMISSIONS AND RADIATION FLUX

- LACK OF EXPERIMENTAL DATA PRECLUDES MORE DETAILED MODEL VALIDATION