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Bill Calhoon " Application of Turbulence Models in Reacting Flows" **(Statement A)**

APPLICATION OF TURBULENCE MODELS IN REACTING FLOW

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ARL MSRC PET SHORT COURSE ON
TREATMENT OF TURBULENCE MODELS IN
COMPLEX HIGH PERFORMANCE CFD APPLICATIONS,
16 - 17 MAR. 1998

OUTLINE

1. INTRODUCTION
2. OBJECTIVES
3. WHAT IS A "COMPLEX" REACTING FLOW?
4. FLOW MODELING : STEADY VS. UNSTEADY
5. REACTING FLOW EQUATIONS
6. TURBULENCE-CHEMISTRY INTERACTION MODELING
7. SAMPLE PROBLEM

1. INTRODUCTION: APPLICATION OF CFD TO REACTING FLOW

- **REQUIRES CHARACTERIZATION OF THE INTERACTION OF TURBULENCE AND CHEMISTRY**

- **TURBULENT COMBUSTION MODELING:**

  1) IS AN ENTIRE FIELD OF RESEARCH

  2) HAS BEEN THE SUBJECT OF INTENSE RESEARCH FOR ~ 25 YEARS

  3) MOST OF RESEARCH RESTRICTED TO:

     - LOW SPEED FLOWS
     - SMALL MEAN PRESSURE VARIATIONS
     - SIMPLE CONFIGURATIONS

KEY FEATURES OF TURBULENT REACTING FLOW

- **TURBULENT STIRRING:**
  - A PROCESS OF STRETCHING INTERMATERIAL AREA BETWEEN DIFFERENT FLUIDS (E.G., FUEL AND OXIDIZER)
  - CHARACTERIZED BY SCALAR LENGTH SCALE REDUCTION
- **MOLECULAR MIXING:**
  - THE PROCESS OF DIFFUSION OF SUBSTANCES ACROSS INTERMATERIAL AREA (E.G., MOLECULAR DIFFUSION)
- **FLUIDS MAY BE WELL STIRRED BUT NOT MOLECULARLY MIXED:**
  - CRUDE EXAMPLE: MIXING OF OIL AND WATER
- **COMBUSTION ONLY OCCURS WHEN REACTANTS ARE MOLECULAR MIXED**

2. OBJECTIVES

1) PROVIDE A "TIP OF THE ICEBERG" INTRODUCTION TO THE FIELD OF TURBULENT COMBUSTION

2) BRIEFLY COVER TWO MODELS APPLICABLE TO "COMPLEX" FLOWS

3) PROVIDE REFERENCES FOR SELF STUDY

3. WHAT IS A "COMPLEX" TURBULENT REACTING FLOW?

- <u>CHARACTERISTICS OF A "COMPLEX" REACTING FLOW:</u>
  - MULTIPLE SOURCES OF REACTANTS AND FUEL STREAMS
  - NONUNIFORM COMPOSITIONS IN THE FUEL STREAMS
  - CHEMICAL NONEQUILIBRIUM
  - HIGH SPEED FLOWS
    1) COMPRESSIBILITY EFFECTS
    2) LARGE PRESSURE VARIATIONS
    3) SHOCK WAVE HEATING
    4) HEATING DUE TO VISCOUS ENERGY DISSIPATION
  - COMPLEX MIXING
    1) SHOCK-SHEAR LAYER INTERACTIONS
    2) SEPARATED/RECIRCULATING FLOWS

CHARACTERISTICS OF A "COMPLEX" REACTING FLOW, CONT'D

- **THESE COMPLEX CHARACTERISTICS ELIMINATE TURBULENT COMBUSTION MODELS BASED ON:**

  1) **MIXTURE FRACTION FORMULATIONS**
     - **E.G., TWO STREAM CONFIGURATIONS**

  2) **INFINITE/FAST CHEMISTRY ASSUMPTIONS**

  3) **TABULARIZED FORMULATIONS**
     - **E.G., LAMINAR FLAMELET MODEL**

  4) **REDUCED FORMS OF THE ENERGY EQUATIONS**
     - **E.G., LOW SPEED, ~ CONSTANT PRESSURE FLOWS**

EXAMPLE OF A "COMPLEX" REACTING FLOW: MISSILE EXHAUST PLUMES

- **SIGNATURES IMPORTANT TO MISSILE DEFENSE SYSTEMS:**

  - **TYPING, TRACKING AND INTERCEPTOR AIMPOINT SELECTION**

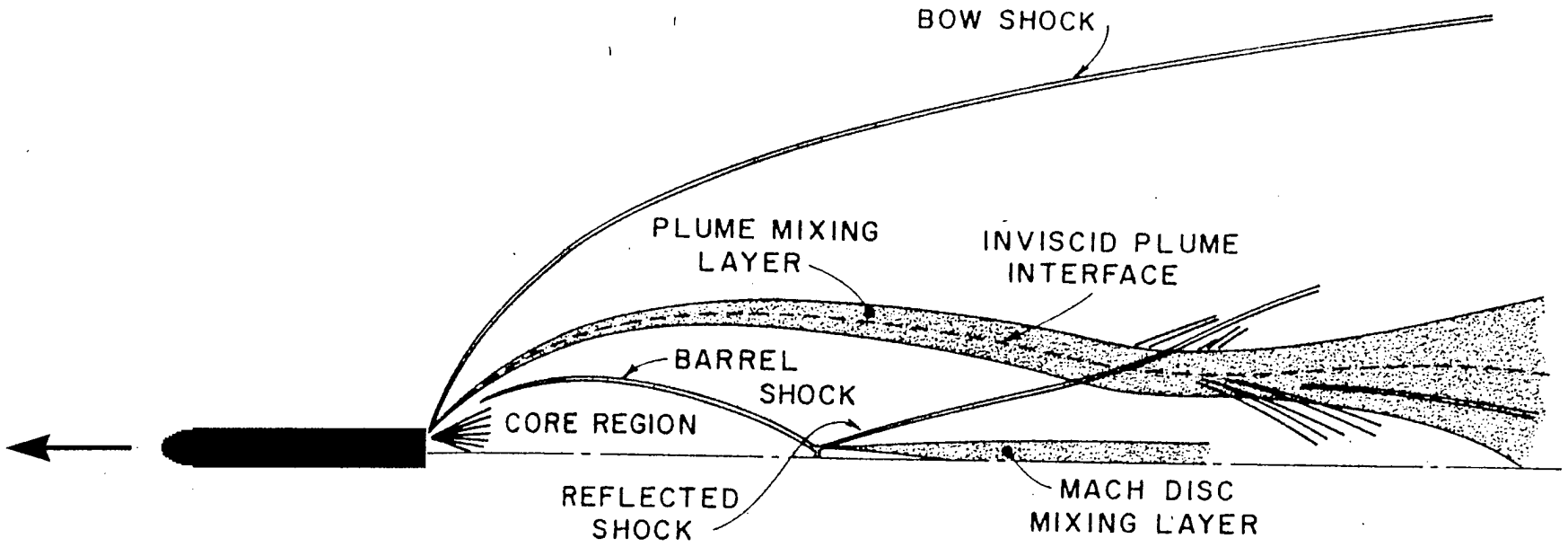
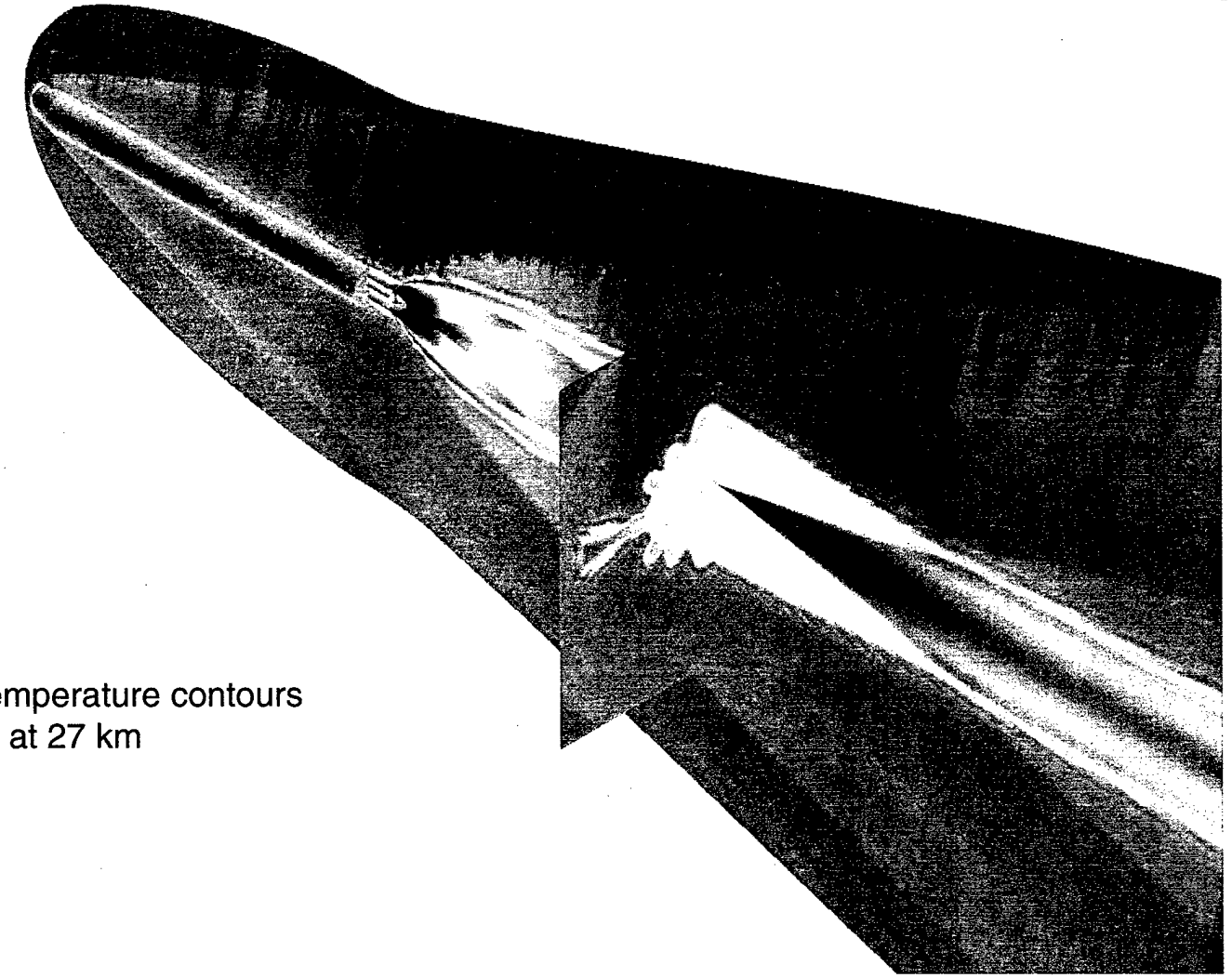


Fig. 1 Schematic of viscous/inviscid structure in plume nearfield.

EXAMPLE OF A "COMPLEX" REACTING FLOW: MISSILE EXHAUST PLUMES



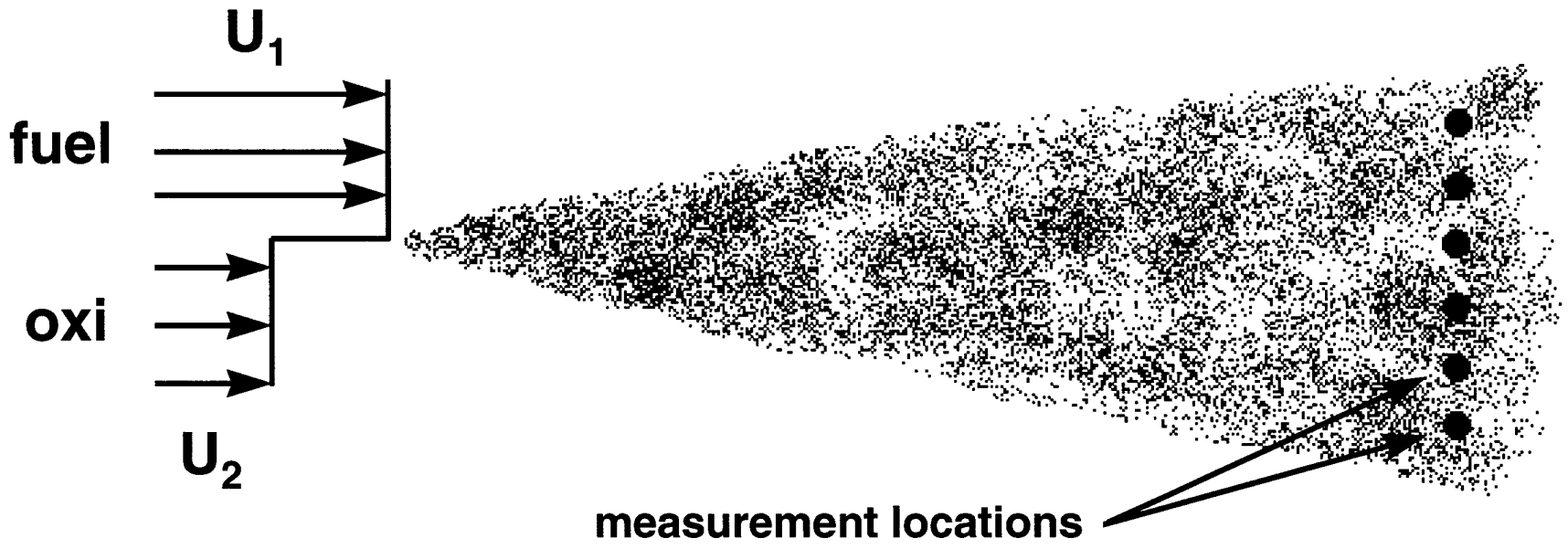
Titan II Temperature contours
at 27 km

4. FLOW MODELING : STEADY STATE VS. UNSTEADY STATE

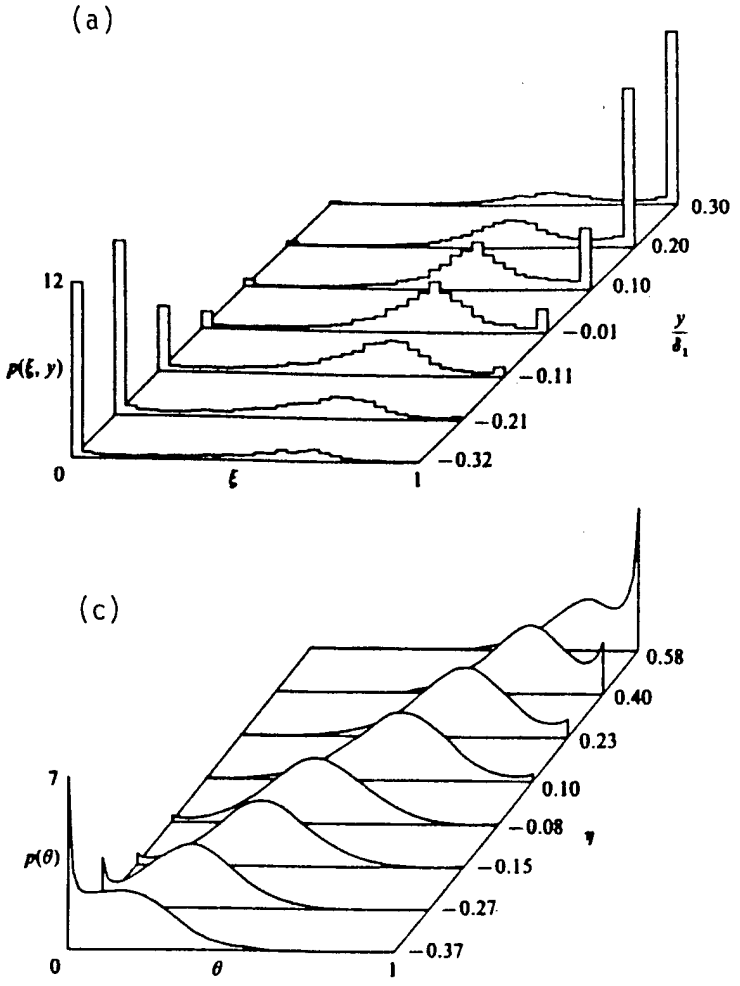
- **STEADY STATE VS. UNSTEADY**
  - TURBULENCE BY DEFINITION IS UNSTEADY
  - UNSTEADY SIMULATION METHODS PREFERABLE
- **STEADY STATE METHOD:**
  - REYNOLDS AVERAGED NAVIER-STOKES (RANS)
- **UNSTEADY METHODS:**
  - UNSTEADY RANS
  - LARGE-EDDY SIMULATION (LES)

STEADY STATE VS. UNSTEADY

- **STEADY STATE METHODS LIMITED BY TURBULENT TRANSPORT MODELS FOR SCALARS**
  - **EXAMPLE : NONREACTING SHEAR LAYER MIXING**



SHEAR LAYER MIXING CHARACTERISTICS



Mixing layer normalized fuel probability density functions in the cross stream direction (a) liquid, Re = 23,000, (b) gas, Re = 25,000, (c) steady state calculation (Broadwell, J.E. and Mungal, M.G., 1991)

STEADY STATE VS. UNSTEADY

- **UNSTEADY METHODS:**
  - GOOD REPRESENTATION OF SCALAR TURBULENT TRANSPORT
  - HIGH RESOLUTION REQUIRED
  - COSTLY TIME ACCURATE SIMULATION REQUIRED
  - LES MODELS FOR COMPLEX FLOWS IMMATURE
- **STEADY STATE METHODS:**
  - LOWER RESOLUTION REQUIREMENTS
  - CONVERGENCE ACCELERATION TECHNIQUES APPLICABLE
  - THE ONLY ALTERNATIVE FOR MANY COMPLEX FLOWS
  - POOR REPRESENTATION OF TURBULENT TRANSPORT PRODUCED BY CURRENT MODELS

5. REACTING FLOW EQUATIONS

- **EQUATION SET (GAS PHASE):**
  - MASS, MOMENTUM, ENERGY AND SPECIES CONSERVATION
  - SUPPLEMENTED WITH STATE EQUATIONS
- **MASS, MOMENTUM AND ENERGY EQUATIONS THE SAME AS FOR NONREACTING EXCEPT:**
  - ADDITION HEAT FLUX TERM IN ENERGY EQUATIONS:

$$q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{K} Y_k h_k V_{k,j} + q_j^R$$

  - MOLECULAR PROPERTIES (VISCOSITY, THERMAL CONDUCTIVITY) ARE A FUNCTION OF THE LOCAL MIXTURE

SPECIES CONSERVATION AND STATE EQUATIONS

- **SPECIES CONSERVATION:**
  - $$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = -\frac{\partial \rho V_{k,j} Y_k}{\partial x_j} + \dot{w}_k$$
  - $$Y_k = \rho_k / \rho \quad , \quad \sum_{k=1}^{k} \rho_k = \rho \quad , \quad \dot{w}_k = f(\rho, Y_k, T)$$
- **STATE EQUATIONS:**
  - $$p = \rho R^o T \sum_{k=1}^{K} \frac{Y_k}{W_k}$$
  - $$h = e + \frac{p}{\rho} = e + R^o T \sum_{k=1}^{K} \frac{Y_k}{W_k} = \sum_{k=1}^{K} Y_k \left[\Delta h_k^o + \int_{T^o}^{T} c_{p,k}(T') dT' \right]$$
  - $$c_{p,k}(T) = \sum_{n=0}^{N} a_{n,k} T^N$$

RANS SPECIES AND STATE EQUATIONS

- **VARIABLE DECOMPOSITION:** $\phi = \overline{\phi} + \phi' = \tilde{\phi} + \phi''$

- **SPECIES CONSERVATION:**

  - $$\frac{\partial \overline{\rho}\tilde{Y}_k}{\partial t} + \frac{\partial \overline{\rho}\tilde{u}_j\tilde{Y}_k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\overline{\rho} D_K \frac{\partial \tilde{Y}_k}{\partial x_j}\right] - \frac{\partial}{\partial x_j}\left[\overline{\rho u_j'' Y_k''}\right] + \overline{\dot{w}}_k$$

- **STATE EQUATIONS:**

  - $$\overline{p} = \overline{\rho} R^o \sum_{k=1}^{K} \frac{\tilde{T}\tilde{Y}_k}{W_k} + R^o \sum_{k=1}^{K} \frac{\overline{\rho T'' Y_k''}}{W_k}$$

  - $$\tilde{e} + R^o \sum_{k=1}^{K} \frac{\tilde{T}\tilde{Y}_k}{W_k} + \frac{1}{\overline{\rho}} R^o \sum_{k=1}^{K} \frac{\overline{\rho T'' Y_k''}}{W_k} = \sum_{k=1}^{K} \tilde{Y}_k \Delta h_k^o + \tilde{h}^s$$

  - $$\tilde{h}^s = \frac{1}{\overline{\rho}} \sum_{k=1}^{K} \overline{\rho Y_k \int_{T^o}^{T} c_{p,k}(T')dT'} = f\left(\overline{\rho T'' Y_k''}, \overline{\rho T''^{n+1} Y_k''}\right)$$

RANS UNCLOSED TERMS

- **TURBULENT TRANSPORT:** $\overline{\rho u_j'' Y_k''}$
  - **MODELED BY:**
    1) **GRADIENT DIFFUSION :**

$$\overline{\rho u_j'' Y_k''} = -\frac{\overline{\rho}\, \nu_T}{Sc_T} \frac{\partial \tilde{Y}_k}{\partial x_j}$$

    2) **SECOND ORDER CLOSURE**

- **SCALAR MOMENTS:**
  - **MEAN REACTION RATE:** $\overline{\dot{w}_k}$
  - **TEMPERATURE-SPECIES CORRELATIONS:** $\overline{\rho T'' Y_k''}$, ..., ...
  - **MODEL THE SINGLE POINT JOINT PDF OF** ρ , T **AND** Y_k **:** $P(\rho, T, Y_k)$
  - $$\overline{\dot{w}_k} = \int_0^\infty \int_0^\infty \int_0^1 \cdots \int_0^1 \dot{w}_k P(\rho', T', Y_k') dY_1' \ldots dY_k' d\rho' dT'$$

6. TURBULENCE-CHEMISTRY INTERACTION MODELING

- **INTERACTION OF TURBULENCE AND CHEMISTY CONTAINED IN THE SINGLE POINT PDF** $P(\rho,T,Y_k)$
- $P(\rho,T,Y_k)$ **REPRESENTS THE COMBINED EFFECTS OF:**
  - **TURBULENT TRANSPORT (LARGE AND SMALL SCALE)**
  - **MOLECULAR DIFFUSION**
- **ESTABLISHED MODELS FOR** $P(\rho,T,Y_k)$**:**
  - **LAMINAR MODEL**
  - **EDDY DISSIPATION CONCEPT**

LAMINAR MODEL FOR THE PDF

- **LAMINAR MODEL FOR** $P(\rho,T,Y_k)$**:**
  - $P(\rho,T,Y_k) = \delta(\rho-\overline{\rho})\delta(T-\tilde{T})\sum_{k=1}^{K}\delta(Y_k-\tilde{Y}_k)$
  - $\overline{\dot{w}_k} = \overline{\dot{w}}_k(\overline{\rho},\tilde{T},\tilde{Y}_k)$
  - $\overline{\rho T'' Y_k''} = 0$

- **COMMENTS:**
  - **CAN BE IN ERROR BY AN ORDER OF MAGNITUDE**
  - **WIDELY USED AS A FIRST APPROXIMATION**
  - **CAN GIVE GOOD RESULTS WHEN FLUCTUATIONS ARE UNIMPORTANT**
  - **NO GENERAL CRITERIA OF THE APPLICABILITY RANGE OF THE MODEL**

EDDY DISSIPATION CONCEPT (EDC)

- **OBSERVATIONS:**
  - REACTIONS ONLY OCCUR WHEN SPECIES MOLECULARLY MIXED
  - MICROSCALE STRUCTURES, WHERE MOLECULAR EFFECTS ARE IMPORTANT, ONLY OCCUPY A SMALL FRACTION OF THE TOTAL FLUID VOLUME
- **EDC MODEL:**
  - FLUID CONSISTS OF FINE SCALE STRUCTURES AND SURROUNDING FLUID
  - CHEMICAL REACTIONS ONLY OCCUR IN THE FINE SCALES
  - FINE SCALES ASSUMED HOMOGENEOUSLY MIXED
  - FINE SCALES REPRESENT BY A "PERFECTLY STIRRED REACTOR" (PSR)
  - $$P(\rho,T,Y_k) = \delta(\rho-\hat{\rho})\delta(T-\hat{T})\sum_{k=1}^{K}\delta(Y_k-\hat{Y}_k) + \delta(\rho-\rho^*)\delta(T-T^*)\sum_{k=1}^{K}\delta(Y_k-Y_k^*)$$

EDDY DISSIPATION CONCEPT (EDC)

- **MEAN REACTION RATE:**
  - $\overline{\dot{w}}_k = A_{EDC}\,\dot{f}\,\Delta m_k$
  - $\dot{f}$ - **FLOW RATE TO FINE SCALES PER UNIT MASS**
  - Δm_k - **MASS PER UNIT VOLUME CHANGE IN FINE SCALE SPECIES**
  - A_{EDC} - **MODEL PARAMETER**

- **MOST ELEMENTARY FORM FOR FAST CHEMISTRY:**
  - $F + rO \rightarrow P$
  - $\varphi_p = W_F / rW_O$
  - $\varphi_{st} = (W_F + rW_O) / W_F$
  - A_{EDC} **= CONSTANT**

$$\overline{\dot{w}}_F = -A_{EDC}\overline{\rho}(\tilde{\varepsilon} / \tilde{k}) \min\left[\tilde{Y}_F, \tilde{Y}_O \varphi_{st}\right]$$

$$\overline{\dot{w}}_O = -A_{EDC}\overline{\rho}(\tilde{\varepsilon} / \tilde{k}) \min\left[\tilde{Y}_F / \varphi_{st}, \tilde{Y}_O\right]$$

$$\overline{\dot{w}}_P = -\overline{\dot{w}}_F \varphi_p$$

EDDY DISSIPATION CONCEPT (EDC)

- **MORE GENERAL FORMS OF EDC MODEL:**
  - A_{EDC}, $\dot{f}$ - ESTIMATED FROM ENERGY CASCADE THEORY
  - CAN INCLUDE REVERSIBLE REACTIONS
  - Δm_k FROM PSR CALCULATION FOR FINITE RATE CHEMISTRY
  - CAN FORMULATE AN EXTINCTION MODEL

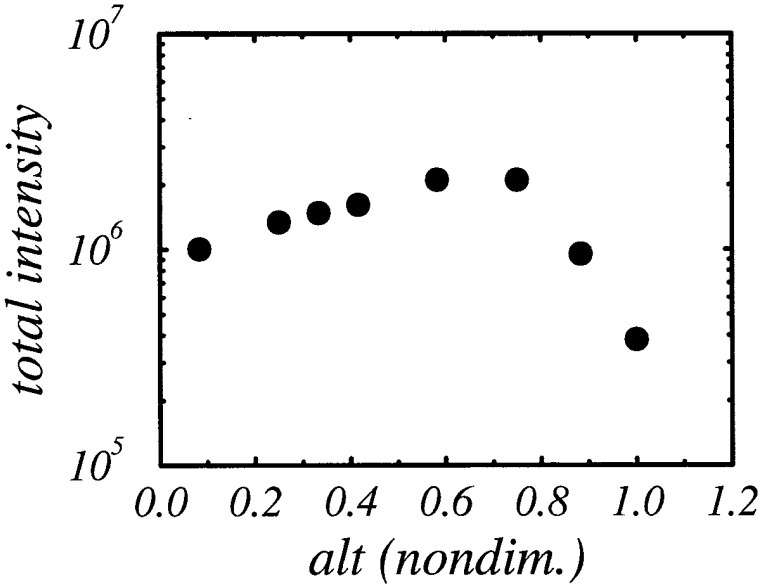
- **COMMENTS:**
  - VERY INEXPENSIVE FOR FAST CHEMISTRY
  - HIGH SENSITIVITY TO MODEL PARAMETER, A_{EDC}, AND INFLOW TURBULENCE
  - GOOD FOR RUNNING PERMUTATIONS AROUND A KNOWN CALIBRATION POINT

EXAMPLE OF THE IMPORTANCE OF TURBULENCE CHEMISTRY INTERACTIONS: MISSILE PLUME AFTERBURNING CESSATION

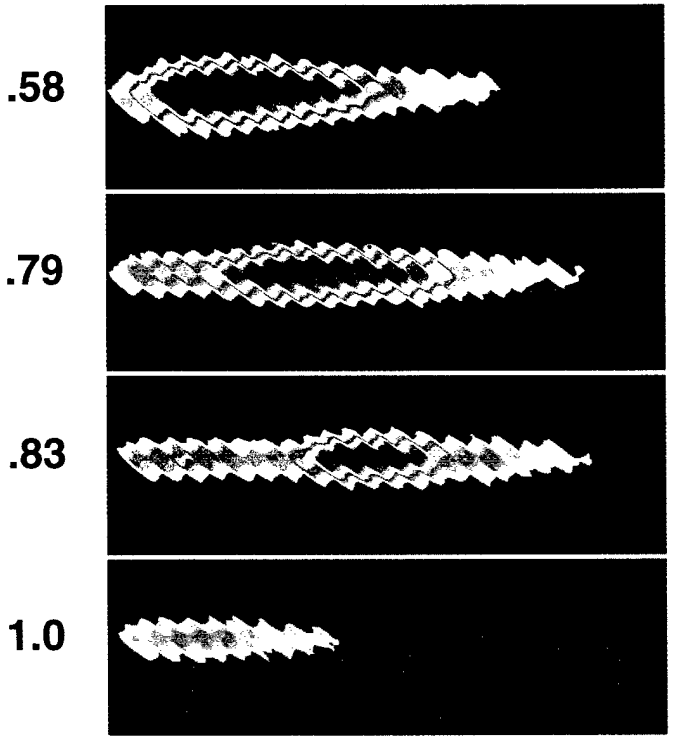
AFTERBURNING CESSATION IMPORTANT TO:

- SURVEILLANCE SENSOR DEVELOPMENT
  - DETERMINATION OF NOISE EQUIVALENT TARGET THRESHOLD
  - SENSOR DYNAMIC RANGE
- MISSILE TYPING
- PLUME-TO-HARDBODY HANDOVER AND AIMPOINT SELECTION ALGORITHMS

EXAMPLE OF RAPID CESSATION EVENT



TOTAL INTENSITY AS A FUNCTION OF ALTITUDE



SPATIAL RADIANT INTENSITY

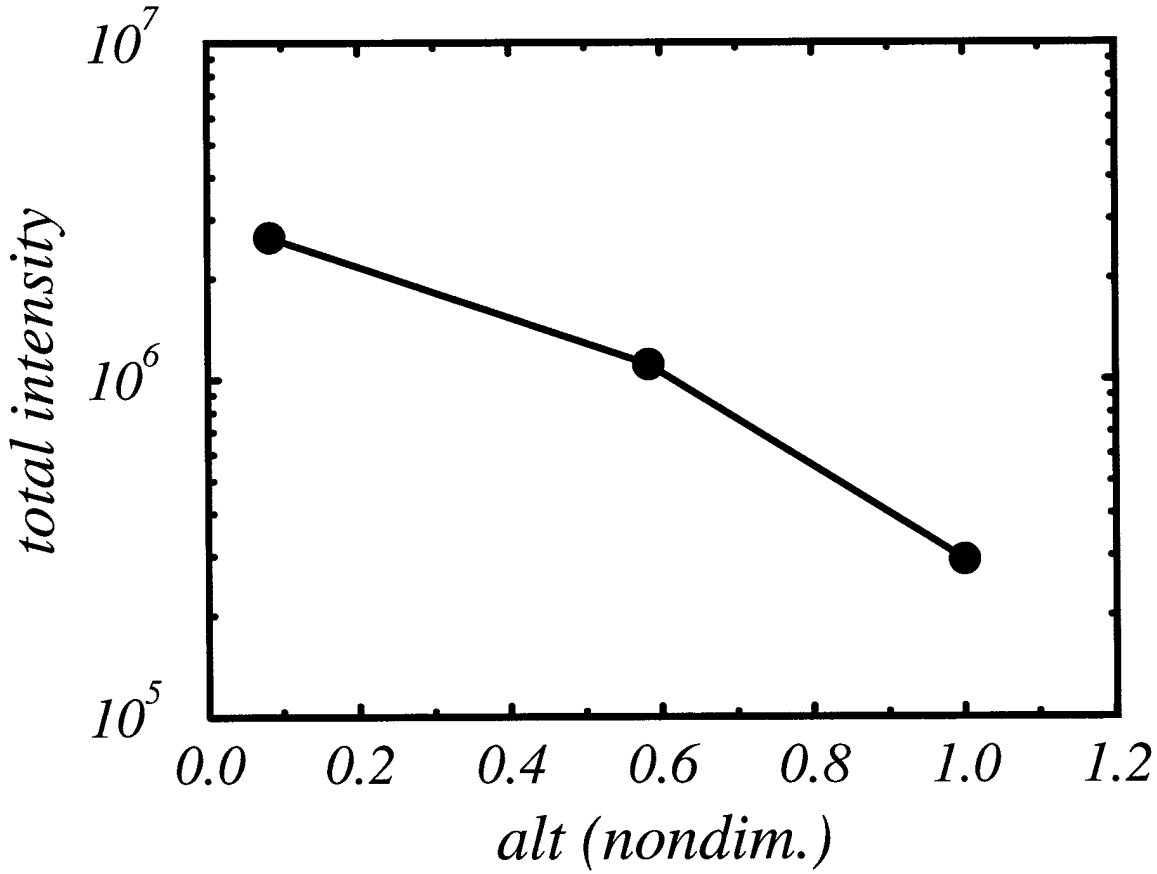
POSSIBLE MECHANISMS FOR RAPID AFTERBURNING CESSATION

- **SHEAR LAYER RELAMINARIZATION (VELOCITY MATCHING):**
  - AFTERBURNING INHIBITED BY LACK OF TURBULENT MIXING
- **DAMKOHLER NUMBER EFFECT:**
  - DAMKOHLER NUMBER IS RATIO OF MIXING AND CHEMICAL TIME SCALES
  - LARGE SCALE TURBULENT MIXING COOLS PLUME FASTER THAN AFTERBURNING HEATS THE PLUME (LOW DAMKOHLER NUMBER)
- **CLASSICAL FLAME EXTINCTION MECHANISM:**
  - HIGH TURBULENT MIXING RATES AT THE SMALL SCALES CAUSES LOCAL FLAME EXTINCTION AND EVENTUAL AFTERBURNING CESSATION

COMPUTATIONAL METHODOLOGY

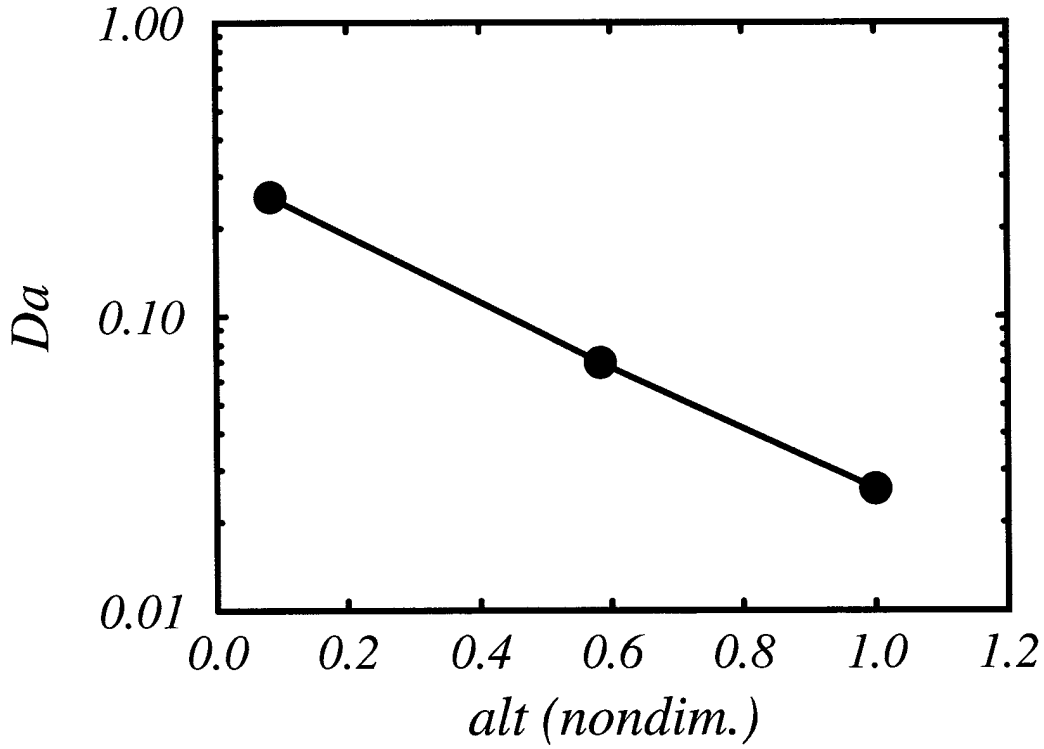
- **SIMULATIONS ACCOMPLISHED USING THE "GASP" CODE:**
  - GENERAL AERODYNAMIC SOLVER FOR COMPRESSIBLE REACTING FLOWS
  - INCLUDES MODERN, WIDELY ACCEPTED TURBULENCE MODELS
  - DRAWBACK: NEGLECTS THE EFFECT OF TURBULENCE-CHEMISTRY INTERACTIONS
  - FINITE RATE/EXTINCTION VERSION OF EDC MODEL IMPLEMENTED TO ACCOUNT FOR TURBULENCE-CHEMISTRY INTERACTIONS
- **MISSILE MODELING:**
  - SIMULATE THE ENTIRE MISSILE BODY, BASE AND PLUME
  - ASSUME ONLY AXISYMMETRIC BODY CONFIGURATION

PREDICTED TOTAL RADIANT INTENSITY

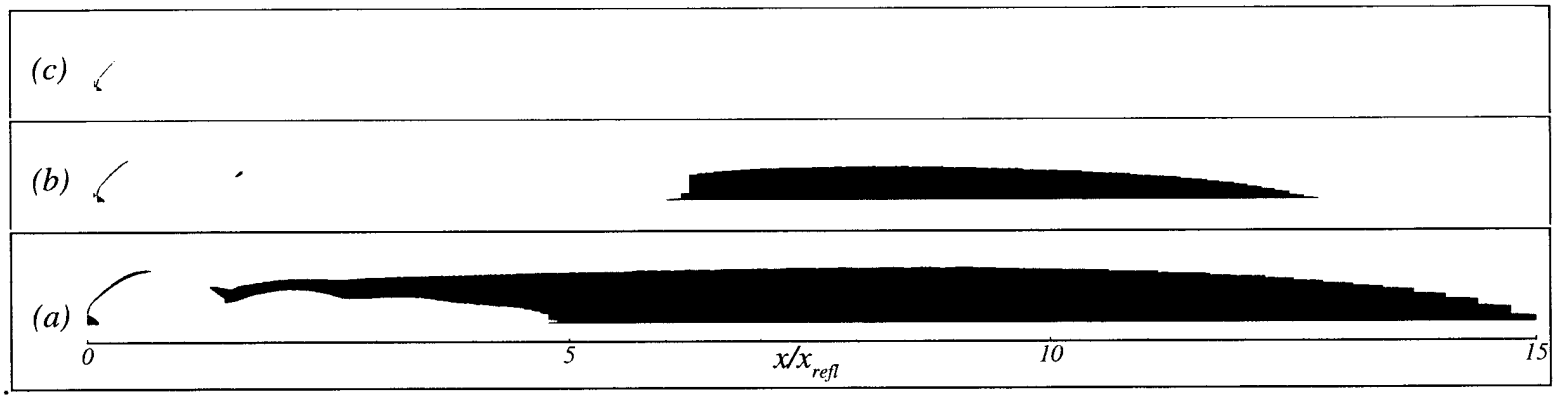


DAMKOHLER NUMBER VARIATION WITH ALTITUDE ENGINE MODELS

$$Da = \tau_{mix}/\tau_{chem}$$

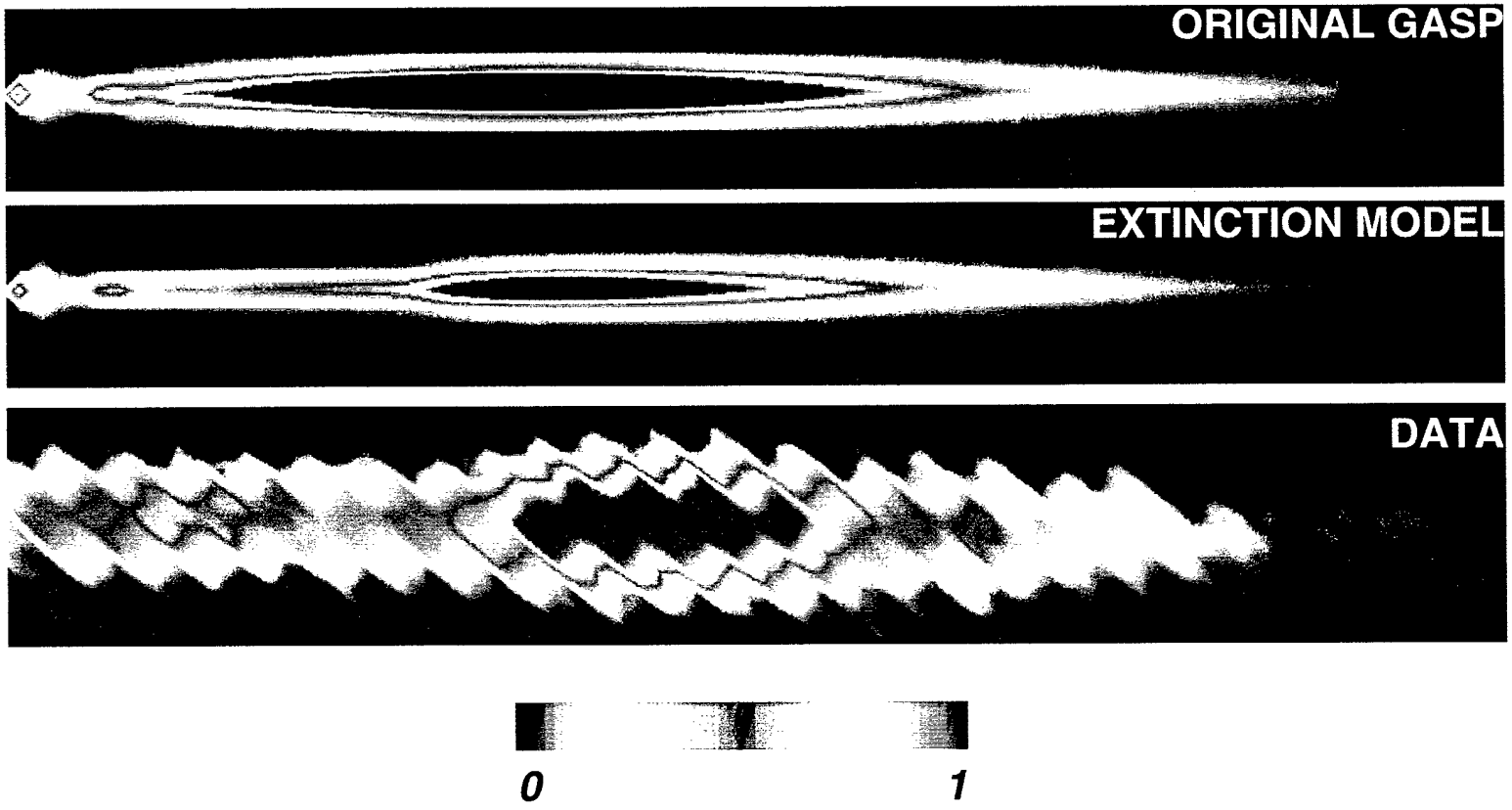


CONTOUR PLOT OF THE EXTINCTION MODEL BINARY SWITCH



COMPARISON OF TEMPERATURE CONTOURS USING EXTINCTION MODEL

EFFECT OF EXTINCTION MODEL ON SPATIAL RADIANT INTENSITY PREDICTIONS DURING THE CESSATION EVENT



CONCLUSIONS

- PROPERLY ACCOUNTING FOR TURBULENCE-CHEMISTRY INTERACTIONS IN REACTING FLOW SIMULATIONS CAN BE CRITICAL

- TURBULENT COMBUSTION MODELS HAVE BEEN DEVELOPED FOR COMPLEX FLOWS

- TURBULENT COMBUSTION MODELS EFFICIENT ENOUGH FOR ROUTINE APPLICATION