NUMERICAL MODELING OF SPRAY COMBUSTION
WITH AN UNSTRUCTURED-GRID METHOD

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ABSTRACT

The present unstructured-grid method follows strictly the basic finite volume forms of
the conservation laws of the governing equations for the entire flow domain. High-order
spatially accurate formulation has been employed for the numerical solutions of the
Navier-Stokes equations. A two-equation k-ε turbulence model is also incorporated in the
unstructured-grid solver. The convergence of the resulted linear algebraic equation is
accelerated with preconditioned Conjugate Gradient method. A statistical spray
combustion model has been incorporated into the present unstructured-grid solver. In this
model, spray is represented by discrete particles, rather than by continuous distributions.
A finite number of computational particles are used to predict a sample of total population
of particles. Particle trajectories are integrated using their momentum and motion
equations and particles exchange mass, momentum and energy with the gas within the
computational cell in which they are located. The interaction calculations are performed
simultaneously and eliminate global iteration for the two-phase momentum exchange. A
transient spray flame in a high pressure combustion chamber is predicted and then the
solution of liquid-fuel combusting flow with a rotating cup atomizer is presented and
compared with the experimental data. The major conclusion of this investigation is that the
unstructured-grid method can be employed to study very complicated flow fields of
turbulent spray combustion. Grid adaptation can be easily achieved in any flow domain
such as droplet evaporation and combustion zone. Future applications of the present
model can be found in the full three-dimensional study of flow fields of gas turbine and
liquid propulsion engine combustion chambers with multi-injectors.
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OUTLINE

- INTRODUCTION
- MOTIVATION AND OBJECTIVE
- UNSTRUCTURED GRID FLOW SOLVER
- PHYSICAL MODELS AND NUMERICAL APPROACHES
- COMPUTATIONAL RESULTS
- CONCLUSIONS
INTRODUCTION

- APPLICATION OF SPRAY COMBUSTION
  - LIQUID-FUELED ROCKET ENGINES
  - GAS-TURBINE COMBUSTORS
  - INDUSTRIAL FURNACES
  - DIESEL ENGINES
- MODELING IN LIQUID-FUELED ROCKET ENGINES
  - COAXIAL, IMPINGING JETS AND SWIRLING INJECTORS ...
  - ATOMIZATION PROCESS
  - DROPLET VAPORIZATION, DISPERSION AND COLLISION
  - TURBULENT COMBUSTION

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INTRODUCTION . . .

- STRUCTURED GRID
  - BODY-FITTED COORDINATES, MULTI-ZONE
  - AUTOMATIC INDEXING
  - HIGH EFFICIENCY AND LESS MEMORY
  - TIME-CONSUMING GRID GENERATION FOR COMPLEX GEOMETRY

- UNSTRUCTURED GRID
  - SIMULATION OF ANY COMPLEX GEOMETRIES
  - FLEXIBLE SOLUTION ADAPTIVITY
  - LESS GRID GENERATION EFFORTS
  - HIGH MEMORY AND COMPUTATION EFFORT
MOTIVATION AND OBJECTIVE

- SIMULATE MULTI-INJECTOR COMPLEX SPRAY COMBUSTION PROCESS IN ROCKET PROPULSION ENGINES
- A MAJOR STRUCTURED GRID CAN BE GENERATED ABOUT THE MAIN COMBUSTION CHAMBER
- EACH INJECTOR REGION CAN BE A SUBDOMAIN (A HOLE IN MAJOR GRID) WHERE STRUCTURED OR UNSTRUCTURED GRID CAN BE GENERATED
- THE OVERLAPPED REGION OR GAP BETWEEN MAJOR- AND SUB-GRID CAN BE FILED UP WITH UNSTRUCTURED GRIDS
- TAKE THE ADVANTAGE OF GRID FLEXIBILITY OF UNSTRUCTURED GRID METHOD
- DEVELOP AND INCORPORATE ADVANCED SPRAY COMBUSTION MODEL IN UNSTRUCTURED CODE

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UNSTRUCTURED GRID FLOW SOLVER

- CELL-CENTERED FINITE VOLUME ALGORITHM
- HYBRID UNSTRUCTURED CELL
  - TRIANGLE AND QUADRANGLE FOR 2D
  - PRISM, TETRAHEDRAL AND HEXAHEDRAL FOR 3D
- PRESSURE-CORRECTION ALGORITHM
- CONJUGATE GRADIENT SQUARED (CGS) MATRIX SOLVER
- VISCOUS OR INVISCID, LAMINAR OR TURBULENT, INCOMPRESSIBLE OR COMPRESSIBLE FLOW
- HIGH-ORDER SCHEME WITH FLUX LIMITER
- STEADY STATE OR TRANSIENT FLOW
2D UNSTRUCTURED CELLS

Main Point
Boundary Point
Node Point
Flux
Cell Surface

1,2,...

F
S

620
JOINT HYBRID CELLS

Hexahedron: 1 2 3 4 5 6 7 8
Prism: 2 3 9 6 10 7
Pyramid: 5 6 7 8 11
Tetrahedron: 6 10 7 11
DOUGLAGS MULTI-ELEMENT AIRFOIL
GOUGLAS MULTI-ELEMENT AIRFOIL
PRESSURE CONTOUR
Pressure Coefficient

- Experiment
- Prediction

$M=0.2$
$\alpha=16.2^\circ$
BOEING 747 AIRPLANE
PHYSICAL MODELS AND NUMERICAL APPROACHES

- STRONGLY-COUPLED EULERIAN-LAGRANGIAN TWO-PHASE FLOW APPROACH
- STOCHASTIC SEPARATED FLOW (SSF) MODEL FOR PARTICLE TURBULENT DISPERSION
- DROPLET BREAK-UP, EVAPORATION AND COLLISION MODEL
- LIQUID JET ATOMIZATION MODEL
- VOF (VOLUME OF FLUID) MODEL FOR COAXIAL OR IMPINGING JETS INJECTORS
- $K$-$\varepsilon$ TWO-EQUATION TURBULENCE MODEL
- INSTANTANEOUS, FINITE-RATE AND EQUILIBRIUM CHEMISTRY MODEL

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COMPUTATIONAL RESULTS

- TRANSIENT SPRAY COMBUSTION
  - EXPERIMENT OF YOKOTA ET AL.
  - LIQUID FUEL TRIDECANE ($C_{13}H_{28}$) INJECTED INTO HIGH-PRESSURE (3.0 MPA) AND TEMPERATURE (900 K) AIR CHAMBER
  - SINGLE STEP AND EDDY-BREAK-UP COMBUSTION MODEL
  - FIVE SPECIES WERE CONSIDERED: $C_{13}H_{28}$, $O_2$, $N_2$, $CO_2$ AND $H_2O$
  - THE IGNITION DELAY AND TRANSIENT CONFIGURATION OF THE SPRAY FLAME ARE REASONABLY PREDICTED

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TRANSIENT SPRAY COMBUSTION

TEMPERATURE CONTOUR

$t=1.0\, \text{ms}$

$t=2.6\, \text{ms}$

$t=1.4\, \text{ms}$

$t=3.8\, \text{ms}$
TRANSIENT SPRAY COMBUSTION

$t=3.8$ ms

FUEL MASS FRACTION

CO2 MASS FRACTION

O2 MASS FRACTION

TEMPERATURE
TRANSIENT SPRAY COMBUSTION

SPRAY + GRIDS + TEMPERATURE CONTOUR
COMPUTATIONAL RESULTS...

- SPRAY FLAME IN A COMBUSTION CHAMBER
  - EXPERIMENT OF EL-BANHAWY AND WHITELAW
  - MONO-SIZED (D=47 \( \mu \)M) LIQUID KEROSENE INJECTED AT ROOM TEMPERATURE WITH FLOW RATE 1.32\( \times \)10\(^3\) KG/S
  - AIR INLET SWIRL NUMBER 1.2 WITH FLOW RATE 0.0556 KG/S
  - SINGLE STEP AND EDDY-BREAK-UP COMBUSTION MODEL
  - FIVE SPECIES WERE CONSIDERED: C\(_{13}\)H\(_{28}\), O\(_2\), N\(_2\), CO\(_2\) AND H\(_2\)O
  - FAVORABLE AGREEMENT WITH EXPERIMENTAL MEASUREMENT
  - HIGHER TEMPERATURE PREDICTED DUE TO THE LACK OF RADIATION HEAT TRANSFER MODEL AND DISSOCIATION OF CHEMICAL RADICALS AND SOOT

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SPRAY FLAME IN A COMBUSTION CHAMBER

FUEL MASS FRACTION

O2 MASS FRACTION
SPRAY FLAME IN A COMBUSTION CHAMBER

CO2 MASS FRACTION

TEMPERATURE
CONCLUSIONS

- A SPRAY COMBUSTION MODEL HAS BEEN INCORPORATED IN A PRESSURE-BASED HYBRID UNSTRUCTURED GRID CODE
- FAVORABLE AGREEMENT WITH EXPERIMENTAL RESULTS HAS BEEN ACHIEVED
- CONTINUE VALIDATE AND EXTEND THE CURRENT MODEL IN 3D MULTI-INJECTOR COMBUSTION MODELING
- DEVELOP HYBRID UNSTRUCTURED GRID GENERATION TECHNIQUE
- RADIATION HEAT TRANSFER EFFECT MUST BE INCLUDED IN FUTURE DEVELOPMENT FOR HYDROCARBON COMBUSTION