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*GASFLOW: A Computational
Fluid Dynamics Code for Gases,
Aerosols, and Combustion*

VOLUME 1

Theory and Computational Model

Los Alamos
NATIONAL LABORATORY

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*GASFLOW: A Computational
Fluid Dynamics Code for Gases,
Aerosols, and Combustion*

VOLUME 1

Theory and Computational Model

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CONTENTS

	Page
ACKNOWLEDGMENTS.....	xi
NOMENCLATURE	xiii
EXECUTIVE SUMMARY	xix
 1 INTRODUCTION	 1
1.1 Background.....	1
1.2 Computational Methodology	4
REFERENCES.....	6
 2 MATHEMATICAL AND PHYSICAL MODELS.....	 7
2.1 The Generalized Conservation Equation.....	7
2.2 The Mass Conservation Equations.....	8
2.3 The Momentum Transport Equations	10
2.4 The Internal Energy Transport Equation	11
2.5 Constitutive Relationships	12
2.5.1 Thermochemical and Transport Properties	12
2.5.1.1 Internal Energy and Specific Heats	13
2.5.1.2 Transport Properties	15
2.5.2 Equation of State.....	16
2.6 Heat-Transfer and Phase-Change Relationships.....	16
2.6.1 Gas-Structure Heat Transfer.....	16
2.6.2 Condensation and Vaporization.....	18
2.6.3 Phase Change in the Fluid Mixture—The Homogeneous Equilibrium Model (HEM).....	20
2.6.4 Droplet Depletion or Droplet "Rainout".....	22
2.6.5 Structural Heat Conduction.....	22
2.6.6 Wall Shear Stress.....	23
2.7 Turbulence Modeling.....	24
2.7.1 Algebraic Model.....	26
2.7.2 κ - ϵ Model.....	27
2.7.3 Turbulence Effects on the Transport Coefficients	28
2.8 Chemical Kinetics.....	29
2.8.1 One-Step Model	29
2.8.2 Two-Step Model.....	32
2.8.2.1 Induction Parameter Model.....	32
2.8.2.2 Coupling of Induction Parameter Model with κ - ϵ Model	33
2.9 Recombiner Models.....	34
2.9.1 NIS Recombiner Model.....	37
2.9.2 Siemens Recombiner Model.....	39

CONTENTS (cont)

	Page
2.9.3 Siemens Correlation for Siemens Type FR-90/1 Recombiner	40
2.9.4 GRS Recombiner Correlation	41
2.10 Ignitor Model	41
2.11 Ventilation System Modeling	42
2.11.1 Ducts and Pipes	42
2.11.2 Junctions	47
2.11.3 Blowers and Fans	47
2.11.4 Dampers and Valves	48
2.11.5 Filters	49
2.12 Aerosol Model	49
2.12.1 Particle Transport	49
2.12.2 Particle Turbulent Diffusion	51
2.12.3 Particle Deposition	51
2.12.4 Particle Entrainment	56
2.12.5 Boundary Layer Thickness	60
2.12.6 Particle Cloud Model	60
REFERENCES	61
 3 COMPUTATIONAL MODEL	 67
3.1 Beginning of Time Cycle Initialization	69
3.2 Phase A: Explicit Lagrangian Phase for the Multidimensional Finite Control Volumes	70
3.2.1 Volume Equation	70
3.2.2 Momentum Equations	70
3.2.3 Mixture and Species Mass Equations	71
3.2.4 Internal Energy Equation	72
3.2.5 Gas Mixture Temperature	72
3.2.6 Equation of State	72
3.2.7 Structural Heat Conduction	73
3.2.8 Mass and Energy Transfer	74
3.2.8.1 Structural Convective Heat Transfer	74
3.2.8.2 Structural Convective Heat and Mass Transfer	75
3.2.8.3 Structural Convective Heat and Mass Transfer with Phase Change in the Fluid Mixture - HEM	80
3.2.9 Liquid Droplet Depletion or "Rainout"	86
3.2.10 Hydrogen Combustion	87
3.2.10.1 One-Step Model	87
3.2.10.2 Two-Step Model	89
3.2.11 Hydrogen Recombination	90
3.2.12 Ventilation System	91
3.3 Phase B: Implicit Pressure Iteration Phase	93
3.3.1 Three-Dimensional Developments	93
3.3.2 Ventilation System Developments	97
3.4 Phase C: Rezone Phase	97

CONTENTS (cont)

	Page
3.4.1 Multidimensional Developments.....	97
3.4.2 Ventilation System Developments.....	104
3.5 Turbulence Transport.....	104
3.5.1 Algebraic Model.....	104
3.5.2 κ - ϵ Model.....	104
3.6 Time-Step Controls.....	105
3.6.1 Courant Condition for Material Velocity.....	105
3.6.2 Diffusional Condition for Mass, Momentum, and Energy.....	106
3.6.3 Ignition Conditions.....	106
3.6.4 Pressure Iteration Considerations.....	106
3.6.5 Maximum Time Step.....	107
3.7 Particle Computational Model.....	107
3.7.1 Particle Equations of Motion.....	107
3.7.2 Particle Diffusion.....	108
3.7.3 Deposition/Rebound.....	109
3.7.4 Entrainment.....	110
3.7.5 Numerical Solution Method.....	112
REFERENCES.....	113
4 SUMMARY.....	115

APPENDICES

A	The Gauss Divergence Theorem.....	A-1
B	Structural Heat Conduction Algorithm.....	B-1
C	Preconditioned Conjugate Residual Algorithm.....	C-1

FIGURES

1-1	Typical dry containment.....	2
1-2	Cross section of the Heiss Dampf Reactor near Frankfurt, Germany.....	3
1-3	Example of four independent multiblock computational volumes connected at each of the 3D volume's external boundaries by a complex ventilation system.....	5
2-1	Schematic diagram for the recombiner box model.....	35
2-2	Siemens (Ref. 2-31) and NIS (Refs. 2-32 and 2-33) recombiner.....	36
2-3	Ventilation system for a waste tank farm.....	44
2-4	Change in elevation for two neighboring one-dimensional cells.....	45
2-5	Gradual flow area change from A_s to A_l	45
2-6	Definitions for α and r	47

FIGURES (cont)

	Page
2-7 Illustration of a junction component.....	48
2-8 Forces acting on a single sphere at rest on a wall with a steady, fully developed turbulent flow.....	57
3-1 GASFLOW three-dimensional computational cell. Velocity components are located at face centers[W] west (-x), [E] east (+x), [S] south (-y), [N] north (+y), [B] bottom (-z), and [T] top (+z).....	68
3-2 A two-dimensional mesh slice showing the u and v staggered momentum control volumes associated with cell (i, j, k).....	69
3-3 Geometry for one-dimensional structural heat conduction.....	73
3-4 Slab and sink discretization.....	73
3-5 Wall discretization.....	74
3-6 Schematic diagram of van Leer second-order advection algorithm when face velocity is positive.....	99
3-7 Schematic diagram of van Leer second-order advection algorithm when face velocity is negative.....	100
3-8a A monotonicity condition shown by plotting the slope distribution of (slope of i lies outside the zero slope values for i - 1 and i + 1).....	102
3-8b A monotonicity condition shown by plotting the slope distribution of ϕ (slope of i is reduced to zero when its mesh value reaches an extreme).....	102
3-8c A monotonicity condition shown by plotting the slope distribution of ϕ (slope of i is reduced to zero when it doesn't agree with the trend of the adjacent slopes).....	103
B-1 Diagram of structural heat conductor elements and nodes.....	B-2
B-2 Slab and sink discretization.....	B-2
B-3 Wall discretization.....	B-2
B-4 Interior Elements ($1 \leq j \leq N$), Cartesian Coordinates—Backward Euler Method.....	B-3
B-5 Configuration for a wall, or two-sided heat-conduction problem.....	B-5
B-6 Configuration for a cylindrical heat-conducting element.....	B-7
B-7 Configuration for a two-sided cylindrical heat-conducting element.....	B-9

TABLES

	Page
2-1 Stress tensor components for a Newtonian fluid (Cartesian coordinates).....	11
2-2 Stress tensor components for a Newtonian fluid (cylindrical coordinates).....	11
2-3 Gas properties at temperature equaling 298.15 K [extracted from the JANAF (Ref. 2-7) Tables].....	13
2-4 Constants used in the κ - ϵ turbulence model.....	28
2-5 Siemens recombiner constants of FR-90/1.....	40
2-6 L/D values for 90° bends.....	45
2-7 L/D values for miter bend.....	46
2-8 L/D values for standard elbow.....	46
3-1 Comparison of standard ALE and GASFLOW ALE features.....	68
B-1 Coefficients and Terms for Heat-Conduction Algorithm.....	B-12

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NOMENCLATURE

a	Gordon and McBride coefficient for specific heat polynomial, CHEMKIN coefficients for transport properties, and coefficient for internal energy polynomial
A	Hamaker constant and generalized polynomial coefficients for internal energy approximation
A	Fractional flow-area vector
Ar	Archimedes number
A_r	Recombiner surface area (cm^2)
A_s	Wall or structural surface area (cm^2)
A	Area of fluid cell in contact with GRS recombiner foil (cm^2)
b	Coefficient for internal energy polynomial
b	Velocity of control surface (cm/s)
B	Constant for wall shear stress
c	Coefficient for internal energy polynomial and for water saturation curve
C	Relaxation coefficient for phase-change model (HEM) or droplet rainout model (s^{-1})
C_a	Concentration of species a (moles/ cm^3)
C_c	Energy of combustion (ergs/mole)
CD	Fluid drag coefficient
C_D	Vector structural drag coefficient
C_f	Frequency (or pre-exponential) factor in Arrhenius law ($\text{cm}^3/\text{mole s}$)
C_p	Specific heat at constant pressure (erg/g K)
C_v	Specific heat at constant volume (erg/g K)
d	Coefficient for internal energy polynomial
d	Particle (sphere) diameter (cm)
D	Hydraulic diameter of duct (cm)
Dd	Structural drag vector (g/cm s^2)
$D_{\alpha \rightarrow \text{mix}}$	Molecular diffusion coefficient of species α into the mixture (cm^2/s)
$D_{\alpha \rightarrow \beta}$	Binary molecular diffusion coefficient of species α into species β (cm^2/s)
D_t	Turbulent mass diffusivity (cm^2/s)
e	Coefficient for internal energy polynomial
e	Coefficient of restitution
E	Activation energy (ergs/mole)
E_i	Potential energy well depth on impact (ergs)
E_r	Potential energy well depth on rebound (ergs)
f	Duct friction factor
F	Force (g cm/s^2)
f_s	Static friction coefficient
g	Acceleration of gravity (cm/s^2)
h	Apparent particle penetration depth (cm)

h_d	Structural mass-transfer coefficient ($\text{g}/\text{cm}^2 \text{ s}$)
h_d^*	Structural mass-transfer coefficient, corrected for effect of water vapor ($\text{g}/\text{cm}^2 \text{ s}$)
h_f	Penetration depth (cm)
h_s	Structural heat-transfer coefficient ($\text{g}/\text{s}^3 \text{ K}$) or ($\text{ergs}/\text{cm}^2 \text{ K s}$)
h_s^*	Corrected structural heat-transfer coefficient for effect of water vapor ($\text{g}/\text{s}^3 \text{ K}$)
h_α	Enthalpy for species α (ergs/g)
h_2	Hydrogen
h_{2o}	Water vapor
H	Heaviside function or blower head (cm)
i	x- (or r-) direction index
I	specific internal energy (ergs/g)
$I_{reference}$	Specific internal energy at reference temperature of 298.15 K (ergs/g)
j	y- (or θ -) direction index
$\mathbf{J}_\alpha$	Mass flux vector for species α ($\text{g}/\text{cm}^2 \text{ s}$)
k	z-direction index or thermal conductivity ($\text{ergs}/\text{cm K s}$ or $\text{g cm}/\text{K s}^3$)
$k(T)$	Chemical rate constant ($\text{cm}^3/\text{mole s}$)
K	Bulk mechanical property = $(1-N^2)/Y$ (cm^2/dyne) or momentum form loss coefficient
KE_i	Kinetic energy from incident normal velocity (ergs)
KE_r	Kinetic energy from rebound normal velocity (ergs)
l	Turbulence length scale (cm)
L	Effective length of duct (cm)
m	Mass of bulk material or aerosol particles (g)
m_{lim}	Smallest of fuel, oxygen, burnt fuel mass fractions
$\dot{m}_s$	Mass-transfer rate to and from structural surface (g/s)
M	Molecular weight (g/mole)
n	Mole fraction
$\mathbf{n}$	Unit normal vector
n_2	Nitrogen
o_2	Oxygen
p	Pressure (Pa)
P	Induction parameter for combustion model
Pr	Prandtl number
Q	Volumetric flow rate into recombiner (cm^3/s)
$\mathbf{q}$	Energy flux vector ($\text{ergs}/\text{cm}^2 \text{ s}$)
$q_{p,h2o}$	Energy lost or gained by the structure due to phase change (ergs/s)
q_s	Convected energy to structural surface (ergs/s)
r	Radial coordinate
R	Flux ratio
R	Radius of curvature (cm)
R_α	Gas constant for species α ($\text{ergs}/\text{mole K}$)

Re	Reynolds number
R_{h_2}	Recombination reaction rate for hydrogen (g/s)
$\mathcal{R}^2$	Universal gas constant (ergs/mole K or g cm ² /mole s ²)
S	Fluid cell surface area (cm ²), or blower speed (radian/s)
S^*	Moving control surface (cm ²)
Sc	Schmidt number
SI	Energy source or sink (ergs/s)
S_m	Momentum source or sink (g/cm ² s ²)
$S\Phi$	Arbitrary source term
$S\rho$	Mass source or sink resulting from phase change involving structures (g/s)
$S\rho, \alpha$	Mass source or sink resulting from chemical reactions and HEM (g/s)
t	Time (s)
T	Temperature (K)
u	x- (or r-) direction velocity component (cm/s)
$\mathbf{u}$	Fluid velocity vector (cm/s)
$\mathbf{u}_g$	Grid velocity vector (cm/s)
u_y	Velocity component tangent to and a distance y from wall (cm/s)
u_*	Shear velocity (cm/s)
U	Velocity into recombiner (cm/s)
U_g	Gas velocity (cm/s)
U_{gcp}	Gas velocity at center of particle (cm/s)
U_{gpu}	Minimum particle pickup velocity predicted by the semi-empirical model (cm/s)
U_{gpuo}	Minimum particle pickup velocity predicted by the single particle model (cm/s)
U_i	Incident normal velocity (cm/s)
U_i^*	Critical normal rebound velocity (cm/s)
U_p	Particle velocity (cm/s)
U_r	Rebound normal velocity (cm/s)
U_t	Tangential velocity (cm/s)
v	y- (or θ -) direction velocity component (cm/s)
V	Volume (cm ³)
V^*	Moving control volume (cm ³)
w	z-direction velocity component (cm/s)
$\mathbf{x}$	Position vector (cm)
x	Cartesian coordinate
x_α	Mass fraction of species α
y	Cartesian coordinate
y	Distance normal to surface and perpendicular to flow direction (cm)
y_c	Distance from wall to cell center (cm)
Y	Young's modulus (dyne/cm ²)

Y_α	Molar or volume fraction for species α
z	Cartesian coordinate
z_0	Separation distance of sphere and substrate (cm)
α	Coefficient of thermal expansion Random number for particle bounce; angle of miter bend (degrees)
β	Wall thermal diffusivity
δ	Boundary layer or film thickness (cm)
δx	Mesh cell size for fluid cells in x- or r- coordinate direction (cm)
δy	Mesh cell size for heat cells in y- or θ - coordinate direction (cm)
δz	Mesh cell size for heat cells in z-coordinate direction (cm)
Δt	Time step (s)
Δx	Mesh cell size for heat conduction grid (cm)
ε	Dissipation of turbulent kinetic energy per unit mass (cm^2/s^3)
η	Molecular viscosity (g/cm s) and recombiner efficiency
θ	Azimuthal coordinate, gas mixture volume, fraction, or gas mixture void fraction
θ_m	Mass-transfer correction factor
θ_T	Heat-transfer correction factor
κ	Square root of turbulent kinetic energy per unit mass (cm^2/s^2)
λ	Second coefficient of molecular viscosity (g/cm s)
μ	First coefficient of molecular viscosity (g/cm s)
ν	Kinematic viscosity (cm^2/s)
N	Poisson ratio
ξ	Geometry coefficient
ρ	Density (g/cm^3)
ρ_g	Gas density (g/cm^3)
ρ_p	Particle density (g/cm^3)
σ	Turbulence coefficient and standard deviation
τ	Relaxation constant
τ_{ind}	Induction time
τ	Viscous stress tensor ($\text{g}/\text{cm s}^2$)
τ_s	Wall or structural shear stress ($\text{g}/\text{cm s}^2$)
ϕ	Molecular thermal conductivity ($\text{ergs}/\text{cm K s}$ or $\text{g cm}/\text{K s}^3$)
ϕ_t	Turbulent thermal conductivity ($\text{ergs}/\text{cm K s}$ or $\text{g cm}/\text{K s}^3$)
ϕ_T	Rate factor
Φ	General (arbitrary) scalar or vector function
Ψ	General molecular transport coefficient and turbulence variable
ω	Reaction rate ($\text{moles}/\text{cm}^3 \text{ s}$)

Superscripts

A	Lagrangian Phase A computational level
B	Lagrangian Phase B computational level
n	Old time level

n+1	New time level
*	Moving control surface or volume and corrected heat and mass Transfer coefficients for water vapor effect
o	Reference value; or thermodynamic or microscopic density

Subscripts

b	Bulk fluid property
c	Cell-centered value; or related to combustion, condensation/vaporization; or convection
d	Related to mass-transfer coefficient
f	Cell face
g	Gas
h ₂	Hydrogen component
h ₂ o	Water vapor component
h ₂ ol	Water liquid component
i	x- (or r-) direction index
in	Recombiner inlet
I	Related to the energy conservation equation
j	y- (or θ -) direction index
k	z-direction index
m	Momentum control volume, or related to the momentum conservation equations
max	Maximum droplet loading of the atmosphere
mixture	Refers to fluid mixture
out	Recombiner outlet
o ₂	Oxygen component
0	Reference; or related to droplet rainout
p	Particle
ref	Reference
s	Structure surface; or saturation
t	Turbulent and total or apparent
total	Total heat flux to structures, convection plus phase change
w	Wall-temperature distribution in structures
x	Vector component in x- or r-coordinate direction
y	Vector component in y- or θ -coordinate direction
z	Vector component in z-coordinate direction
α	Species
ϵ	Related to the turbulence coefficients
κ	Related to the turbulence coefficients
μ	Related to the turbulence coefficients
ρ	Related to the mass conservation equations

GASFLOW: A Computational Fluid Dynamics Code for Gases, Aerosols, and Combustion

by

**J. R. Travis, J. W. Spore, P. Royle, K. L. Lam, T. L. Wilson,
C. Müller, G. A. Necker, B. D. Nichols, and R. Redlinger**

EXECUTIVE SUMMARY

Los Alamos National Laboratory (LANL) and Forschungszentrum Karlsruhe (FzK) are developing GASFLOW, a three-dimensional (3D) fluid dynamics field code as a best-estimate tool to characterize local phenomena within a flow field. Examples of 3D phenomena include circulation patterns; flow stratification; hydrogen distribution mixing and stratification; combustion and flame propagation; effects of noncondensable gas distribution on local condensation and evaporation; and aerosol entrainment, transport, and deposition.

An analysis with GASFLOW will result in a prediction of (1) the gas composition and discrete particle distribution in space and time throughout the facility and (2) the resulting pressure and temperature loadings on the walls and internal structures with or without combustion. A major application of GASFLOW is for predicting the transport, mixing, and combustion of hydrogen and other gases in nuclear reactor containments and other facilities. It has been applied to situations involving transporting and distributing combustible gas mixtures. It has been used to study gas dynamic behavior (1) in low-speed, buoyancy-driven flows, as well as sonic flows or diffusion dominated flows; and (2) during chemically reacting flows, including deflagrations. The effects of controlling such mixtures by safety systems can be analyzed.

The code version described in this manual is designated GASFLOW 2.1, which combines previous versions of the United States Nuclear Regulatory Commission code HMS (for Hydrogen Mixing Studies) and the Department of Energy and FzK versions of GASFLOW. The code was written in standard Fortran 90. This manual comprises three volumes. Volume I describes the governing physical equations and computational model. Volume II describes how to use the code to set up a model geometry, specify gas species and material properties, define initial and boundary conditions, and specify different outputs, especially graphical displays. Sample problems are included. Volume III contains some of the assessments performed by LANL and FzK. GASFLOW is under continual development, assessment, and application by LANL and FzK. This manual is considered a living document and will be updated as warranted.

GASFLOW is a finite-volume code based on robust computational fluid dynamics numerical techniques that solve the compressible Navier-Stokes equations for 3D volumes in Cartesian or cylindrical coordinates. The code can model geometrically complex facilities with multiple compartments and internal structures in a computational domain of multiple 3D blocks of cells connected by one-dimensional flow paths. GASFLOW has transport equations for multiple gas species, liquid water droplets, and total fluid internal energy. A built-in library contains 23 gas species and 1 liquid water species.

GASFLOW can simulate the effects of two-phase dynamics with the homogeneous equilibrium model, two-phase heat transfer (steam condensation and water evaporation) to walls and internal structures, chemical kinetics from catalytic hydrogen recombination and combustion processes, and fluid turbulence. The code can model two-phase heat transfer to and from walls and internal structures by convection and mass diffusion.

Wall shear stress models are provided for bulk laminar and turbulent flow. Two turbulence models available: algebraic and κ - ϵ , which provide zero- and two-transport-equation models, respectively, that determine turbulent velocity and length scales needed to compute the turbulent viscosity. Terms for the turbulent diffusion of different species are included in the mass and internal energy equations.

Chemical energy of combustion involving hydrogen provides a source of energy within the gaseous regions. A one-step global chemical kinetics model based on a modified Arrhenius law accounts for local hydrogen and oxygen concentrations. A two-step chemical kinetics model divides the chemical reaction into two parts: (1) an induction phase, which builds radicals and releases little energy; and (2) an energy release phase, where the radicals recombine. Hydrogen is ignited using a generalized ignitor model that represents both spark- and glow-plug-type designs. A catalytic hydrogen combination with oxygen is modeled using data from both the Nuclear Ingenieur Service and Siemens recombiner box designs.

The aerosol model comprises the following models: Lagrangian discrete particle transport, stochastic turbulent particle diffusion, particle deposition, particle entrainment, and particle cloud. These models incorporate the physics of particle behavior to model discrete particle phenomena and allow the code user to track the transport, deposition, and entrainment of discrete particles, as well as clouds of particles.

GASFLOW 2.1 models have been extended beyond GASFLOW 1.0 with the following developments:

- independent multiblock computational domains;
- independent multiblocks connected on external boundaries by a ventilation system;
- a fractional area treatment to model flow areas smaller than a cell face area;
- accurate internal energy as a function of temperature to fourth-degree polynomials;
- gas properties library of thermochemical and transport extended to 30 species;
- homogeneous equilibrium model for fluid mixture;
- droplet depletion or "rainout";
- two-phase heat and mass transfer to structural components;
- both spark- and glow-plug ignitor models;
- empirical hydrogen combustion limits;
- hydrogen recombiner models; and
- transport, deposition, and entrainment of discrete particles.

Each version of GASFLOW is tested with a Standard Test Matrix of 126 problems in four categories: (1) feature tests for the computer science aspects of the code; (2) functional tests for code algorithms, equations, logic paths, and decision points; (3) comparisons with analytical solutions; and (4) comparisons with data. During the development of GASFLOW 2.1, many experiments were modeled and analyzed. All 19 analytical solutions and the following 6 experiments are documented in Volume III: (1) the Bureau of Mines Spherical Test Chamber; (2) the Sandia FLAME Experiment; (3) Battelle Model Containment (BMC) Test GX6; (4) Battelle Model Containment Test HYJET JX7; (5) Heißdampfreaktor (HDR) Test T31.5; and (6) Phebus Tests 4A, 4B, 6A, and 10A. All of the problems in the Standard Test Matrix and in the initial set of assessments were executed successfully by GASFLOW 2.1 without modification, and the results are in agreement with the analytical solution or the test data. For example, other assessment analyses of the HDR, BMC, Russian RUT, and LANL TA-55 facilities are documented in the literature.

The Bureau of Mines Spherical Test Chamber (having a volume of 120 L) has been used to investigate the flammability of hydrogen, ammonia, nitrous oxide, and air mixtures under quiescent and turbulent conditions. GASFLOW calculated combustion of mixtures of hydrogen concentrations for 5 to 40 vol % diluted in air,

1:1 ratios of hydrogen and nitrous oxide in air, and very low hydrogen and nitrous oxide concentrations in air with 1 and 2% ammonia added. Beginning with ambient temperature and pressure, GASFLOW accurately calculated that the behaviors of both fuel-lean and fuel-rich mixtures for hydrogen are (1) little pressure rise for very low hydrogen concentrations, (2) downward flame propagation and nearly complete combustion for approximately 8% hydrogen, and (3) and maximum pressure for a stoichiometric (29.6% hydrogen) mixture. Good results were obtained for the mixtures where nitrous oxide was added, although the pressure rise rate was conservatively high by up to 20%. In conclusion, the one-step finite-rate chemical kinetics model yields good results but is limited. For more complex combustion problems, a reduced set of chemical kinetics mechanisms or a two-step method based on an induction parameter model should be used. Both improved models are derived from detailed chemical kinetics mechanisms.

The FLAME facility (1.8 m wide, 2.4 m high, 30 m long = 136 m³) at Sandia National Laboratories was used to study flame acceleration and deflagration-to-detonation transition of hydrogen-air mixtures. In experiment F-21, 13% hydrogen was added and mixed with a fan. After 30 min, gas samples indicated stratification ranging from 15% at an upper location to 10% at a lower location. The test was chosen to assess transient mixing and stratification calculations by GASFLOW, beginning with stagnant air and followed by hydrogen injection, mechanical mixing, and natural stratification. The algebraic turbulence model was used, and results were not very sensitive to the chosen turbulent length scale because mixing was largely achieved by molecular diffusion. GASFLOW showed that the hydrogen jet does not penetrate very far before it becomes a buoyant plume that gradually expands. At 100 s after injection ends, stratification is maximum (approximately 17% at the top and approximately 4% at the bottom) in the early part of the mixing phase, which lasted for 1800 s, or 30 min. When the gas samples were taken, GASFLOW calculated upper and lower volume fractions of 15.4% and 9.8%, respectively, within the reported uncertainty of 0.5%.

The Battelle Model Containment (BMC) Test GX6 was used to validate the catalytic recombiner model in GASFLOW. This test was conducted using the central cylindrical room R1/R3 and the annular segment compartments R5 through R8; these rooms were sealed off from the remainder of the BMC. Each compartment has a gas volume of 49 m³; the total for test GX6 was 209 m³. A Siemens catalytic recombiner was placed next to the inner wall of R5, not far from the opening to R6. Steam was injected into rooms R5, R6, and R7. Hydrogen was injected into R8. Ten hours of the test was calculated with GASFLOW. The calculated pressure was slightly higher than measured and stayed more level, indicating a combination of too much in-leakage in the calculation and slightly different boundary condition pressures. The drop in pressure at approximately 6 h into the transient, which was caused by terminating the inflow of steam, was calculated to be slightly earlier and larger. This drop indicated that the condensation rate in GASFLOW is slightly larger than is inferred from the test data. The overall agreement is good and captures the dominant trends in the data. Temperature comparisons at several different

locations are excellent and capture dominant trends in the data. In particular, the temperature rise through the recombiner was calculated quite accurately.

The BMC Test JX7, also known as HYJET, was used to validate the capability to model small- and large-scale effects of a turbulent jet and convection with containment within one calculation. This test used all of the rooms in the BMC, except the annular segment compartment R7, which has a total gas volume of 600 m^3 . Near the bottom of R6, a helium mass of 9.25 kg was injected vertically under the openings to R5 and to the dome over a period of 200 s. The nozzle had a diameter of 95 mm and an average injection velocity of 42 m/s. The jet from the nozzle extended all the way from the source location into the dome region, where the helium then stratifies as a cloud. Using a model with 50,000 computational cells, GASFLOW calculated the helium concentrations at four sensor locations: in the dome, near the bottom of the central room, and in the upper and lower parts of the ring room. In general, GASFLOW predicts the dominate trends well and predicts the helium stratification consistently with the data. Good agreement was obtained in the central room and in the lower part of the ring room. GASFLOW overpredicted the helium concentration in the dome region; this is attributed to insufficient air entrainment along the jet surface.

HDR Test T31.5, also known as an International Standard Problem, ISP-23, was used to validate the capability to model hydrogen and steam transport and distributions in a large-scale containment during a simulated large-break loss-of-coolant accident. The containment has a steel shell with a height of 60 m, an internal diameter of 20 m, and a free volume of $11,300 \text{ m}^3$. The containment has 72 compartments connected with about 200 passageways below the approximately 5000-m^3 volume of the open hemispherical-dome region. In this test, a blowdown from the pressure vessel injected 30,000 kg of a steam-water mixture over the first 50 s at the 22-m level. From 21 to 36 min, superheated steam was injected at a rate of 2.2 kg/s. From 36 to 48 min, a light gas (14% hydrogen and 85% helium) was injected. The GASFLOW model for T31.5 used 12,300 computational cells with obstacles and barriers to model all major floors and walls and all compartments. Heat structures were modeled extensively through the containment. An isentropic expansion model was used for the blowdown. GASFLOW predicts the dominate trends well for pressure, temperature, and concentration for this complex test.

Pressure peaks and rapid pressure equilibrium calculated by GASFLOW throughout the containment agreed quite well with the data. After 5 min, GASFLOW starts predicting a slower pressure decay, reaching a difference of 0.08 bars after about 15 min. One explanation is the lack of a film relocation model. The film vaporization model provides a continuous steam source that slows down the pressure decay; however, that should be cut off as dryout occurs. Calculated temperature histories reflect the somewhat higher asymptotic pressures. Calculated values are high by about 10°C in the middle and upper containment and by 20° to 25°C in the bottom containment. Three effects could cause high bottom temperatures; the most likely is that a significant amount of water collects in the

bottom, creating an additional heat sink, especially after passing over cold surfaces on the way down. GASFLOW calculations of light-gas concentrations in the spiral staircase and in the dome are in excellent agreement with data. In two places, GASFLOW concentrations vary significantly from the data. One is near the source, where concentration gradients vary strongly and the computational mesh is not fine enough to resolve them well. Another is at the bottom, where the concentration is very low (only about 0.5%).

Four steady-state tests (4A, 4B, 6A, and 10A) in the Phebus facility were used to validate the condensation model in GASFLOW. The facility (approximately 5.7 m high and 1.8 m in diameter = 10 m³) has a insulated double skinned wall through which coolant flows to maintain a homogeneous inner wall temperature of approximately 110°C. Inside the top part of the facility is (1) a wet condenser, which consists of three steel rods internally cooled to a specific temperature, and (2) a dry condenser, which is heated to prevent condensation. Initial conditions were air diluted with 39 vol % steam at 110°C and 1.9 bars. Steam sources for this set of tests varied from 1 g/s at 114°C and 1.65 bar to 4 g/s at 125°C and 2.3 bar, directly vertically upward from the bottom. A GASFLOW model of 715 computational cells modeled a 60-degree sector. Condensation parameters were set to standard values. The calculated final pressures during the condensation process were found to agree with the data within 1% to 5% for the various cases.

1 INTRODUCTION

1.1 Background

Combustion in nuclear facility buildings, such as light-water reactor (LWR) containments, can cause high pressures or temperatures that can, in turn, damage the containment or affect important safety-related equipment. After the Three Mile Island accident (a severe, or degraded-core, accident), it was found that significant quantities of hydrogen had been generated from the chemical reaction between the zirconium cladding (the thin protective covering of the nuclear fuel) and the water vapor. When released into the containment, this hydrogen burned by one or more combustion modes and threatened the containment integrity, internal structures, and safety-related equipment.

The principal design basis for containment integrity is peak pressure. Local temperature is important for the safe operation of instrumentation and equipment. Local concentrations of hydrogen, air, and water vapor are the important parameters for determining safe levels of hydrogen with respect to potential deflagration or detonation. Thus, the primary parameters of interest are pressure, temperature, and concentrations of gas species. A secondary parameter of interest is a concentration of aerosol particles. Containment pressure is usually of interest as a global parameter; however, the detailed spatial distribution of temperatures and concentrations is important for safety analyses.

It is common to differentiate between two types of multidimensional fluid dynamics codes. A "field code" uses correlations for wall flow resistance and heat transfer. A "computational fluid dynamics (CFD) code" calculates the heat and momentum transfer through the boundary layer at a wall instead of using correlations. Although GASFLOW is capable of calculating flow and heat transfer gradients near surfaces, thereby resolving boundary layers, noding for such calculations is too fine for use with full-size containment structures. Thus, for containment analyses, GASFLOW is characterized as a "field code."

Modeling the geometry of a containment building can be difficult. One example is a pressurized water reactor (PWR) containment, such as H. B. Robinson (Ref. 1-1), shown in Figure 1.1. The net free volume in the containment is 2,100,000 ft³. The containment cylinder and dome of steel-lined concrete has an area of 78,000 ft², of which 58,000 ft² is insulated, and is 30-42 in. thick. The top part of the containment is open, but the lower part is divided into compartments housing steam generators, pumps, reactor, and auxiliary equipment. Interior concrete walls, 12 in. thick, have an area of 165,000 ft². Interior steel walls and structures, 0.1 to 4.0 in. thick, have a surface area of 185,000 ft². All of these walls and surfaces serve as passive heat sinks. Active cooling equipment include two spray systems and four fan coolers.

Figure 1-1. Typical dry containment

Another example is the Heiss Dampf Reactor (HDR) containment (Ref. 1-2), shown in Figure 1-2, near Frankfurt, West Germany. Data from HDR Tests T31.5 and E11.2 were used for GASFLOW assessment. The HDR building is 60 m high and 20 m in diameter. It contains two stairwells, an elevator shaft, several vertical open hatchways, and ~70 rooms. This particular containment has roughly 11,300 m³ of free volume, or approximately one-sixth to one-eighth the free volume of a typical

Figure 1-2. Cross section of the Heiss Dampf Reactor near Frankfurt, Germany

United States (US) or German Konvoi-type pressurized water reactor (PWR) containment.

The US Department of Energy (DOE), the US Nuclear Regulatory Commission (NRC), and the German government and nuclear utility industry are supporting research at Los Alamos National Laboratory (LANL) and Forschungszentrum Karlsruhe to develop GASFLOW to evaluate design basis and beyond design basis severe accidents in nuclear reactor containments as well as in other nuclear facility buildings and the consequences on safety-related equipment and the containment

structure itself. Current research coordinates model development with validation using experiments performed in Germany, the European Communities, and the US.

1.2 Computational Methodology

This report documents the theoretical and computational aspects of GASFLOW, a finite-volume computer code for solving transient, three-dimensional (3D), compressible, Navier-Stokes equations for multiple gas species. The code is designed to be a best-estimate tool for predicting the transport, mixing, and combustion of hydrogen gas in nuclear reactor containments and other nuclear facility buildings and structures.

An example of GASFLOW's capabilities is shown in Figure 1-3. Here we show an arrangement of three cylindrical tanks and one small hexahedral tank connected by a complex ventilation system. The four tanks represent the independent multiblock computational domains, each composed of a single 3D array of cells. The one-dimensional (1D) ventilation system connecting the four tanks indicates the coupling of the tanks through attachments at external boundaries on the 3D blocks or at "T" junctions within the 1D network itself. Within the ventilation system, there are components that may be arbitrarily included. These components include fans or blowers, dampers or valves, and filters. With this additional capability, GASFLOW has modeled nuclear waste tank farm behavior and provided safety analyses for the DOE nuclear waste depository sites at Hanford, Washington.

GASFLOW is based on the governing physical laws and modeling assumptions that are described in Chapter 2. In Chapter 3, we describe the Los Alamos linearized Implicit Continuous-Fluid Eulerian Arbitrary-Lagrangian-Eulerian numerical methodology (ICE'd ALE) field-model approach that provides the basis of the computational method used to integrate the equations in time and space. Briefly, each computational step is divided into three phases.

- (1) An explicit Lagrangian phase computes changes in material volume, density, velocity, and internal energy caused by pressure gradients, combustion ignited with a generalized ignitor model, condensation and vaporization within the assumptions of the two-phase homogeneous equilibrium model, a structural two-phase heat transfer, catalytic recombiner hydrogen mitigation, structural heat conduction, and turbulence.
- (2) An implicit Lagrangian phase calculates pressures at the advanced time level by solving simultaneously for pressure, density, velocities, and internal energy.

Figure 1-3. Example of four independent multiblock computational volumes connected at each of the 3D volume's external boundaries by a complex ventilation system

- (3) A rezone phase computes the mass, momentum, and energy exchange between Eulerian cells that has occurred in the Lagrangian phase and repartitions or rezones these variables onto the original mesh.

The computational time step is completed with the evaluation of turbulence quantities—kinetic energy, dissipation, and viscosity—which are calculated explicitly. Then, the discrete particle transport, deposition, and entrainment governing equations are solved, independently of the fluid flow equations. Finally, a global analysis of the stability of the time step is performed.

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- 1-2 L. Wolf and L. Valencia, "Results of the Preliminary Hydrogen Distribution Experiment at HDR and Future Experiments for Phase III," 16th Water Reactor Safety Information Meeting, Gaithersburg, Maryland, October 1988, 189-222, Vol. 5, NUREG.CP-0097 (March 1989).

2 MATHEMATICAL AND PHYSICAL MODELS

The equations of motion for a compressible fluid are derived from the physical laws that require the conservation of mass, momentum, and energy. The equations of change, which are presented in this section, relate the dynamics of the fluid to temporal and spatial influences such as viscous stress, body force, turbulence, structural resistance, heat transfer, phase change, and combustion. This includes relations for the transport of individual gas species. An equation of state is included to relate pressure (p) to density (ρ), mixture temperature (T), and volume fraction occupied by the gaseous mixture (θ).

As suggested by the "ALE" name, GASFLOW uses both the Lagrangian and Eulerian methodologies. The Lagrangian (or material) specification considers specific elements of matter and describes the motion as functions of space (x) and time (t). This approach is useful because the conservation laws refer to specific parcels of matter. However, the Eulerian (or spatial) viewpoint is often more convenient because it describes flow in terms of volumes fixed in space. Because the computational method used to model the flow is facilitated by dividing the problem domain into parallelepiped Eulerian volumes (cells) in either Cartesian or cylindrical geometry, it is natural to present the continuous equations in integral form (Refs. 2-1 and 2-2). This makes it easier to see how the integration of continuous volume and surface integrals presented in this section is approximated by the discrete or finite-volume equations given in Chapter 3.

2.1 The Generalized Conservation Equation

The conservation of any arbitrary extensive variable (for example, mass, momentum, or energy) is

$$\frac{d}{dt} \int_V \Phi dV = \int_V S_\Phi dV, \quad (2-1)$$

where $\Phi(x, t)$ is any continuously summable function, V is a material volume, and S_Φ is a source term. We use the Reynolds Transport Theorem, which may be expressed as

$$\int_V \frac{\partial \Phi}{\partial t} dV = \oint_S \Phi(\mathbf{u} \cdot \mathbf{A}) dS + \int_V S_\Phi dV, \quad (2-2)$$

where $\mathbf{u}(x, t)$ is the fluid velocity and $\mathbf{A}$ and dS are the outward normal fractional area vector and differential area, respectively, of material surface S bounding V . We introduce the fractional area methodology of the FAVOR (Fractional Area Volume Obstacle Representation) algorithm due to Hirt (Ref. 2-3) to more easily and

accurately model variable flow areas involved in complex geometrical representations. Applying the transport theorem to an arbitrary control volume V^* (Ref. 2-2) (not necessarily a material volume) enclosed by surface S^* moving at velocity $\mathbf{b}$ gives

$$\frac{d}{dt} \int_{V^*} \Phi dV = \int_{V^*} \frac{\partial \Phi}{\partial t} dV + \oint_{S^*} \Phi (\mathbf{b} \cdot \mathbf{A}) dS + \int_{V^*} S_\Phi dV \quad (2-3)$$

If V^* is chosen to be instantaneously coincident with V , Equations (2-2) and (2-3) may be combined to give

$$\frac{d}{dt} \int_{V^*} \Phi dV = \oint_{S^*} \Phi (\mathbf{b} - \mathbf{u}) \cdot \mathbf{A} dS + \int_{V^*} S_\Phi dV \quad (2-4)$$

the integral form of the generalized conservation law. This is the basic kinematic relation used in the following three subsections and states that the time-rate-of-change of F in an arbitrary control volume V^* (left side) is equal to the inflow of F through the boundary plus the source term (right side). The term $\mathbf{b} - \mathbf{u}$ is the relative velocity between the control surface and the fluid. When $\mathbf{b} = \mathbf{u}$, we recover the Lagrangian form [Equation (2-1)]. For a control volume that is fixed with respect to the coordinate axes, $\mathbf{b} = 0$ and we recover the Eulerian form

$$\frac{d}{dt} \int_{V^*} \Phi dV = - \oint_{S^*} \Phi (\mathbf{u} \cdot \mathbf{A}) dS + \int_{V^*} S_\Phi dV \quad (2-5)$$

or

$$\int_{V^*} \frac{\partial \Phi}{\partial t} dV = - \oint_{S^*} \Phi (\mathbf{u} \cdot \mathbf{A}) dS + \int_{V^*} S_\Phi dV \quad (2-6)$$

2.2 The Mass Conservation Equations

The mixture mass conservation equation follows directly from Equation (2-4) by letting $\Phi = \rho$

$$\frac{d}{dt} \int_V \rho dV = \oint_S \rho (\mathbf{b} - \mathbf{u}) \cdot \mathbf{A} dS + \int_V S_\rho dV \quad (2-7)$$

where ρ is the mixture density or the sum of the macroscopic densities for each individual species; $\mathbf{u}$ is the mass-average velocity vector; and S_ρ is the mass source or sink due to condensation, vaporization, and liquid droplet depletion (rainout) per unit volume and time. Similarly, setting $\Phi = 1$ in Equation (2-4) gives an expression for the change in volume:

$$\frac{\partial V}{\partial t} = \oint_S \mathbf{b} \cdot \mathbf{A} dS \quad (2-8)$$

The transport equation for individual species α is given by

$$\frac{d}{dt} \int_V \rho_\alpha dV = \oint_S \rho_\alpha (\mathbf{b} - \mathbf{u}) \cdot \mathbf{A} dS - \oint_S (\mathbf{J}_\alpha \cdot \mathbf{A}) dS + \int_V S_{\rho,\alpha} dV \quad (2-9)$$

where α denotes the gas species, ρ_α is the mass per unit volume (macroscopic density), $\mathbf{J}_\alpha \cdot \mathbf{A}$ is the mass diffusion flux vector with Cartesian geometry components $(A_x J_{x,\alpha}, A_y J_{y,\alpha}, A_z J_{z,\alpha})$, and the source or sink term, $S_{\rho,\alpha}$, represents the species mass created or destroyed by chemical reactions and two-phase change dynamics of the liquid and vapor water components.

The diffusion of species α is represented by the second integral on the right side of Equation (2-9), which is often reported in the literature (Refs. 2-4 and 2-5) as

$$\mathbf{J}_\alpha \cdot \mathbf{A} = \begin{bmatrix} -A_x \rho D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial x} \left(\frac{\rho_\alpha}{\rho} \right) \\ -A_y \rho D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial y} \left(\frac{\rho_\alpha}{\rho} \right) \\ -A_z \rho D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial z} \left(\frac{\rho_\alpha}{\rho} \right) \end{bmatrix} \quad (2-10)$$

for Cartesian geometry, where $D_{\alpha \rightarrow \text{mix}}$ is the mass diffusion coefficient of species α into the gaseous mixture. The reader is referred to Sections 2.5.1.2 (Transport Properties) and 2.7.3 (Turbulence Effects on the Transport Coefficients) to see what models are used to compute molecular mass diffusion coefficients of the binary coefficients and what effects turbulence has on these coefficients, respectively.

It is essential that the diffusion fluxes identically sum to zero, so Equation (2-10) is

$$\sum_\alpha \mathbf{J}_\alpha \cdot \mathbf{A} = \sum_\alpha \sum_i -A_i \rho D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial x_i} \left(\frac{\rho_\alpha}{\rho} \right) \equiv 0 \quad (2-11)$$

As pointed out by Ramshaw (Ref. 2-6), the condition of Equation (2-11) is only exact for Equation (2-10) when binary mixtures are involved or for multicomponent mixtures when all the diffusion coefficients are equal. This is in general not the case

(see Ref. 2-6), so a correction to Equation (2-10) is incorporated that properly reflects the physical content of Equation (2-10) while providing full symmetry in all species:

$$\mathbf{J}_\alpha \cdot \mathbf{A} = \begin{Bmatrix} -A_x \left[cM_\alpha D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial x} \left(\frac{c_\alpha}{c} \right) - \left(\frac{c\rho_\alpha}{\rho} \right) \sum_\beta M_\beta D_{\beta \rightarrow \text{mix}} \frac{\partial}{\partial x} \left(\frac{c_\beta}{c} \right) \right] \\ -A_y \left[cM_\alpha D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial y} \left(\frac{c_\alpha}{c} \right) - \left(\frac{c\rho_\alpha}{\rho} \right) \sum_\beta M_\beta D_{\beta \rightarrow \text{mix}} \frac{\partial}{\partial y} \left(\frac{c_\beta}{c} \right) \right] \\ -A_z \left[cM_\alpha D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial z} \left(\frac{c_\alpha}{c} \right) - \left(\frac{c\rho_\alpha}{\rho} \right) \sum_\beta M_\beta D_{\beta \rightarrow \text{mix}} \frac{\partial}{\partial z} \left(\frac{c_\beta}{c} \right) \right] \end{Bmatrix} \quad (2-12)$$

When Equation (2-9) is summed over all species, the result is the mixture mass equation [Equation (2-7)].

2.3 The Momentum Transport Equations

The mixture-momentum conservation equations are given by

$$\begin{aligned} \frac{d}{dt} \int_V \rho \mathbf{u} dV = \oint_S \rho \mathbf{u} (\mathbf{b} - \mathbf{u}) \cdot \mathbf{A} dS \\ - \oint_S p d\mathbf{S} + \int_V \rho \mathbf{g} dV - \oint_S (\boldsymbol{\tau} \cdot \mathbf{A}) dS - \oint_S (\mathbf{D}_d \cdot \mathbf{A}) dS + \int_V \mathbf{S}_m dV \end{aligned} \quad (2-13)$$

where p is the pressure, $\boldsymbol{\tau}$ is the viscous stress tensor, $\mathbf{g}$ is the gravitational vector, $\mathbf{D}_d$ is the internal structure drag tensor, and $\mathbf{S}_m$ is a momentum source or group of sources, such as one or more fans. The right-side integrals represent, respectively, the flux of momentum through the control surface; the sum of pressure gradient, gravity, and viscous forces on the control volume; fluid drag forces acting on structural surfaces; and any additional momentum sources.

The Cartesian and cylindrical components of $\boldsymbol{\tau}$ for a Newtonian fluid are given in Tables 2-1 and 2-2, respectively. The components of $\mathbf{u}$ are (u, v, w) in the x -, y -, and z -directions (Cartesian coordinates) or r -, θ -, and z -directions (cylindrical coordinates); subscripts on $\boldsymbol{\tau}$ indicate the surface normal direction and the direction of the stress component.

The reader is referred to Sections 2.5.1.2 (Transport Properties) and 2.7.3 (Turbulence Effects on the Transport Coefficients) to see how the mixture viscosity is computed and what effects turbulence has on the viscosity, respectively. Here we have used the second viscosity coefficient, $\lambda = -2\mu/3$, which is equivalent to assuming the bulk viscosity to be zero.

Table 2-1. Stress tensor components for a Newtonian fluid (Cartesian coordinates)

$$\begin{aligned}\tau_{xx} &= -\mu \left[2 \frac{\partial u}{\partial x} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \right] & \tau_{xy} &= -\mu \left[\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right] \\ \tau_{yy} &= -\mu \left[2 \frac{\partial v}{\partial y} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \right] & \tau_{xz} &= -\mu \left[\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right] \\ \tau_{zz} &= -\mu \left[2 \frac{\partial w}{\partial z} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \right] & \tau_{yz} &= -\mu \left[\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right]\end{aligned}$$

Table 2-2. Stress tensor components for a Newtonian fluid (cylindrical coordinates)

$$\begin{aligned}\tau_{rr} &= -\mu \left[2 \frac{\partial u}{\partial r} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \right] & \tau_{r\theta} &= -\mu \left[r \frac{\partial}{\partial r} \left(\frac{v}{r} \right) + \frac{1}{r} \frac{\partial u}{\partial \theta} \right] \\ \tau_{\theta\theta} &= -\mu \left[2 \left(\frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right) - \frac{2}{3} (\nabla \cdot \mathbf{u}) \right] & \tau_{z\theta} &= -\mu \left[\frac{\partial v}{\partial z} + \frac{1}{r} \frac{\partial w}{\partial \theta} \right] \\ \tau_{zz} &= -\mu \left[2 \frac{\partial w}{\partial z} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \right] & \tau_{rz} &= -\mu \left[\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \right]\end{aligned}$$

2.4 The Internal Energy Transport Equation

The equation of change for total internal energy is

$$\begin{aligned}\frac{d}{dt} \int_V \rho I dV &= \oint_S \rho I (\mathbf{b} - \mathbf{u}) \cdot \mathbf{A} dS \\ &\quad - \oint_S p (\mathbf{u} \cdot \mathbf{A}) dS - \int_V \left[\frac{p}{V} \frac{\partial V_{h_2o}}{\partial t} \right] dV - \oint_S (\mathbf{q} \cdot \mathbf{A}) dS + \int_V S_I dV \quad ,\end{aligned}\tag{2-14}$$

where I is the mixture specific internal energy, and S_I is the energy source or sink per unit volume and time as a result of combustion, phase change, and energy exchange with internal structures, floors, ceilings, and walls. Because phase-change effects can dominate the $p \nabla \cdot \mathbf{u}$ work term, we must account for the remaining gas in

a computational cell expanding or compressing into the volume change associated with the phase change process. We account for this effect by using the ideal gas equation of state to arrive at

$$\frac{p}{V} \frac{\partial V_{h_2o}}{\partial t} = -R_{h_2o} T S_{\rho, h_2o} ,$$

where R_{h_2o} is the gas constant for steam, T is the gas mixture temperature, V_{h_2o} is the steam volume, and S_{ρ, h_2o} is the sum of all steam mass per unit time lost or gained due to phase change in the fluid mixture and to mass transfer on all surfaces internal to or bounding the computational cell V . Note that S_{ρ, h_2o} is the same mass source per unit volume and time as Equation (2-7), i.e., the water vapor component conservation equation. The energy flux vector $\mathbf{q}$ is given by

$$\mathbf{q} \cdot \mathbf{A} = \begin{Bmatrix} -A_x \left[\phi_x \frac{\partial T}{\partial x} - \sum_{\alpha} h_{\alpha} J_{x,\alpha} \right] \\ -A_y \left[\phi_y \frac{\partial T}{\partial y} - \sum_{\alpha} h_{\alpha} J_{y,\alpha} \right] \\ -A_z \left[\phi_z \frac{\partial T}{\partial z} - \sum_{\alpha} h_{\alpha} J_{z,\alpha} \right] \end{Bmatrix} , \quad (2-15)$$

where ϕ_i is the molecular conductivity and h_{α} is the enthalpy for species α . The reader is referred to Sections 2.5.1.2 (Transport Properties) and 2.7.3 (Turbulence Effects on the Transport Coefficients) to see what models are used to compute the mixture conductivity and what effects turbulence has on these coefficients, respectively.

2.5 Constitutive Relationships

2.5.1 Thermochemical and Transport Properties

GASFLOW 2.1 has incorporated a library of 25 species, which are listed in Table 2-3. Two of them are gas mixtures: (1) air, a mixture of 79% nitrogen and 21% oxygen and (2) LG, a "light-gas" consisting of a mixture of 15% hydrogen and 85% helium. Some of the species are not stable molecules, for example, H, O, and OH, but they are included because of the possibility of implementing detailed hydrogen-oxygen chemical kinetics mechanisms which require intermediate reaction species.

Two of the species are not gases: (1) H_2O_l , which is the water liquid component required for the two-phase homogenous equilibrium model, and (2) C, which is solid carbon or soot being produced in the event of hydrocarbon combustion.

Table 2-3. Gas properties at temperature equaling 298.15 K [extracted from the JANAF (Ref. 2-7) Tables]

Species	Molecular Weight M_α (g/mole)	Gas Constant R_α (J/g-K)	Specific Heat $C_{v,\alpha}$ (J/g-K)	Enthalpy of Formation $h_{f,\alpha}^\circ$ (J/g)
H ₂	2.01588	4.12416	10.179479	0.000
O ₂	31.99880	0.25983	0.658068	0.000
N ₂	28.01340	0.29680	0.742878	0.000
air	28.85033	0.28819	0.723125	0.000
He	4.00260	2.07705	3.115522	0.000
LG	3.70459	2.24411	3.690719	0.000
H ₂ O	18.01528	0.46150	1.402215	-13422.869
OH	17.00734	0.48886	1.274294	2320.372
H	1.00794	8.24856	12.373200	216262.790
O	15.99940	0.51964	0.849832	15574.679
HO ₂	33.00674	0.25189	0.805014	633.786
H ₂ O ₂	34.01468	0.24442	1.023102	-4001.221
NH ₃	17.03052	0.48820	1.603728	-2695.058
NH ₂	16.02258	0.51891	1.576402	10471.333
NH	15.01464	0.55374	1.387406	22571.525
HNO	31.01404	0.26807	0.848757	3210.575
N ₂ O	44.01280	0.18889	0.688477	1864.055
NO	30.00610	0.27707	0.717481	3008.888
CH ₄	16.04276	0.51825	1.703236	-4667.000
CO	28.01040	0.29683	0.743551	-3946.416
CO ₂	44.00980	0.18892	0.654727	-8941.658
Ar	39.94800	0.20813	0.312192	0.000
Xe	131.29	0.06333	0.094993	0.000
H ₂ OI	18.01528	0.00000	4.179300	-15865.897
C	12.01100	0.00000	0.017708	0.000

2.5.1.1 Internal Energy and Specific Heats

The specific internal energy of species α is related to the temperature by

$$I_\alpha = (I_{reference})_\alpha + \int_{T_{reference}}^T (C_v)_\alpha dT \quad , \quad (2-16)$$

where we have arbitrarily defined our reference temperature 298.15 K and set the reference internal energy equal to zero.

One can approximate the specific heat in Equation (2-16) by polynomials of various degrees. In fact, Gordon and McBride (Ref. 2-8), basing their approximations on the JANAF Tables (Ref. 2-9), give specific heats at constant pressure as a function of temperature in the form of least squares coefficients as follows:

$$\frac{C_p^o}{\mathcal{R}} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (2-17)$$

We have based the GASFLOW approximations for the specific heats at constant volume upon polynomials of up to the third degree. When Equation (2-16) is then integrated for the species specific internal energy, we approximate the resulting fifth-degree polynomial with a polynomial of up to the fourth degree,

$$I_\alpha = a_\alpha + b_\alpha T + c_\alpha T^2 + d_\alpha T^3 + e_\alpha T^4 \quad (2-18)$$

which allows analytically inverting this function for the temperature field when the internal energy and species densities are known. Therefore, GASFLOW provides the possibility of internal energy as a function of temperature representation from linear to the fourth-degree polynomial shown in Equation (2-18). It must be stated that the selection of accuracy, i.e., the degree of the polynomial, is related to the computer time to invert Equation (2-18), and the user will be reminded of this fact in the User's Manual.

The total specific internal energy then is given by

$$\begin{aligned} I &= \sum_{\alpha} x_{\alpha} I_{\alpha} = \\ &= \sum_{\alpha} x_{\alpha} a_{\alpha} + T \sum_{\alpha} x_{\alpha} b_{\alpha} + T^2 \sum_{\alpha} x_{\alpha} c_{\alpha} + T^3 \sum_{\alpha} x_{\alpha} d_{\alpha} + T^4 \sum_{\alpha} x_{\alpha} e_{\alpha} = \\ &= \sum_{\alpha} x_{\alpha} a_{\alpha} + T \left\{ \sum_{\alpha} x_{\alpha} b_{\alpha} + T \left[\sum_{\alpha} x_{\alpha} c_{\alpha} + T \left(\sum_{\alpha} x_{\alpha} d_{\alpha} + T \sum_{\alpha} x_{\alpha} e_{\alpha} \right) \right] \right\} \quad (2-19) \end{aligned}$$

where x_{α} is the mass fraction for species α . In order that homogeneous equilibrium model thermodynamics be correct, the expression for the liquid water specific internal energy is derived such that the difference between the vapor and liquid specific internal energies is matched by the same difference between the vapor and liquid saturation curve from the steam tables (Ref. 2-10).

We recommend, for consistency between Equations (2-17) and (2-18), that each species' specific heat be obtained by differentiating Equation (2-18) with respect to temperature, but there are other possibilities that will be described in the User's Manual.

The interrelationships between enthalpy, internal energy, and specific heats are given by the usual thermodynamic relations

$$I_{\alpha} = h_{\alpha} - R_{\alpha}T$$

$$C_{v,\alpha} = C_{p,\alpha} - R_{\alpha}$$

2.5.1.2 Transport Properties

The molecular transport properties, i.e., heat conductivities, dynamic viscosities, and binary diffusion coefficients, for all gaseous species are included in the GASFLOW properties library. We have used the data base of the CHEMKIN (Ref. 2-11) code to provide the GASFLOW relationships. We use the CHEMKIN model

$$\ln(\Psi) = a_0 + a_1 \ln(T) + a_2 \ln(T)^2 + a_3 \ln(T)^3 + a_4 \ln(T)^4 \quad (2-20)$$

for the desired transport property Ψ , as well as perhaps less accurate, but simplified polynomials discussed in the User's Manual.

When the individual transport properties are determined, the mixture values can also be computed. For the mixture thermal conductivity, the relationship of Mathur et al. (Ref. 2-12), is used:

$$\phi = \frac{1}{2} \left(\sum_{\alpha=1}^N Y_{\alpha} \phi_{\alpha} + \frac{1}{\sum_{\alpha=1}^N Y_{\alpha} / \phi_{\alpha}} \right) \quad (2-21)$$

The modified semi-empirical formulas of Wilke (Ref. 2-13), modified by Bird et al. (Ref. 2-4), can be used to compute the mixture viscosity as

$$\mu = \sum_{\alpha=1}^N \frac{Y_{\alpha} \mu_{\alpha}}{\sum_{\beta=1}^N Y_{\alpha} \Phi_{\alpha\beta}} \quad (2-22)$$

where

$$\Phi_{\alpha\beta} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_{\alpha}}{M_{\beta}} \right)^{-\frac{1}{2}} \left[1 + \left(\frac{\mu_{\alpha}}{\mu_{\beta}} \right)^{\frac{1}{2}} \left(\frac{M_{\beta}}{M_{\alpha}} \right)^{\frac{1}{4}} \right]^2 \quad (2-23)$$

We determine the diffusion coefficient of species α into the mixture by the following well-known relationship (Ref. 2-14):

$$D_{\alpha \rightarrow \text{mixture}} = \frac{\sum_{\beta \neq \alpha} Y_{\beta}}{\sum_{\beta \neq \alpha} Y_{\beta} / D_{\alpha \rightarrow \beta}} \quad (2-24)$$

2.5.2 Equation of State

The pressure field, p , is obtained by applying the Gibbs-Dalton law of partial pressures to an ideal gas mixture in the available gas volume (void volume):

$$p = \frac{T \sum_{\alpha}^{h_2, ol} R_{\alpha} \rho_{\alpha}}{1 - \theta} = \frac{\rho T \sum_{\alpha}^{h_2, ol} R_{\alpha} x_{\alpha}}{1 - \theta} \quad (2-25)$$

where R_{α} is the gas constant for species α . The volume fraction, θ , of the gas phase is computed from

$$\theta = 1 - \frac{\rho_{h_2, ol}}{\rho_{h_2, ol}^{thermo}} \quad (2-26)$$

where the thermodynamic liquid water density, $\rho_{h_2, ol}^{thermo}$, is usually approximated as a constant value of 1 g/cm³.

2.6 Heat-Transfer and Phase-Change Relationships

Heat transfer between a gas mixture and a structure may occur by three means: convection, condensation (or evaporation), and radiation. GASFLOW contains models convection and condensation. A user may add a radiation model by coding the FORTRAN as part of the input model. Within a gas mixture, heat transfer may occur between the gas and liquid phases, and a liquid phase may be depleted through droplet rainout.

2.6.1 Gas-Structure Heat Transfer

The convective heat exchange between a gas mixture and a solid boundary (referred to generically as a wall, but it may in fact be, in addition, a ceiling, floor, or internal structure) is given by

$$\int_V S_{I, convection} dV = \sum_s h_s A_s (T_s - T) \quad (2-27)$$

where T_s is the structure surface temperature, T is the gas temperature, h_s is the heat-transfer coefficient between the gas mixture and the internal structures, and A_s is the cell face area for walls or the exposed area for internal structures in a computational cell. The rate of thermal energy delivered to the wall surface, $q_{s,convection}$, has the opposite sign of energy flow to the gas mixture, so the thermal energy delivery rate becomes

$$q_{s,convection} = h_s A_s (T - T_s) \quad (2-28)$$

The thermal boundary layer is taken into account by using a modified Reynolds analogy formulation (Ref. 2-15), which is simplified and combined with a Chilton-Colburn empirical analogy (Ref. 2-4) between the momentum and thermal boundary layers to obtain the heat-transfer coefficient:

$$h_s = \frac{\tau_s}{|\mathbf{u}_c|} C_p \cdot \text{Pr}^{-\frac{2}{3}} \quad (2-29)$$

See Section 2.6.6 (Wall Shear Stress) below for a more detailed discussion of this heat-transfer coefficient.

The rates of heat transfer and condensation increase when the mass fraction of steam becomes a relatively large fraction of the mass of the gas mixture. As the mass-transfer rate increases, the thermal and concentration boundary layers become thinner because of the suction effect of the condensation process. This reduction in the boundary layer thickness further increases the temperature and concentration gradients near the boundary and consequently increases the heat- and mass-transfer coefficients. The opposite effect occurs at a surface where vaporization of a liquid film is taking place; hence, the heat- and mass-transfer coefficients decrease during these conditions. Bird, Stewart, and Lightfoot (Ref. 2-4, Section 21.5) develop correction factors based on film theory that can be used to determine the increase in the heat- and mass-transfer coefficients. The corrected heat-transfer coefficient then becomes

$$h_s^* = \Theta_T h_s \quad (2-30)$$

where

$$\Theta_T = \frac{\phi_T}{e^{\phi_T} - 1} \quad (2-31)$$

and the rate factor, ϕ_T , is given by

$$\phi_T = \frac{-\dot{m}_s C_{p,h_2o}}{h_s A_s} \quad (2-32)$$

where $\dot{m}_s$ is the wall condensation or vaporization rate, equal to one of the surface contributions involving the term $\int_V S_{p,h_2o} dV$ in Equation (2-9), and C_{p,h_2o} is the specific heat of the water vapor at constant pressure. Note that in the presence of condensing water vapor, ϕ_T is negative which increases the correction factor, Θ_T and the heat-transfer coefficient, h_w^* ; the opposite effect occurs during evaporation of a surface film when ϕ_T is positive. The internal structure heat-transfer coefficient is computed in an analogous fashion.

2.6.2 Condensation and Vaporization

Phase change between the gas and structures can occur on any structural surface (walls, ceiling, floors, and internal structures) can occur under one of these two conditions: (1) the surface temperature is less than the saturation temperature of the water vapor next to the surface (condensation), or (2) condensate exists on any given structural surface and the condensate surface (i.e., the surface temperature as well) is greater than the saturation temperature of the gas mixture adjacent to the surface (vaporization).

The phase-change rate on any structural surface is described as

$$\dot{m}_s = h_d^* A_s (\rho_{h_2o} - \rho_{s,saturation}) \quad , \quad (2-33)$$

where h_d^* is the corrected mass-transfer coefficient, ρ_{h_2o} is the water vapor density in the gas mixture, and $\rho_{s,saturation}$ is the saturation water vapor density at the structural surface conditions.

The saturation density in the above relationship is computed from the saturation pressure and the structural surface temperature by

$$\rho_{s,saturation} [T_s, p_{s,saturation}(T_s)] = \frac{p_{s,saturation}(T_s)}{R_{h_2o} \cdot T_s} \quad , \quad (2-34)$$

where the saturation pressure as a function of temperature is evaluated from the integrated Clausius-Clapeyron equation for the water component saturation curve in the form

$$p_{sat}(T) = 10^6 \cdot e^{\frac{-c_1 + c_2 \cdot T}{c_3 \cdot T}} \quad , \quad (2-35)$$

and the coefficients are defined

$$\begin{aligned}
c_1 &= 2258.0 \\
c_2 &= 6.05963 \\
c_3 &= 0.4579742
\end{aligned}
\tag{2-36}$$

The mass-transfer coefficient, h_d , then can be expressed in terms of the heat-transfer coefficient, h_s (Ref. 2-16), as

$$h_d = \frac{h_s}{\rho C_p} \frac{Sc^{-\frac{2}{3}}}{Pr^{-\frac{2}{3}}} \tag{2-37}$$

when we make use of a Chilton-Colburn empirical analogy between heat and mass transfer (Ref. 2-4).

Following similar ideas as with the heat-transfer coefficient for relatively large steam mass fractions, we correct the mass-transfer coefficient by

$$h_d^* = \Theta_m h_d, \tag{2-38}$$

where

$$\Theta_m = \frac{\log(R+1)}{R}, \tag{2-39}$$

and the flux ratio R is expressed as

$$R = \frac{n_{s,h_2o} - n_{h_2o}}{1 - n_{s,h_2o}}, \tag{2-40}$$

where n_{s,h_2o} is the steam mole fraction at the wall, and n_{h_2o} is the steam mole fraction in the gas mixture.

For the situation where "dryout" of a surface may occur, i.e., the liquid film totally evaporates leaving the surface dry, a better formulation of the surface mass transfer equation (2-33) is

$$\dot{m}_s = \max \left[-\frac{\delta A_s \rho_{h_2o}^{thermo}}{2 \Delta t}, h_d^* A_s (\rho_{h_2o} - \rho_{s,saturation}) \right], \tag{2-41}$$

where δ is the film thickness and Δt is the computational time step in seconds. Note the sign of Equation (2-41): positive indicates condensation, whereas negative means vaporization of the liquid film, where, at the point of near dryout, we allow only half of the available film to evaporate in a time step. The first term inside the

max function in Equation (2-41) represents the total mass of liquid in the film on a given heat structure surface, divided by two times the time step size. This max function ensures that the model will not evaporate all of the liquid film in a single time step for this heat structure. Note that the film thickness is calculated based on the mass of liquid film calculated to be on a heat-transfer surface and the liquid phase density and the available heat-structure surface area (i.e. film thickness = mass of liquid film/liquid phase density/heat structure surface area). The mass of liquid film on a given heat-structure surface is calculated based on the mass conservation equation for the liquid film including all sources and sinks for the liquid film. The total mass source or sink term due to phase change involving structural surfaces in Equations (2-7) and (2-9) for all surfaces then becomes

$$\int_V S_{\rho, h_2o, condensation/vaporization} dV = - \sum_s \max \left[-\frac{\delta A_s \rho_{h_2o}^{thermo}}{2\Delta t}, h_d^* A_s (\rho_{h_2o} - \rho_{s, saturation}) \right] . \quad (2-42)$$

The amount of energy resulting from phase change and the structural wall surface is then

$$q_{s, condensation/vaporization} = \max \left[\begin{array}{l} -\frac{\delta A_s \rho_{h_2o}^{thermo}}{2\Delta t} I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o} - \rho_{s, saturation}) I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o} - \rho_{s, saturation}) I_{h_2o}(T) \end{array} \right] , \quad (2-43)$$

where $I_{h_2o}(T)$ is the specific internal energy of the water vapor in the computational cell adjacent to the wall with volume V_c , and $I_{h_2o}(T_s)$ is the specific internal energy of the liquid water film that is on the surface. (Note that we assume the film temperature is equal to the surface temperature of the wall.) In this case, the energy lost or gained in the gas mixture is

$$\int_V S_{I, condensation/vaporization} dV = - \sum_s \max \left[\begin{array}{l} -\frac{\delta A_s \rho_{h_2o}^{thermo}}{2\Delta t} I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o} - \rho_{w, saturation}) I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o} - \rho_{s, saturation}) I_{h_2o}(T) \end{array} \right] . \quad (2-44)$$

2.6.3. Phase Change in the Fluid Mixture—The Homogeneous Equilibrium Model (HEM)

The Homogeneous Equilibrium Model (HEM) assumes that within a given cell, that the noncondensable gases, steam, and water droplets are well mixed and that the

mixture, given enough time, will reach an equilibrium state with the non-condensable gases, steam, and water droplets at the same temperature, and the density of the steam will correspond to the saturation density at the saturation pressure of the cell. During a transient calculation, nonequilibrium conditions can occur because of changes in the system pressure, injection of steam, condensation of steam as a film on heat structures, evaporation of liquid water from the film on heat structures, etc. However, the HEM predicts that the mixture of gases, steam, and water droplets will attempt to move back toward an equilibrium condition by either condensation of steam or evaporation of water droplets. The rate at which the mixture approaches equilibrium is determined by the phase or mass exchange models. It should be noted that the dropout model is not explicitly contained within the HEM, but rather is an attempt to address the experimental observations that water droplet density entrained within a noncondensable gas/steam mixture is finite and cannot grow without bounds.

The nonequilibrium phase exchange function between the vapor and liquid phases is presented here as a relaxation-type function. The mass exchange between the phases, shown as a source and sink term in Equation (2-9), is given for the water vapor phase by

$$\int_V S_{\rho, h_2o, fluid} dV = VC [\rho_{saturation}(T, p_{saturation}) - \rho_{h_2o}] \quad (2-45)$$

and for the water liquid phase as

$$\int_V S_{\rho, h_2ol, fluid} dV = -VC [\rho_{saturation}(T, p_{saturation}) - \rho_{h_2o}] \quad (2-46)$$

where the saturation pressure is again given by

$$p_{saturation}(T) = 10^6 \cdot e^{\frac{-c_1 + c_2 \cdot T}{c_3 \cdot T}} \quad (2-47)$$

and the saturation density is then computed by

$$\rho_{saturation}(T, p_{saturation}) = \frac{p_{saturation}(T)}{R_{h_2o} \cdot T} \quad (2-48)$$

The relaxation coefficient C , which has units of inverse time, is a user input value (see **cbulkrlx** in the User's Manual), but GASFLOW checks to see if this input value produces an acceptable stable solution for the current time step. The relaxation coefficient C , is related to rate at which a nonequilibrium mixture (i.e. superheated steam injected into an air environment) relaxes back to an equilibrium condition and must be specified based on experimental data.

The work due to the production or loss of steam on the internal energy control volume in Equation (2-12) can now be computed from

$$\begin{aligned}
 -\int_V \left[\frac{p}{V} \frac{\partial V_{h_2o}}{\partial t} \right] dV &= \int_V \left[R_{h_2o} T S_{h_2o} \right] dV = R_{h_2o} T \int_V S_{h_2o} dV = \\
 &= R_{h_2o} T \left[\int_V S_{\rho, h_2o, \text{condensation/vaporization}} dV + \int_V S_{\rho, h_2o, \text{fluid}} dV \right] = \\
 &= R_{h_2o} T \left\{ -\sum_s \max \left[-\frac{\delta A_s \rho_{h_2o}^{\text{thermo}}}{2 \Delta t}, h_d^* A_s (\rho_{h_2o} - \rho_{s, \text{saturation}}) \right] \right. \\
 &\quad \left. + VC [\rho_{\text{saturation}}(T, p_{\text{saturation}}) - \rho_{h_2o}] \right\} \quad (2-49)
 \end{aligned}$$

2.6.4 Droplet Depletion or Droplet "Rainout"

When the nonequilibrium phase exchange function between the vapor and liquid phases is active, conditions may exist that could produce large amounts of liquid water (water droplets). It has been observed experimentally that a certain droplet loading rainout of liquid droplets will occur. This can be simulated with a relaxation-type function, where the liquid droplet mass, when the liquid water exceeds a certain loading, relaxes toward the accepted loading value. The loss or sink term to account for this event in Equation (2-9) is given for the liquid phase by

$$\int_V S_{\rho, h_2ol, \text{mixture}} dV = VC_{h_2ol, \text{mixture}} \cdot \min[0, (\rho_{h_2ol, \text{max}} - \rho_{h_2ol})] \quad (2-50)$$

The relaxation coefficient, $C_{h_2ol, \text{mixture}}$, which has units of inverse time, and the maximum loading density, $\rho_{h_2ol, \text{max}}$, are user input values (see **crelax** and **rholiqmx**, respectively, in the User's Manual), but GASFLOW checks to see if these input values produce an acceptable stable solution for the current time step.

The loss of droplets on the internal energy control volume in Equation (2-12) can now be computed from

$$\int_V S_{I, \text{rainout}} dV = VC_{h_2ol, \text{mixture}} \cdot \min[0, (\rho_{h_2ol, \text{max}} - \rho_{h_2ol})] \cdot I_{h_2ol}(T) \quad (2-51)$$

2.6.5 Structural Heat Conduction

For every computational cell side interfacing with a wall, ceiling, or floor and any defined distributed heat sinks, the 1D transient heat-conduction equation

$$\frac{\partial}{\partial t} \int_V q dV = \int_S k \frac{\partial T}{\partial x} dS \quad (2-52)$$

with the wall boundary condition from Equations (2-28) and (2-43)

$$q_{s,convection} + q_{s,condensation/vaporization} = -kA_s \left. \frac{\partial T_w}{\partial x} \right|_{x=s} \quad (2-53)$$

is solved from the temperature distribution, $T_w(x,t)$, and the wall surface temperature, T_s . The term k in Equations (2-52) and (2-53) is the thermal conductivity of the structure. On the left side of Equation (2-53), the two terms represent energy delivered to a wall section by convection and phase change, respectively.

A detailed development of the structural heat conduction is presented in Appendix B.

2.6.6 Wall Shear Stress

The heat-transfer coefficient expression [Equation (2-29)] contains the computational cell-centered average velocity, $\mathbf{u}_c$, a vector with the two wall tangential velocity components, and the wall shear stress, τ_s , which is related to the fluid density and the wall shear speed, u_* , by

$$\tau_s = \rho u_*^2 \quad (2-54)$$

If GASFLOW were used as a CFD code, we could resolve the boundary layer with a fine computing mesh. However, for engineering problems involving a nuclear containment or other facility, GASFLOW is used as a field code, and a practical computing mesh is too large to resolve a turbulent boundary layer near a solid wall. Thus, we match our solution near solid boundaries or internal structures with the turbulent law-of-the-wall (Ref. 2-17):

$$\frac{|\mathbf{u}_c|}{u_*} = A \ln \left(\frac{y_c u_*}{\nu} \right) + B \quad (2-55)$$

This expression requires an iterative solution for u_* . We find that it is more convenient and almost as accurate to use an approximation obtained by replacing u_* in the argument of the logarithm in Equation (2-55) by the one-seventh-power law (Ref. 2-18). The one-seventh-power law may be rearranged to give

$$\frac{y_c u_*}{\nu} = 0.15 \left(\frac{y_c |\mathbf{u}_c|}{\nu} \right)^{\frac{7}{8}} \quad (2-56)$$

which yields

$$\frac{|u_c|}{u_*} = 2.19 \ln \left(\frac{y_c |u_c|}{\nu} \right) + 0.76 \quad (2-57)$$

when substituted into Equation (2-55) and when $A = 2.5$ and $B = 5.5$. It is now straightforward to find the shear speed, u_* , where y_c is the distance from the wall to the cell-centered average tangential speed, $|u_c|$, and ν is the gas mixture molecular kinematic viscosity.

The local Reynolds number, $(y_c |u_c| / \nu)$, may be small, indicating that the cell center lies in the laminar sub layer and the law-of-the-wall formulation is not valid. In this case, Equation (2-57) is replaced by the corresponding laminar formula:

$$\frac{|u_c|}{u_*} = \left(\frac{y_c |u_c|}{\nu} \right)^{\frac{1}{2}} \quad (2-58)$$

The transition between Equations (2-57) and (2-58) is made at the value where they predict the same wall surface shear speed, u_* , which is $(y_c |u_c| / \nu) = 130.7$. Therefore, u_* is calculated by Equation (2-57) when $(y_c |u_c| / \nu) \geq 130.7$ and by Equation (2-58) when $(y_c |u_c| / \nu) < 130.7$. In the laminar case, the wall heat-transfer coefficient [Equation (2-29)] reduces to $h_w = \rho \nu C_p / y_c$, which results in a simple difference approximation to the laminar heat flux for a molecular Prandtl number of unity when substituted into Equation (2-28).

Therefore, the uncorrected heat-transfer coefficient calculated from Equation (2-29) becomes

$$h_s = \begin{cases} \frac{\nu \rho C_p}{y_c}, & \frac{y_c |u_c|}{\nu} < 130.7 \\ \frac{\rho C_p |u_c|}{\left[2.19 \ln \left(\frac{y_c |u_c|}{\nu} \right) + 0.76 \right]^2 \text{Pr}^{\frac{2}{3}}}, & \frac{y_c |u_c|}{\nu} \geq 130.7 \end{cases} \quad (2-59)$$

2.7 Turbulence Modeling

Most flows of engineering interest, including the flows of concern here, are turbulent. Turbulence may be described qualitatively as the superposition of an irregular fluctuating motion on the mean flow, which, for an arbitrary variable y , may be expressed as

$$\psi(\mathbf{x}, t) = \bar{\psi}(\mathbf{x}) + \psi'(\mathbf{x}, t) \quad , \quad (2-60)$$

where ψ is the instantaneous value, ψ' is the fluctuating (turbulent) component, and $\bar{\psi}$ is the mean value defined as time average

$$\bar{\psi}(\mathbf{x}) = \lim_{t \rightarrow \infty} \frac{1}{t} \int_{t_0}^{t_0+t} \psi(\mathbf{x}, t) dt \quad . \quad (2-61)$$

In practice, t is taken to be much larger than the characteristic times associated with ψ' . Formally, this time Reynolds averaging is only appropriate for stationary turbulence (Ref. 2-19). In practice, virtually all the problems involving turbulent flows that we are interested in are classified as inhomogeneous turbulent flows. Therefore, in order to make use of the Reynolds-averaged equations, we assume nearly stationary or quasi-stationary turbulent conditions, which are discussed below.

When the instantaneous values of p , ρ , μ , and u_i ($u_i \equiv u, v, w$ for $i = 1, 2, 3$) are substituted into the mixture-momentum equations [Equation (2-13)], the resulting equations contain additional products of terms involving u'_i , $\bar{u}_i$, ρ' , and $\bar{\rho}$. The terms $-\bar{\rho} u'_i u'_j$, called the Reynolds stresses, are the focus of attention in the turbulent equations. [Other correlations such as $\bar{u}_i \rho' u'_j$ are discussed, for example, by Cebeci and Smith (Ref. 2-20, Chapter 2).] Defining $-\bar{\rho} u'_i u'_j$ as the components of the turbulent stress tensor τ_t and combining them with the laminar viscous stress, $\bar{\tau}$, the total stress tensor may be written as

$$\tau = \bar{\tau} + \tau_t \quad . \quad (2-62)$$

The effect of τ_t in most flows is a large increase in the apparent (turbulent) resistance of the flow; in other words, τ_t results in increased momentum transport. With the addition of the unknown turbulence quantities, Equations (2-9), (2-13), and (2-14) no longer form a closed set and modeling τ_t becomes the major problem in simulating turbulent motion.

To understand the general approach to modeling τ_t , it is useful to consider two observations about the eddies that characterize the turbulent motion. First, the largest eddies (whose size is determined by the geometry of the flow) carry most of the turbulent kinetic energy. The smallest eddies, with sizes determined by molecular viscosity, dissipate turbulent kinetic energy. The qualitative dynamics of the eddies and their interaction with the mean flow are described by Rodi (Ref. 2-21):

The large eddies interact with mean flow (because the scales of both are similar), thereby extracting kinetic energy from the mean motion and

feeding it into the large-scale turbulent motion. The eddies can be considered as vortex elements which stretch each other. Due to this vortex stretching, which is an essential feature of the turbulent motion, the energy is passed on to smaller and smaller eddies until viscous forces become active and dissipate the energy. This process is called energy cascade. The rate at which mean-flow energy is fed into the turbulent motion is determined by the large-scale motion; only this amount of energy can be passed on to smaller scales and finally be dissipated. Therefore, the rate of energy dissipated is also determined by the large-scale motion although dissipation is a viscous process and takes place at the smallest eddies. It is important to note that viscosity does not determine the amount of dissipated energy but only the scale at which dissipation takes place. The smaller the effective viscosity (i.e., the larger the Reynolds number), the smaller are the dissipative eddies relative to the large-scale eddies. When buoyancy forces are present, there is also an exchange between potential energy of the mean flow and turbulent kinetic energy, which can go in both directions but is also effected through the large-scale motion.

The preceding observations are the basis for modeling the effects of turbulence on the mean flow, specifically in choosing the relevant velocity and length scales that characterize the local state of turbulence. Postulating an analogy between laminar stresses and Reynolds stresses (Boussinesq's idea), that is,

$$(\tau_{ij})_t = -\overline{\rho u_i' u_j'} = \mu_t \frac{\partial u_i}{\partial x_j} \quad , \quad (2-63)$$

the turbulence closure problem is seen as one of finding a turbulent or eddy viscosity μ_t . The effects of turbulence on the mean flow come down to modeling μ_t as a function of fluid properties, the dynamics of the flow, and the geometry. The two turbulence models used in GASFLOW—algebraic and κ - ϵ —are, respectively, zero- and two-transport-equation models that predict the velocity and length scales that are used to compute μ_t . The models are described in order of increasing complexity, number of equations, and computational effort and, as a rule, in order of accuracy.

Turbulence effects in the vicinity of a wall are modeled with the law-of-the-wall formulation (Section 2.6.5).

2.7.1 Algebraic Model

For a turbulent velocity scale, Prandtl suggested that the mean turbulent kinetic energy per unit mass κ is a natural choice, where

$$\kappa = \frac{1}{2} (\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) \quad (2-64)$$

and a length scale l characteristic of the size of the energy-carrying eddies. Thus,

$$\mu_t = C_\mu \rho \kappa^{1/2} l \quad , \quad (2-65)$$

where C_μ is a constant (typically 0.05). It is often estimated that 10% or less of the mean flow energy is contained in the turbulent kinetic energy, so

$$\kappa = [0.1(1/2)u^2]^{1/2} \quad . \quad (2-66)$$

For containment studies, the length scale usually is set equal to 0.25–0.5 m, based on the containment modeling experiences with GASFLOW. Length scale must be based on engineering judgment, and available data or simulations with two-equation turbulence models can be used to estimate a given length scale for the flow configuration of interest.

2.7.2 κ - ϵ Model

The Navier-Stokes equations may be manipulated to produce exact expressions for κ , the turbulent kinetic energy, and ϵ , the rate of dissipation of turbulent kinetic energy (Ref. 2-22) defined as

$$\epsilon = \nu \sum_i \sum_j \left(\frac{\partial \overline{u_i}}{\partial x_j} \right)^2 \quad . \quad (2-67)$$

The exact κ and ϵ equations are modeled by a pair of approximate transport equations developed by Launder and Spalding (Ref. 2-15), with an extension to treat buoyancy effects. Again, $\kappa^{1/2}$ is the characteristic velocity scale, and the length scale is proportional to $\kappa^{3/2}/\epsilon$. The transport equation for the product $\rho\kappa$ is given by

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \rho \kappa dV = & \oint_S \left[\rho \kappa (\mathbf{b} - \mathbf{u}) + \left(\frac{\mu}{\sigma_\kappa} \nabla \kappa \right) + \boldsymbol{\tau} \cdot \nabla \mathbf{u} \right] \cdot \mathbf{A} dS \\ & + \int_V [\mu \alpha \mathbf{g} \cdot \nabla T - \rho \epsilon + \kappa S_\kappa] dV \quad , \end{aligned} \quad (2-68)$$

where α is the coefficient of thermal expansion. The advection, diffusion, and shear production of turbulent kinetic energy are given by the three terms in the first integral on the right side; the three terms in the second integral represent its production by buoyancy, dissipation, and generation from sources, respectively.

The transport equation for the product of the density and the dissipation of the turbulent kinetic energy, $\rho\epsilon$, is

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \rho \epsilon dV = \oint_S \left[\rho \epsilon (\mathbf{b} - \mathbf{u}) + \left(\frac{\mu}{\sigma_\epsilon} \nabla \epsilon \right) + C_1 \frac{\epsilon}{\kappa} \boldsymbol{\tau} : \nabla \mathbf{u} \right] \cdot \mathbf{A} dS \\ + \int_V \left[C_1 \frac{\epsilon}{\kappa} \mu \alpha \mathbf{g} \cdot \nabla T - C_2 \rho \frac{\epsilon^2}{\kappa} + \epsilon S_\epsilon \right] dV \end{aligned} \quad (2-69)$$

The terms on the right-hand side have meanings analogous to those in Equation (2-68). The turbulent viscosity is calculated using the Kolmogorov hypothesis:

$$\mu_t = \frac{C_\mu \rho \kappa^2}{\epsilon} \quad (2-70)$$

The values of the five new constants ($C_1, C_2, C_\mu, \sigma_\kappa, \sigma_\epsilon$) appearing in Equations (2-68) through (2-70) and listed in Table 2-4 are those suggested by Launder and Spalding (Ref. 2-15) following an extensive examination of experimental data for free turbulent flows.

Table 2-4. Constants used in the κ - ϵ turbulence model

C_1	C_2	C_μ	σ_κ	σ_ϵ
1.44	1.92	0.09	1.0	1.3

2.7.3 Turbulence Effects on the Transport Coefficients

By postulating the Boussinesq analogy (Ref. 2-18) between molecular stresses and Reynolds stresses, we can replace the molecular diffusion coefficients for mass [Equations (2-9) and (2-12)], energy [Equations (2-14) and (2-16)], and momentum [Equation (2-13), Tables 2-1 and 2-2] with the sum of the molecular and turbulent values. The resulting diffusion coefficient is often referred to as the "total" or "apparent" diffusivity, thermal conductivity, and viscosity, respectively, for the mass, energy, and momentum diffusion terms. Therefore, we represent these three transport coefficients in the following way:

$$\begin{aligned}
D_{\alpha \rightarrow \text{mix}} &\rightarrow D_{\text{apparent}} = D_{\alpha \rightarrow \text{mix}} + D_t \\
\phi &\rightarrow \phi_{\text{apparent}} = \phi + \phi_t \\
\mu &\rightarrow \mu_{\text{apparent}} = \mu + \mu_t
\end{aligned}
\tag{2-71}$$

The turbulent thermal conductivity, ϕ_t , is

$$\phi_t = \frac{\mu_t C_p}{Pr_t} \tag{2-72}$$

and the turbulent mass diffusivity, D_t , is

$$D_t = \frac{\mu_t}{\rho Sc_t} \tag{2-73}$$

which involve the turbulent Prandtl and Schmidt numbers.

The turbulent Prandtl number, Pr_t , can usually be assumed constant. Values of 0.90 for shear flows and 0.50 for free shear layers are usually satisfactory, whereas the turbulent Schmidt number, Sc_t , is normally selected between 0.5 and 1.0. Both the turbulent Prandtl and Schmidt numbers are properties of the flow field and hence are not material properties.

2.8 Chemical Kinetics

2.8.1 One-Step Model

We are currently using a simple one-step global chemical kinetics model that grossly oversimplifies the actual chemical processes. In the present implementation of this model, the only reaction modeled is

In modeling nuclear reactor containment buildings, typical computational cell volumes are 1–2 m³; they are larger in some cases. We try to keep cell volumes to about 1 m³ in regions where diffusion flames are expected. For this spatial resolution, there is no attempt to describe flame structure; we simply represent combustion energy release in a complex geometric containment (Ref. 2-22). Furthermore, chemical reaction time scales generally are short compared with fluid motions in these combustion modes, so the many elementary reaction steps and intermediate chemical species can be neglected in this first approximation.

The concentrations of reactants and products in Equation (2-74) are usually defined by

$$-\frac{1}{2} \frac{dc_{h_2}}{dt} = -\frac{dc_{o_2}}{dt} = +\frac{1}{2} \frac{dc_{h_2o}}{dt} = \dot{\omega} \quad , \quad (2-75)$$

where rate of reaction or reaction rate, $\dot{\omega}$, is normally proportional to the concentrations of the reactants raised to small powers that are frequently (but not necessarily) integers. The species concentrations (moles/cm³) are related to the macroscopic species densities through the species molecular weight

$$\rho_\alpha = c_\alpha \cdot M_\alpha \quad (2-76)$$

and to the species volume fraction by

$$Y_\alpha = \frac{c_\alpha}{\sum_{\alpha} c_\alpha} \quad (2-77)$$

For the hydrogen-oxygen reaction of Equation (2-74), the reaction rate can be written

$$\dot{\omega} = k(T) c_{h_2}^p c_{o_2}^q \quad , \quad (2-78)$$

where the rate coefficient, k , varies with temperature but is independent of concentration. The exponents of the concentrations in Equation (2-78) are known as the order of the reaction with respect to each reactant, where the sum of the exponents of the rate equation, i.e., order = $p + q$, is called the order of the reaction. There are important points concerning the order of the reaction: (1) it may be a fraction, (2) it is not necessarily related to the stoichiometric coefficients in the balance equation, and (3) it must be determined experimentally.

For this version of GASFLOW, we assume a reaction order 2, i.e., $p = 1$ and $q = 1$, which leads to the equation

$$-\frac{1}{2} \frac{dc_{h_2}}{dt} = -\frac{dc_{o_2}}{dt} = k(T) c_{h_2} c_{o_2} \quad . \quad (2-79)$$

Modeling the rate constant is usually accomplished by implementing a modified Arrhenius law in the form

$$k(T) = C_f \cdot T^n \cdot e^{-\frac{E}{\Re T}} \quad , \quad (2-80)$$

where C_f is the frequency factor (we use $C_f = 5 \times 10^{12}$ cm³/mole-s-K ^{n} in this model), n is the pre-exponential temperature exponent (we use $n = 0$ for this model), $\Re$ is

the universal gas constant, and E is the activation energy (we use 7.8×10^{11} ergs/mole for this model) of Equation (2-74).

Using the method of partial fractions, Equation (2-79) may be analytically integrated to give the solution

$$\frac{1}{c_{h_2}(0) - 2c_{o_2}(0)} \ln \left(\frac{c_{o_2}(0) c_{h_2}(t)}{c_{h_2}(0) c_{o_2}(t)} \right) = k(T) \cdot t \quad (2-81)$$

Another approach is to write two individual equations for the finite-rate chemical kinetics, first for the hydrogen concentration

$$\frac{dc_{h_2}}{dt} = -2k(T)c_{h_2}c_{o_2} \quad (2-82)$$

and then the oxygen concentration

$$\frac{dc_{o_2}}{dt} = -k(T)c_{h_2}c_{o_2} \quad (2-83)$$

The chemical energy of combustion is computed as a source for the energy transport equation [Equation (2-12)] by

$$\int_V S_{l, \text{combustion}} dV = V \cdot C_c \cdot \dot{\omega} \quad (2-84)$$

where $C_c = 4.778 \times 10^{12}$ ergs/mole.

In practice, when solving the finite-rate chemical equations [(2-82) and (2-83)] by this later method, we integrate the fuel [Equation (2-82)] when the fuel-oxidizer mixture is fuel lean and the oxidizer [Equation (2-83)] when the fuel-oxidizer mixture is fuel rich. From the chemical balance Equation (2-74), all components of the combustion process are determined.

We have compared the results of this model with the hydrogen combustion experimental data for the one-fourth-scale test facility (Refs. 2-23 and 2-24), the HDR E12 series and the Battelle Model Containment (BMC) HX series (Ref. 2-25), and an oil pool combustion test in the HDR containment building (Ref. 2-26). We have found good agreement for the general circulation patterns in complex geometries, concentrations of combustion products, and temperature distributions throughout the containment buildings. For the oil pool fires in the HDR (Ref. 2-26), the combustion model was modified to reflect hydrocarbon fuels.

2.8.2 Two-Step Model

Another option for describing the chemical process is to use a two-step model, where the chemical reaction is divided into two parts, an induction phase and an energy release phase.

2.8.2.1 Induction Parameter Model

The induction parameter model provides a simplified approach for the inclusion of chemistry into reacting flow calculations. The primary benefit is the reduction in computation time compared with using detailed chemical mechanisms.

The chemical reaction consists of two phases, an induction phase and an energy release phase. In the first phase, intermediate species build up the radical pool, the radicals that are necessary for chain branching of the reaction. Minimal energy is released. This phase is modeled by an induction time. During the second phase, the radicals recombine, which leads to the release of the main energy of the reaction. This time is called the energy release time.

To formulate an induction parameter model, it is first necessary to determine the characteristic times of the two phases: induction and energy release times. This has been done for a wide range of initial temperatures, pressures, and gas compositions. These parameters were determined from calculations using an integration package for chemical reaction rate equations and an appropriate chemical reaction scheme.

Here, a hydrogen-air system is considered. A detailed chemical mechanism with 48 reactions and 8 reactive species, developed at the Naval Research Laboratory, was used (Refs. 2-27 and 2-28). With GASFLOW using a solver for stiff differential equation systems, this detailed mechanism was solved for one cell over a wide range of initial conditions. The characteristic times were determined from the temperature/time history. As a criterion for completion of the first phase of the reaction and thus the induction time, a temperature rise of 2% was chosen. At 95% of the maximum temperature, the energy release phase was considered to be finished.

Induction and energy release times were then stored in the form of a table. The initial temperature had a range from 800 to 2500 K, the pressure ranged from 0.1 to 0.6 MPa, and the hydrogen concentration ranged from 5 to 30 vol %. An interpolation routine in the code is used to retrieve the needed values from this table.

For the first phase of the reaction, a nondimensional parameter is advanced through time and the computational mesh. The equation for this induction parameter can be represented in the following form:

$$\frac{dP}{dt} = -\mathbf{u} \nabla P + \nabla(D \nabla P) + \frac{1}{\tau_{ind}} \quad (2-85)$$

The first term on the right-hand side is the convective term, the second one describes the diffusion of the parameter, and the third one is the source term.

The term P stands for the induction parameter, $\mathbf{u}$ for the velocity vector with which the parameter can be advected through the domain, D is the diffusion coefficient, and τ_{ind} is the temperature-, pressure-, and composition-dependent induction time. As a diffusion coefficient, the coefficient of a typical radical, OH, was used.

The initial value of P is zero. For P smaller than 1, no energy is released and the fluid composition remains the same. When P reaches one, the induction time is elapsed and the energy release phase begins. We decided to treat this phase as if the energy were released stepwise linearly, depending on the energy release time and the available fuel.

Induction and energy release times are updated for each cell during every time step to reflect the actual condition the fluid is in.

2.8.2.2 Coupling of Induction Parameter Model with κ - ϵ Model

For calculating turbulent flames, the induction parameter model is coupled with the κ - ϵ model. This approach is based on the eddy-dissipation concept by Magnussen and Hjertager (Ref. 2-29) with the ignition/extinction modification introduced by Hjertager (Ref. 2-30).

Experiments have shown that the rate of combustion in flames is mainly dependent on hydrodynamic parameters. The combustion rate is limited by the rate of molecular mixing between the reactants. This mixing is linked to the rate at which turbulent eddies are dissipated. It is therefore assumed that the combustion rate is proportional to the rate of dissipation of kinetic energy of turbulence.

At first, a local turbulent Reynolds number is computed from turbulent and molecular viscosities:

$$Re_t = \frac{v_t}{\nu} \quad (2-86)$$

If this number is smaller than a critical Re number, the energy will be released using the induction parameter model. Otherwise, the Magnussen/Hjertager model is called. The critical value is chosen on the basis of yielding reasonable results, because the approach itself is highly empirical.

Two time scales are defined. One is the turbulent eddy mixing time scale

$$\tau_t = \frac{\kappa}{\varepsilon} \quad , \quad (2-87)$$

where κ is the turbulent kinetic energy and ε is the dissipation rate of turbulent kinetic energy. Both κ and ε are calculated in the code in the κ - ε turbulence model.

The second one is a characteristic chemical time scale which is assumed to be the induction time τ_{ind} . The values for τ_{ind} are interpolated from the table.

A Damkoehler number is defined as the ratio of the chemical time to the turbulent time:

$$Da = \frac{\tau_{ind}}{\tau_t} \quad . \quad (2-88)$$

If this Damkoehler number is greater than the critical value Die , the dissipation time of the turbulent eddies is too short in comparison to the induction time, and the gas will not burn. If the number is smaller than the critical value, the combustion rate is calculated as follows:

$$\dot{\omega} = -\frac{A}{\tau_t} \rho m_{lim} \quad , \quad (2-89)$$

where m_{lim} is the smallest of the three mass fractions, namely fuel, oxygen, or fuel already burnt. The constants A and Die are given the values 16 and 1000, respectively.

2.9 Recombiner Models

We have examined data for both the Siemens (Ref. 2-31) and NIS (Ref. 2-32) recombiner box designs. In addition, we have reviewed the analysis and modeling development of Fischer (Ref. 2-33). For the GASFLOW models of these two systems, which are shown schematically in Figure 2-1, we formulate a geometry that specifies a chimney formed by the vertical walls, and within this enclosure that is open at both the top and bottom, there is a defined reaction zone or volume. The task is to derive a model for the rate of hydrogen recombination with available oxygen in this reaction zone, given the gaseous conditions entering the recombiner at, e.g., location IN (shown in Figure 2-1 at the lower entrance). The model should be developed such that the projected flow area into the box can be scaled to accommodate nearly any recombiner size. We assume that the structure or the porosity for fluid flow of the recombiner members (plates or other configurations) remains uniform of any scale recombiner box. These recombiner structures also provide mass that gives a certain thermal inertia to the system.

Figure 2-1. Schematic diagram for the recombining box model

For the Siemens recombining box, there is considerable performance data available in Ref. 2-31, which we have condensed and presented in Figure 2-2. To understand this figure, one first computes the hydrogen volume percentage at the recombining inlet (location IN in Figure 2-1). Then one reads up to the recombination rate curve and then horizontally to the left vertical axis to determine the hydrogen recombination rate in $\text{g}/\text{m}^2\text{-s}$ (rate of hydrogen consumed per unit area inflow to the recombining box). The recombining efficiency for these conditions, based upon inlet and outlet hydrogen volume fractions, $Y_{h_2, \text{IN}}$ and $Y_{h_2, \text{OUT}}$, respectively, is determined by reading horizontally from the intersection with the hydrogen recombination rate curve to the right to intersect the efficiency curve, where the efficiency is defined as

$$\eta = 1 - Y_{h_2, \text{OUT}} / Y_{h_2, \text{IN}} \quad (2-90)$$

To determine the efficiency percentage as defined by Equation (2-90), one reads vertically to the top horizontal axis.

Fischer (Ref. 2-33) carefully examined the experimental data that was obtained from the Battelle Model Containment for the MC recombiner test series (Ref. 2-32), which focused on the NIS granulated recombiner box design. He found that a correlation showing the flow rate through the recombiner could be established that was dependent on the hydrogen volume fraction at the recombiner inlet and on a time constant which represented the thermal inertia of the device. In addition, Fischer found that, for steady-state operation, the volumetric flow rate was only a function of the hydrogen concentration at the recombiner inlet. Fischer also determined from the data that the efficiency for the NIS recombiner was nearly constant at 84.6% over the operating range of interest. We present Fischer's findings in Figure 2-2.

Figure 2-2. Siemens (Ref. 2-31) and NIS (Refs. 2-32 and 2-33) recombiner

To develop the basis for some of the GASFLOW recombiner models, we summarize Fischer's model here:

- (1) The steady-state volumetric flow through the NIS recombiner, Q_0 , is given by

$$Q_0 = a(Y_{h_2,IN})^b \quad , \quad (2-91)$$

where

$Y_{h_2,IN}$ = hydrogen volume fraction at the box inlet (IN in Figure 2-1)

and the experimentally determined constants are given by

$$a = 0.67 \times 10^6 \text{ (cm}^3/\text{s)}$$

$$b = 0.307 \quad .$$

- (2) The time-dependent behavior of the volumetric flow $Q(t)$ is described by the differential equation

$$\frac{dQ}{dt} = \frac{1}{\tau}(Q_0 - Q) \quad , \quad (2-92)$$

where τ is a relaxation time constant determined by experiment to be roughly 1800 s.

- (3) By carefully examining the time-averaged data at the recombiner inlet and outlet, Fischer found that the hydrogen recombination through the flow passages was incomplete. He determined an efficiency factor based on Equation (2-90) to be $\eta = 0.846$.

2.9.1 NIS Recombiner Model

The Battelle-Frankfurt NIS tests (Ref. 2-32) and Fischer's analysis (Ref. 2-33) were conducted on a 1 m² cross-section inflow recombiner box of high-heat-capacity granulate design. We wish to generalize this model to be able to scale to different inflow areas but of the same or very similar internal design. In addition, we wish to derive the GASFLOW model in terms of inflow velocity, U in Figure 2-1, to conform with the GASFLOW numerical algorithm. Following Fischer's model, the GASFLOW model for NIS recombiner boxes proceeds as follows:

- (1) The reference velocity in cm/s from Equation (2-91) is given by

$$U_0(t) = 67 \cdot [Y_{h_2,IN}(t)]^{0.307} \quad . \quad (2-93)$$

Note that, in the general case, the reference inlet condition (Fischer's "steady-state value") becomes a function of time because containment conditions are nearly always changing.

(2) The time-dependent velocity, $U(t)$, inflowing into the recombiner box is

$$\frac{dU(t)}{dt} = \frac{1}{\tau} [U_0(t) - U(t)] = \frac{1}{\tau} \left\{ 0.67 [Y_{h_2, IN}(t)]^{0.307} - U(t) \right\} \quad (2-94)$$

(3) We define a recombination reaction rate as

$$\dot{R}_{h_2} = -\frac{\delta m_{h_2}}{\delta t} = -(\dot{m}_{h_2, out} - \dot{m}_{h_2, in}) = \dot{m}_{h_2, in} - \dot{m}_{h_2, out} \quad (2-95)$$

which we must relate to the efficiency based upon hydrogen volume fractions shown in Equation (2-88). With a fair amount of algebra, Equation (2-95) can be reformulated to

$$\dot{R}_{h_2} = \eta \cdot \dot{m}_{h_2, in} \left[\frac{1}{1 - \frac{1}{2}(1 - \eta)Y_{h_2, in}} \right] \quad (2-96)$$

which reflects the fact that the number of moles flowing through the recombiner changes during the recombination process. For the conditions we are interested in (see Figure 2-2) the term in brackets is very close to unity, so we can simply write the hydrogen recombination rate as

$$\dot{R}_{h_2} = \eta \dot{m}_{h_2, in} \quad (2-97)$$

We now relate the hydrogen recombination rate from Equation (2-97) to the reaction rate from Equation (2-75) by

$$\dot{R}_{h_2} = 2\dot{\omega}VM_{h_2} \quad (2-98)$$

where $\dot{\omega}$ is the rate of hydrogen recombination in moles- h_2/cm^3 -s. Knowing the efficiency is 0.846, we can compute the rate of recombination, $\dot{\omega}$, as

$$\dot{\omega} = \frac{1}{2} \frac{0.846 \cdot U(t) A_{IN} C_{h_2, IN}(t)}{V} \quad (2-99)$$

(4) We use this recombination rate to solve the chemical kinetics, Equation (2-75), for the consumption of hydrogen and oxygen and the production of water vapor, as well as the combustion energy source term

$$\int_V S_{I, recombination} dV = VC_c \dot{\omega} \quad (2-100)$$

released in the recombiner reaction zone. Since Equation (2-99) is computed to be a constant based on conditions and properties at the recombiner inlet, careful evaluation of the chemical kinetics, Equation (2-75), must follow to ensure non-negative species concentrations.

2.9.2 Siemens Recombiner Model

We have developed a recombiner model for the Siemens recombiner box in a similar fashion. The GASFLOW model for the Siemens recombiner is as follows:

- (1) We first calculate the time-dependent hydrogen and oxygen volume fractions, $Y_{h_2, IN}(t)$ and $Y_{o_2, IN}(t)$, respectively, at the recombiner inlet (location IN in Figure 2-1).
- (2) A check of the species composition is made from

$$Y_{IN}(t) = \min \left[Y_{h_2, IN}(t), 2 \frac{Y_{o_2, IN}(t)}{\eta(t)} \right] \quad (2-101)$$

- (3) Using the volume fraction as a volume percentage, one then determines both the recombination rate, $\dot{R}(t)$, and recombination efficiency, $\eta(t)$, from Figure 2-2.
- (4) A reference velocity is computed as follows:

$$U_0(t) = \frac{\dot{R}(t)}{A_{IN} \eta(t) \rho_{h_2, IN}(t)} \quad (2-102)$$

where A_{IN} is the flow cross-section area into the recombiner box in m^2 .

- (5) The time-dependent velocity, $U(t)$, inflowing into the recombiner box is

$$\frac{dU(t)}{dt} = \frac{1}{\tau} [U_0(t) - U(t)] = \frac{1}{\tau} \left\{ \frac{\dot{R}(t)}{A_{IN} \eta(t) \rho_{h_2, IN}(t)} - U(t) \right\} \quad (2-103)$$

where τ for this model is 10 s. A time constant of 10 s is based on experimental data for the Siemens recombiner.

(6) The chemical kinetics with change of species concentrations, Equation (2-75), is computed from

$$\dot{\omega} = \frac{1}{2} \frac{\eta \cdot U(t) A_{IN} c_{h_2, IN}(t)}{V}, \quad (2-104)$$

and the energy release, Equation (2-97), is updated in the recombiner reaction zone.

Again, care must be taken to insure positive species concentrations with this model because the chemical kinetics in the recombiner reaction zone is dependent on the inflow conditions and properties of the recombiner box.

2.9.3 Siemens Correlation for Siemens Type FR-90/1 Recombiner

The Siemens recombiner correlation (Ref. 2-34) can be used for a Siemens recombiner of the type FR-90/1. This relationship between the species volume fractions, Y_{h_2} and Y_{o_2} , and the pressure p in bars is given by

$$\int_V S_{p, h_2, Siemens_correlation} dV = - \begin{cases} 0, & Y_s < 0.005 \\ Y_s(k_1 p + k_2), & Y_s \geq 0.005 \end{cases} \quad (2-105)$$

where $Y_s = \min(Y_{h_2}, 2Y_{o_2}, 0.08)$ and the empirically determined constants, k_1 and k_2 , are given in Table 2-5.

Table 2-5. Siemens recombiner constants of FR-90/1

Type	k_1 (g/s-bar)	k_2 (g/s)
FR-90/1-320	0.010	0.012
FR-90/1-960	0.031	0.037
FR-90/1-1500	0.137	0.167

In order to utilize this correlation in the GASFLOW methodology, we recast the correlation into

$$\dot{\omega} = \begin{cases} 0, & Y_s < 0.005 \\ \frac{Y_s(k_1 p + k_2)}{2M_{h_2} V}, & Y_s \geq 0.005 \end{cases} \quad (2-106)$$

The chemical kinetics can be evaluated when Equations (2-75) and (2-106) are integrated. Computing the energy from the recombination process with Equation (2-97) completes this model.

2.9.4 GRS Recombiner Correlation

The GRS recombimer correlation model (Ref. 2-35) can be used for a single recombimer plate or foil. This correlation is of an Arrhenius type,

$$\int_V S_{\rho, h_2, GRS_correlation} dV = -A_r k_1 (c_{h_2})^{1.05} e^{-\Delta E(T)/(\mathfrak{R} \cdot T)} \quad (2-107)$$

where A_r is the recombimer surface area, k_1 is a constant equaling 5.0×10^2 , c_{h_2} is the hydrogen concentration, $\mathfrak{R}$ is the universal gas constant, T is the temperature, and $\Delta E(T)$ is an activation function approximated by

$$\Delta E(T) = \begin{cases} 20.271 + \left[2.1771 \cdot 10^{-2} \left(\frac{-1.5078 \cdot 10^{-5}}{9.4707 \cdot 10^{-10} T} - 1 \right) T \right]; & T < 506.9 K \\ 1.8322 + 5.026 \cdot 10^{-2} T; & T \geq 506.9 K \end{cases} \quad (2-108)$$

To cast this relationship into the GASFLOW methodology, we rearrange this expression to

$$\dot{\omega} = \frac{1}{2} \frac{A_r k_1 (c_{h_2})^{1.05} e^{-\Delta E(T)/(\mathfrak{R} \cdot T)}}{M_{h_2} V} \quad (2-109)$$

The chemical kinetics can be evaluated when Equations (2-75) and (2-109) are integrated. Computing the energy from the recombination process with Equation (2-97) completes this model.

2.10 Ignitor Model

The ignitor model is simple, but effective. For a user-specified location, the gaseous composition is first checked to see if a combustible mixture of hydrogen and oxygen exists. We essentially implement the lean combustion limit from the Shapiro Diagram to evaluate the threshold for which a mixture of hydrogen, oxygen, and steam is flammable. To form a flammable mixture, the hydrogen volume fraction must exceed 4% for steam volume fractions up to 30%. For steam volume fractions from 30% to 65%, the hydrogen volume fraction increases from 4% to 12%. Above 65% steam volume fraction, the mixture is considered to be steam inerted. This criteria can be written as

$$\begin{cases} h_2 o \langle \text{Volume}\%_{h_2 o} \rangle < 65 \\ h_2 \langle \text{Volume}\%_{h_2 o} \rangle \geq 4 + \min \left[0, \frac{8}{35} (\text{Volume}\%_{h_2 o} - 30) \right] \end{cases} \quad (2-110)$$

If this condition is met, the temperature in the reaction rate constant of Equation (2-79) is set equal to 2000 K,

$$k(2000) = C_f e^{-\frac{E}{R \cdot 2000}} \quad (2-111)$$

and the chemical kinetics equations are solved with this driving function.

We are able to model both a "glow plug" and a "spark" type of ignitor. With a glow-plug-type ignitor, the reaction rate constant, Equation (2-108), is continuously active for the specified time interval, whereas for the spark-type ignitor, the reaction rate constant is only active at a specified spark interval (sparking frequency) and specified sparking duration.

It should be noted that flame propagation may or may not occur within a GASFLOW simulation after a combustible mixture has been ignited within a given GASFLOW cell. Flame propagation within a GASFLOW simulation is determined by the energy release rate from the chemistry model and the calculation of the hydrodynamics and heat transfer in the vicinity of the flame front. Therefore, once ignition has occurred, flame propagation upward, downward, etc. is determined by the solution of the chemistry model and the hydrodynamics model.

2.11 Ventilation System Modeling

In GASFLOW, ventilation systems are modeled by connecting ventilation system component models together to represent the actual ventilation system (see Figure 2-3). The available ventilation system component models are 1D flow models, with the exception of the junction component. The junction component allows for multidimensional flow from one- to two- or 3D flow, depending upon which faces of the junction component are connected to a duct. The conservation equations solved in the 1D flow components are the same as those in the 3D blocks, except flow is allowed only in the i or x -direction and velocities in the j (y -direction) and k (z -direction) are assumed to be zero. Therefore, the ventilation system component models use the same models for chemistry, diffusion, etc., as used in the 3D block conservation equation solutions. In addition, the same numerical methods are used that result in a coupled and consistent solution between the ventilation system and the 3D blocks.

2.11.1 Ducts and Pipes

The same GASFLOW model is used for both duct and pipe ventilation system components. Ducts/pipes are 1D flow ventilation system components, with the conservation equations collapsed to a single flow direction; however, changes in elevation from one cell to the next are included in the i or x -direction momentum equation by inferring from the user input the $\cos \theta$ for each cell edge, where $\cos \theta$ times the distance between the cell centers of two neighboring cells gives the change

in elevation between those neighboring cells (see Figure 2-4). The gravity term in the collapsed equation set becomes

$$\int \rho \cos \theta dx \quad (2-112)$$

Flow losses due to bends, curves, gradual area changes, abrupt area changes, and user inputs are included in the 1D momentum equation according to the following expression:

$$\frac{K\rho u|u|}{2} \quad (2-113)$$

where K is determined from the appropriate formula or is supplied by the user. For area changes, GASFLOW uses the following formulas to calculate K :

$$\begin{aligned} K &= 0.8 \sin(2\phi)(1-\beta) \text{ for gradual expansion,} \\ K &= 2.6 \sin(2\phi)(1-\beta)^2 \text{ for gradual contraction,} \\ K &= 0.45(1-\beta) \text{ for sudden expansion, and} \\ K &= (1-\beta)^2 \text{ for abrupt contraction,} \end{aligned} \quad (2-114)$$

where ϕ is defined in Figure 2-5 and β is the small flow area divided by the large flow area. These formulas are taken from Ref. 2-36.

Flow losses for elbows and bends in ducts are obtained from the effective length over the hydraulic diameter (L/D), also obtained from Ref. 2-36. The L/D ratio is related to the flow loss according to the following expression:

$$K = \frac{fL}{D} \quad (2-115)$$

where f is the friction factor for the duct and is in general a function of the Reynolds number and surface roughness. All friction factor calculations in GASFLOW assume smooth walls and do not include the effect of surface roughness. The L/D values obtained from Ref. 2-36 are given in Tables 2-6 through 2-8.

The variables α and r in Tables 2-6 through 2-8 are defined in Figure 2-6. For a closed end duct with a 180° bend, GASFLOW uses an L/D of 50.

Figure 2-3. Ventilation system for a waste tank farm

Figure 2-4. Change in elevation for two neighboring 1D cells

Figure 2-5. Gradual flow area change from A_s to A_l

Table 2-6. L/D values for 90° bends

r/D	L/D
1	20
1.5	14
2	12
3	12
4	14
6	17
8	24
10	30
12	34
14	38
16	42
20	50

Table 2-7. L/D values for miter bend

$\alpha(\text{degrees})$	L/D
0	2
15	4
30	8
45	15
60	25
75	40
90	60

Table 2-8. L/D values for standard elbow

$\alpha(\text{degrees})$	L/D
0	0
45	16
90	30
180	50

The friction factor in GASFLOW is calculated from the following formulas obtained from Ref. 2-4:

$$f = 0.3164 \text{Re}^{-0.25}, \text{ for turbulent flow} \quad (2-116)$$

$$f = \frac{64}{\text{Re}}, \text{ for laminar flow}$$

where Re is the Reynolds number and the transition from laminar to turbulent flow in the duct occurs at a Re of 2000.

Ducts must start and end at node points defined in x,y,z space, as defined by the user. The user provides additional input to GASFLOW to indicate whether or not the duct is straight, has a bend, has an area change (gradual or abrupt), etc. Based on this input, GASFLOW calculates the appropriate total flow loss and total effective L/D at each cell edge in the network nodding and includes the momentum losses due to these terms as a momentum sink in the Phase A solution. At the node points a duct must connect to a junction component, a pressure boundary condition, a velocity boundary condition, or a 3D block.

Figure 2-6. Definitions for α and r

2.11.2 Junctions

Junctions are a single, 3D GASFLOW cell at which a single duct can be connected to each of the six cell faces (i.e., +i, -i, +j, -j, +k, and -k cell faces). The conservation equations are the same as developed for the 3D block components in GASFLOW. If a duct is not connected to a junction cell face, then that cell face is assumed to represent a wall through which no mass, energy, or momentum flows. Junctions are centered around node points as shown in Figure 2-7.

2.11.3 Blowers and Fans

The GASFLOW models for blowers and fans are the same. A blower is represented as a momentum source in the 1D duct momentum equation. The momentum source is determined from the user input provided for the blower in terms of a blower head versus the volumetric flow through the blower. The volumetric flow through the blower is determined for each time step. Then the momentum source

Figure 2-7. Illustration of a junction component

is determined from the blower head versus volumetric flow table. The momentum source is included explicitly in the Phase A solution and implicitly in the Phase B solution. The momentum source term used in GASFLOW is

$$M_s = \rho g H \left(\frac{S}{S_R} \right)^2, \quad (2-117)$$

where H is the blower head in cm, S is the blower speed, and S_R is the rated blower speed. The correction factor, the blower speed divided by the rated speed squared, is an attempt to simulate blowers at speeds that are different than rated conditions. The blower head in the above equation is the expected head at rated conditions. Most applications will be at rated blower speeds, so the correction term will be 1.

2.11.4 Dampers and Valves

The GASFLOW models for dampers and valves are the same. A damper is modeled as a location within a duct where the effective flow area can change as a function of time. The resulting flow loss for a damper is given by the following formula:

$$K = 0.5(1 - \beta) + (1 - \beta)^2 + K_o, \quad (2-118)$$

where b is the flow area ratio of the damper flow area over the duct flow area, and K_o is the fully open flow loss for the damper.

2.11.5 Filters

A filter is modeled as a local flow area change based on user input, plus a flow loss developed from experimental observations for filters. The model for the filter loss is the sum of a laminar and turbulent flow loss.* At low fluid velocities through the filter the laminar loss will dominate, and at high velocities through the filter the turbulent flow losses will dominate. The pressure drop associated with a filter can be written as

$$K_l \mu u + K_t \rho u |u|, \quad (2-119)$$

where the first term is the laminar loss and the second term is the turbulent loss.

2.12 Aerosol Model

The GASFLOW 2.1 aerosol model comprises a Lagrangian discrete particle transport model, a stochastic turbulent particle diffusion model, a particle deposition model, a particle entrainment model, and a particle cloud model. These models incorporate the physics of particle behavior to model discrete particle phenomena and allow the code user to track the transport, and deposition and entrainment of discrete particles, as well as, clouds of particles in nuclear systems. This current model does not include agglomeration.

2.12.1 Particle Transport

The inertial force, F_I , of a particle is equal to the sum of the external aerodynamic forces acting on the particle. The external forces modeled are aerodynamic drag, F_d , gravitational, F_{gr} , and centrifugal, F_c . The force balance equation for each particle is

$$F_I = F_d + F_{gr} + F_c = \frac{\pi}{6} d_p^3 \rho_p \frac{dU_p}{dt}, \quad (2-120)$$

where d_p is particle diameter, ρ_p is particle density, U_p is particle velocity, and t is time.

* William S. Gregory, et al., "FIRAC-PC Users Manual," Los Alamos National Laboratory report in preparation.

Convection is the primary means of particle transport. The particle velocity is nearly that of the conveying fluid, but this small difference in velocity gives rise to the primary aerodynamic force, the drag force, acting on particles in motion,

$$F_d = C_D \frac{\pi}{8} d_p^2 \rho_g (U_g - U_p)^2, \quad (2-121)$$

where C_D is the particle drag coefficient, ρ_g is gas density, and U_g is the gas velocity at the particle location. The fluid drag force is computed from Newton's resistance law to determine the form drag for $Re_p > 1000$. (Re_p is the particle Reynolds number, and $Re_p = \rho_g d_p |U_g - U_p| / \mu$, where μ is the gas molecular viscosity.) In this case, the drag coefficient is $C_D \cong 0.44$. Stokes Law, which is derived from the Navier-Stokes equations with many limiting assumptions, is used to calculate the fluid friction drag force when $Re_p < 1$. Here the assumption is that the inertial forces are much less than the viscous forces. For $Re_p < 1$, $C_D = 24/Re_p$. The influence of the Reynolds number on the drag coefficient of spherical particles over a wide range ($1 < Re_p < 1000$) is represented as

$$C_D = 0.4 + \frac{24}{Re_p} + \frac{6}{(1 + \sqrt{Re_p})}$$

(see Ref. 2-37). This formulation is used in the code.

The force from gravity is

$$F_{gr} = \frac{\pi}{6} d_p^3 g (\rho_p - \rho_g), \quad (2-122)$$

where g is gravitational acceleration. When a particle is released in air it quickly reaches a terminal velocity, a condition in which the drag force of the air will be exactly equal and opposite to the force of gravity.

A particle is said to have curvilinear motion when it follows a curved path rather than a straight-line or oscillatory motion. A particle traveling along a curved streamline in flow around an obstacle will have curvilinear motion and will experience a centrifugal force, which can be expressed as

$$F_c = \frac{\pi}{6} d_p^3 \rho_p \frac{U_t^2}{R}, \quad (2-123)$$

where U_t is the tangential velocity at radius of curvature R . Curvilinear motion is characterized by the dimensionless Stokes number (S_{tk}), which is the ratio of the stopping distance (a measure of the inertial range of a particle) to a characteristic dimension of the obstacle. For geometrically similar particle motion to occur

around differently sized obstacles, the flow Reynolds numbers must be equal and the Stokes numbers must be equal.

2.12.2 Particle Turbulent Diffusion

The fluid velocity at the location of a discrete particle is the sum of the mean velocity components and the turbulent velocity components. The turbulent velocity is determined by a stochastic approach suggested by Hotchkiss and Hirt (Ref. 2-38). The idea is to consider the particle as a point source that diffuses for a time Δt . The probability of where the particle is likely to move along a coordinate axis x can be written in the form of a Gaussian probability distribution function

$$n(x,t) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-x^2}{2\sigma^2}} \quad (2-124)$$

where $2\sigma^2$ is the dispersion of the probability distribution, $\sigma = \sqrt{2D_p\Delta t}$ is the standard deviation, and D_p is the turbulent diffusion coefficient. A random number generator selects the actual location used within the possible distribution. The turbulent velocity component is determined from the randomly chosen location. This process is repeated for each of the three coordinate directions.

2.12.3 Particle Deposition

Particle adhesion is poorly understood and its description is partly qualitative. Hinds states that because it is such a complicated phenomenon there is no complete theory that accounts for all the factors that influence adhesion (Ref. 2-39). The main adhesive forces are the van der Waals force, electrostatic forces, and the surface tension of absorbed liquid films. These forces are affected by the following: the material, shape, and size of the particle; the material, roughness, and contamination of the surface; the relative humidity and temperature of the ambient gas; and the duration of particle-surface contact and initial contact velocity.

The theoretical analyses of adhesion forces presented by Hinds (Ref. 2-39) and Dahneke (Refs. 2-40 and 2-41) indicate that the most important adhesion forces are the London-van der Waals forces, the long-range attractive forces that exist between molecules. Hinds explains that these forces arise because the random movement of electrons in any material creates momentary areas of charge concentration called dipoles. At any instant these dipoles induce complementary dipoles in neighboring material, which gives rise to attractive forces. These forces decrease rapidly with separation distance between surfaces; consequently, their influence extends only several molecular diameters away from a surface.

Small particles do not always adhere to a surface after impingement. At "low" velocities a particle may lose all of its kinetic energy on impact by deforming itself

and the surface. In this velocity range, the greater the deformation the greater the adhesive force. At "high" velocities, part of the particle kinetic energy is dissipated in the deformation process and part is converted elastically to kinetic energy of rebound. At some threshold velocity the rebound energy will exceed the adhesion energy and the particle will bounce off the surface. This can occur for particle sizes that would adhere tightly in a static situation. The harder the particle and surface, the larger the particle, and the greater the velocity, the more likely bounce is to occur.

To model particle deposition in GASFLOW, the theory of rebound developed by Dahneke (Refs. 2-40 and 2-41) is used. Dahneke's rebound theory includes an energy balance analysis of the impinging and rebound particle. Consider a particle moving towards a surface, still beyond influence of the surface, with incident normal velocity U_i . The particle kinetic energy due to U_i is KE_i . (Kinetic energy due to motion parallel to the surface is assumed conserved throughout the collision, and kinetic energy due to spinning of the particle is neglected.) Upon nearing the surface the particle will fall into the particle-surface potential energy well of depth E . In general, the depth of the potential well may vary during the collision. Possible causes could be contact charging or particle and surface deformation. Thus two potential well depths are defined: E_i is the depth seen by the incident particle, and E_r is the depth seen by the reflected particle. To obtain the kinetic energy of the particle at the instant of rebound, the concept of the coefficient of restitution, e , is used. This is defined as the ratio of normal particle velocity at the instant of rebound to normal particle velocity at the instant of contact. The kinetic energy at the instant of rebound is

$$KE_{at\ rebound} = (KE_i + E_i)e^2, \quad (2-125)$$

where the sum of KE_i and E_i is the kinetic energy of the particle at the instant of contact, and e^2 is the fraction of this energy recovered by the particle. If the collision is perfectly elastic, $e^2 = 1$.

Upon rebound, the particle must exchange kinetic energy for potential energy as it climbs out of the potential energy well. The final kinetic energy of the reflected particle, beyond influence of the surface, is

$$KE_r = (KE_i + E_i)e^2 - E_r. \quad (2-126)$$

In terms of particle velocity, U , and mass, m , Equation (2-126) can be equivalently written as

$$\frac{U_r}{U_i} = \left[e^2 + \frac{2(E_i e^2 - E_r)}{mU_i^2} \right]^{\frac{1}{2}}, \quad (2-127)$$

where U_r is the rebound velocity. Dahneke (Ref. 2-40) noted that if one could approximate $E = E_r = E_i$, then Equation (2-127) would simplify to

$$\frac{U_r}{U_i} = \left[e^2 + \frac{2E(e^2 - 1)}{mU_i^2} \right]^{\frac{1}{2}} \quad (2-128)$$

When there is no rebound, the particle must fail to climb out of the potential energy well, and thus KE_r is zero, and

$$U_i^* = \left[\frac{2E}{m} \left(\frac{1 - e^2}{e^2} \right) \right]^{\frac{1}{2}} \quad (2-129)$$

This equation determines the critical rebound speed, U_i^* ; it describes the limiting case between particle capture and rebound.

The depth of the potential energy well for a sphere of diameter d and a flat surface adhering to each other is given by Dahneke (Ref. 2-40), quoting as references Bradley (Ref. 2-42) and Hamaker (Ref. 2-43), as

$$E = \frac{Ad}{12z_0}, \quad (2-130)$$

where A is the Hamaker constant, z_0 is the equilibrium separation between the particle sphere and a surface, and d is the particle diameter (see references for more detailed description of terms).

The attractive force between the sphere and a surface is

$$F = -dE / dz = -\frac{Ad}{12z_0^2} \quad (2-131)$$

Combining Equations (2-129) and (2-130) and writing the particle mass in terms of its volume and density, ρ_p , gives

$$U_i^* = \left[\frac{A(1 - e^2)}{\pi z_0 \rho_p d^2 e^2} \right]^{\frac{1}{2}} \quad (2-132)$$

Dahneke (Ref. 2-41) states that the principal deficiency of the Bradley-Hamaker derivation of the adhesion energy is its failure to consider the repulsive portion of

the molecular interactions. Thus, flattening of the sphere tip and deformation of the surface are not considered. Dahneke presents in the 1972 publication (Ref. 2-41) a new theory for the adhesion of particles (spheres) that includes the influence of the repulsive component of force from the elastic flattening of the spheres. The repulsive component of force is expressed in terms of the apparent penetration depth, h , of the impacting sphere into the substrate; the sphere size, d ; and the sphere bulk mechanical properties, $K = (1 - N^2) / Y$, where N is Poisson's ratio and Y is Young's modulus of the particle material. The net force between two impacting spheres (or a sphere and a surface) is written as the sum of the attractive and repulsive forces:

$$F = \left(\frac{Ad}{12z_0^2} \right) \left(1 + \frac{2h}{z_0} \right) + \left(\frac{2\sqrt{2}d}{3K} \right) h^{\frac{3}{2}} \quad (2-133)$$

In order to derive an equation for the maximum adhesive force, F_{max} , Dahneke assumes that some flattening will always occur when two spheres (or a sphere and a flat surface) adhere and exploits the fact that F must obtain a minimum at some value of penetration h . He states that the expression for F_{max} is of practical importance in calculating adhesive force, since a force greater than F_{max} is required to separate two spheres or a sphere from a surface by, for example, centrifuging or blowing, or by dislodgment through inertial forces when a stress in the surface material is reflected to the surface. The maximum adhesive force is

$$F_a = \left(\frac{Ad}{12z_0^2} \right) \left[1 + \left(\frac{A^2 K^2}{108z_0^7} \right) d \right] \quad (2-134)$$

which occurs at the penetration

$$h_f = \left(\frac{A^2 K^2}{72z_0^6} \right) d \quad (2-135)$$

Note that the first term in Equation(2-134) is the adhesive force between two unflattened spheres. The second term is the increase in adhesive force due to flattening of the spheres. Thus, flattening has greater effect for larger particle sizes and softer materials.

In order to obtain an expression for the threshold bounce velocity, U_i^* , including the effect due to flattening, it is first necessary to obtain an expression for the interaction energy. This is obtained directly from Equation (2-133) using the relationship $E = \int Fdh$.

This yields

$$E = \left(\frac{Ad}{12z_0} \right) \left(1 + \frac{h}{z_0} + \frac{h^2}{z_0^2} \right) + \left(\frac{4\sqrt{2d}}{15K} \right) h^{\frac{5}{2}}. \quad (2-136)$$

The potential energy well equivalent to the energy required to overcome the maximum adhesive force expressed in Equation (2-134) is obtained by substituting the penetration depth, h_f , expressed in Equation (2-135) into Equation (2-136). This gives

$$E = \left(\frac{Ad}{12z_0} \right) \left[1 + \left(\frac{A^2 K^2 d}{72z_0^7} \right) + \left(\frac{A^4 K^4 d^2}{72^2 z_0^{14}} \right) \right] + \left(\frac{4\sqrt{2d}}{15K} \right) \left(\frac{A^2 K^2 d}{72z_0^6} \right)^{\frac{5}{2}}. \quad (2-137)$$

Combining Equations (2-129) and (2-137) gives the equation for the critical rebound velocity that determines the threshold particle bounce velocity.

The critical rebound velocity is the value of velocity for a 50% probability of bounce. The concept of the threshold velocity or critical rebound velocity U_i^* being defined as 50% likelihood of particle bounce is presented by Hinds (Ref. 2-39) and Paw U (Ref. 2-44). The incident velocity window outside of which the particle either adheres or bounces is somewhat arbitrary. Data presented by Paw U suggest that plus or minus 50% of U_i^* is a reasonable assumption for this. That is, for $U_i < U_i^*(0.5)$ the particle always adheres, and for $U_i > U_i^*(1.5)$ the particle always bounces. With these specified limits the probability of particle bounce for the velocity range $0.5 U_i^* < U_i < 1.5 U_i^*$ is expressed as

$$0 \leq \left[\frac{(-0.5U_i^* + U_i)}{U_i^*} \right] \leq 1 \quad (2-138)$$

A determination of whether or not specific particles will bounce or adhere can be made by generating a random number, α , with a value between 0 and 1, and testing for

$$\alpha \leq \left[\frac{(-0.5U_i^* + U_i)}{U_i^*} \right] \quad (3-139)$$

When this condition is met, the particle will bounce.

Dahneke's data (Refs. 2-45 and 2-46) show the trend for the coefficient of restitution, e , to reach a maximum value, in this case 0.96, at the threshold bounce velocity of about 10 cm/s. Almost immediately the ratio of rebound velocity to incident velocity begins to decrease as the incident velocity increases. At an incident velocity of 100 cm/s, e is 0.68; at 400 cm/s, e is 0.15. An approximately 70% decrease in e

results in an increase in incident velocity of 100 cm/s. The following equation models this data relatively well:

$$e = e_0(0.60)^{\exp} \quad , \quad (3-140)$$

where

$$\exp = \frac{U_i - U_i^*}{10.0 U_i^*} \quad ,$$

and e_0 is the coefficient of restitution at the threshold bounce velocity.

Particle deposition and bounce are not understood well enough that a totally mechanistic model can be developed. The phenomena simulated in this deposition model are based on theoretical models that are necessarily restricted by a wide range of assumptions and experimental data that are limited to specific conditions. Deposition is in a real sense a stochastic process that follows the general trend of the theoretical and empirical models developed and compared with available experimental data. Because of this, it is a reasonable assumption that some small, unknown percentage of the particles that impact a surface will adhere. To account for this, currently 5% of all particles that impact a surface do adhere. The particles that adhere are randomly chosen.

2.12.4 Particle Entrainment

The mechanisms involved in the entrainment of deposited particles from a surface into the suspension fluid are not well understood. Suspension is associated with the aerodynamic detachment of particles for which the principal force holding them onto a surface is the intersurface molecular force (adhesion force).

Suspension is initiated by flows when the fluid velocity equals or exceeds the particle threshold suspension velocity value. As pointed out by Halow (Ref. 2-47), most treatments of particle suspension have provided correlation of a largely empirical nature and, while perhaps describing the available experimental data, do not have a sound enough fundamental basis to permit confident extrapolation of the data to uninvestigated systems and conditions. Most theoretical work has considered the balance of forces acting on a suspension particle, considering the fluid-particle interaction in the shear flows in the viscous sublayer, which are assumed to be steady. A force balance approach modified by experimental data is used in this model.

Criteria for determining the fluid velocity at which a particle initially at rest on a surface will become suspended can be determined from a force balance equation that includes gravity, adhesion, fluid lift, fluid drag, and friction forces. A particle adhering to a surface will be dislodged when the removal forces *equal or exceed* the force of particle adhesion. This model is based on a force balance approach plus

experimental data reported by Cabrejos and Klinzing.* They present a technique for finding the minimum pickup (suspension) velocity of solid particles in horizontal pneumatic conveying. This general semi-empirical correlation is based on the Archimedes number and is valid over a range of particle sizes from 10 to 1000 μm .

When the size of the particle is smaller than the thickness of the viscous sub-layer, that is, $d_p < d_l$, the forces acting on the sphere are as shown in Figure 2-8, where a horizontal flow is assumed.

Gravitational, buoyant, and adhesive forces depend only on the physical properties of the particle and the gas density, and they are independent of the gas stream velocity. The drag and lift forces depend on the gas stream velocity, whereas the frictional force is proportional to the coefficient of sliding friction. The adhesive force is the van der Waals intersurface molecular force.

Figure 2-8. Forces acting on a single sphere at rest on a wall with a steady, fully developed turbulent flow

The forces acting on a small sphere, immersed in the viscous sublayer are as follows:

(1) Gravitational force:
$$F_g = \frac{\pi}{6} d_p^3 \rho_p g$$

* Francisco J. Cabrejos and George E. Klinzing, "Incipient Motion of Solid Particles in Horizontal Pneumatic Conveying," Dept. of Mech. Engr., University of Pittsburgh, unpublished paper (1991).

(2) Buoyant force: $F_b = \frac{\pi}{6} d_p^3 \rho_g g$,

(3) Adhesive force: $F_a = \left(\frac{A d_p}{12 z_0^2} \right) \left[1 + \left(\frac{A^2 K^2}{108 z_0^7} \right) d_p \right]$,

(4) Drag force: $F_D = C_D \frac{\pi}{8} d_p^2 \rho_g U_{gcp}^2$,

(5) Lift force: $F_l = 6.46 \rho_g \sqrt{\nu} U_{gcp} \sqrt{\frac{\partial U_g}{\partial y} \frac{d_p^2}{4}}$, and

(6) Friction force: $F_f = f_s F_n = f_s (F_g + F_a - F_b - F_l)$

where U_{gcp} is the gas stream velocity at the center ($y = d_p/2$) of the stationary particle, which is typically in the viscous sublayer. The shear velocity, U_t , is known, so U_{gcp} can be computed from

$$U_{gcp} = \frac{d_p U_t^2}{2\nu} . \quad (2-141)$$

The adhesive and lift forces are from Dahneke (Ref. 2-41) and Saffman (Ref. 2-48), respectively.

The small sphere will begin moving when the forces acting on the particle are zero. Applying Newton's second law, motion will take place when

$$F_d = f_s (F_g + F_a - F_b - F_l) . \quad (2-142)$$

Substituting the above force equations into the force balance equation gives

$$C_D \frac{\pi}{8} d_p^2 \rho_g U_{gcp}^2 / f_s = \frac{\pi}{6} d_p^3 (\rho_p - \rho_g) g + \left(\frac{A d_p}{12 z_0^2} \right) \left[1 + \left(\frac{A^2 K^2}{108 z_0^7} \right) d_p \right] - 6.46 \rho_g \sqrt{v} U_{gcp} \sqrt{\frac{\partial U_g}{\partial y} \frac{d_p^2}{4}} \quad (2-143)$$

A Newton-Raphson solver can be used to solve this implicit equation for U_{gcp} , which is the minimum pickup velocity for the single particle.

This model follows the derivation of the force balance model presented by Cabrejos and Klinzing.* However, they derived the equations for pipe flow. They also used Munroe's equation to model the effect that the pipe would have on large particles and used Blasius' correlation for the friction factor inside a smooth pipe for the effect the pipe would have on small particles, that is, for those totally immersed in the viscous sublayer. The equations presented here are for flow over a flat plate. The shear velocity, U_t , is used to determine the velocity at the small particle center in the viscous sublayer.

Cabrejos and Klinzing modified the pickup velocity predicted by these fundamental equations with experimental data. Although this data was obtained in pipe flow, we believe it can be used for a more general flow model. Comparison of minimum pickup velocities predicted by the modified Cabrejos-Klinzing model with experimental measurements of the threshold suspension velocity, for flow over thick beds of a wide range of material sizes and densities (Ref. 2-49), shows good agreement. The predicted pickup velocity is modified by an empirical equation that is a function of the Archimedes number,

$$Ar = \frac{g}{v^2} \frac{(\rho_p - \rho_g)}{\rho_g} d_p^3 \quad (2-144)$$

The magnitude of this correction factor ranges from about 2.5 for high-density, large particles to about 250 for low-density, small particles. Cabrejos and Klinzing show that this semi-empirical model agrees well with experimental data.

Combining the single particle model, which predicts a pickup velocity, U_{gpu0} , with the experimental data for the minimum pickup velocity of a layer of particles gives

* Francisco J. Cabrejos and George E. Klinzing, "Incipient Motion of Solid Particles in Horizontal Pneumatic Conveying," Dept. of Mech. Engr., University of Pittsburgh, unpublished paper (1991).

a general correlation. This semi-empirical correlation is believed to be valid over a range of particle sizes from 10 to 1000 μm . It is expressed as

$$U_{gpu} = \left(1.27 Ar^{-\frac{1}{3}} + 0.036 Ar^{\frac{1}{3}} + 0.45 \right) \left(0.70 Ar^{-\frac{1}{5}} + 1.0 \right) U_{gpu0}. \quad (2-145)$$

The first term on the right-hand side takes into account the effects of particle interactions with the other particles, and the second term accounts for the particle shape.

2.12.5 Boundary Layer Thickness

The boundary layer thickness, δ_l , is approximated by

$$\frac{\delta_l}{x} = 0.370 R_x^{-\frac{1}{5}}, \quad (2-146)$$

where $R_x = u_y x / \nu$, and x is the distance along the wall from the point at which the turbulent fluid initially contacts the wall. To estimate the magnitude of the boundary layer thickness, assume a 300 cfm flow through a 2 ft by 2 ft duct, which is a flow velocity of about 40 cm/s. Then, 10 m from the duct entrance ($x = 10$ m) the boundary layer thickness, δ_l , is about 30 cm. Since the inner layer is approximately 2% of δ_l , the inner layer is approximately 0.6 cm or 6 mm. For a flow velocity of only 10 cm/s and at a distance of 1.0 m from the duct entrance, the boundary layer thickness is only 5 cm, and the inner layer is 1 mm. These examples indicate that generally the deposited particles available for resuspension will be immersed in the inner layer of the boundary layer.

2.12.6 Particle Cloud Model

The particle cloud model permits each discrete computational particle to represent a cluster of particles that can disperse as a Gaussian cloud. The density and size of the particles in the cloud of particles are the same as the computational particle with which the cloud is associated. The particle cloud density, ρ_{pc} , at a selected point that is a distance r from the cloud center is given by

$$\rho_{pc}(r, t) = M_{pc} f(r, \sigma), \quad (2-147)$$

where

$$f(r, \sigma) = \left(\frac{1}{(2\pi)^{\frac{3}{2}} \sigma^3} \right) e^{\frac{-r^2}{2\sigma^2}}, \quad (2-148)$$

and

$$\sigma = r_{pci} + \sqrt{2D_{pc}t}. \quad (2-149)$$

The term M_{pc} is the mass of the particle cloud, D_{pc} is the particle diffusion coefficient of the cloud, r_{pci} is the initial radius of the particle cloud, and t is the elapsed cloud growth time. The radius of the cloud at any elapsed time is $r_{pc} = 3$ s. The cloud density at any given point is determined by the summation of all density contributions of individual particle clouds at that point.

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3 COMPUTATIONAL MODEL

The computational model and solution algorithm for solving the multidimensional, time-dependent fluid-flow equations follows the ICE'd-ALE methodology first introduced by Hirt et al. (Ref. 3-1) and used later in other computational fluid dynamics efforts at Los Alamos (Refs. 3-1 through 3-7).

The computational domain is defined by regular, 3D arrays of regular parallelepiped cells in 3D computing domains, and 1D arrays of either square cross-sections or cylindrical cross-sections in the piping or duct networks. First, each coordinate axis is divided into intervals that define cell faces in that direction. The location of each interval is identified by its physical mesh coordinate (x , y , or z in Cartesian geometry or r , θ , or z in cylindrical geometry) and a corresponding logical coordinate (i , j , or k) called the mesh index. The domain is divided up in the x -direction by planes passing through the x -direction mesh coordinates and normal to the x -axis. Similarly, sets of planes normal to the other directions divide up space in the y - and z - directions. The intersections of the three families of planes define a 3D arrangement of cells ("finite volumes"). Figure 3-1 shows a typical cell, along with conventions for identifying faces and vertices.

Values of the scalar variables ρ , I , and p are computed at cell centers, and the face-normal component of velocity is computed at cell faces or edges. Initial values for each variable and appropriate boundary conditions are set at all locations. The continuous integral equations of motion described in Section 2 are approximated by finite-volume expressions (discrete algebraic equations) on the computational mesh. Thus, the dynamic state in the problem domain can be approximated by integrating the finite-volume equations in space and time.

In the standard ALE method (Ref. 3-1), both fluid and grid ($\mathbf{u}_g$) velocities are located at cell vertices. By specifying $\mathbf{u}_g$ to be different from $\mathbf{u}$, the shape and spatial distribution of the mesh may be changed to model a problem with a deformable boundary. Mass, momentum, and energy are exchanged between cells by averaging vertex velocities to produce a cell-face fluxing velocity. Because GASFLOW is designed to compute flows with fixed geometries, this general mesh motion feature is not needed; therefore, we locate fluid velocities directly on cell faces. Other differences between the standard ALE method and the ALE method implemented in GASFLOW are given in Table 3-1.

Mesh cells serve as control volumes for cell-centered variables and thus serve as the finite volumes for solving the mass and energy equations. Because velocity components are located at cell faces, a different treatment is needed for the

Figure 3-1. GASFLOW 3D computational cell. Velocity components are located at face centers: [W] west (-x), [E] east (+x), [S] south (-y), [N] north (+y), [B] bottom (-z), and [T] top (+z); all other variables, the scalar variables, are located at the cell center.

Table 3-1. Comparison of standard ALE and GASFLOW ALE features

Standard ICE'd ALE	GASFLOW linearized ICE'd ALE
Cell-centered ρ , I , p	Cell-centered ρ , I , p
Vertex-centered u , momentum	Face-centered u , momentum
Total energy (E)	Internal energy (I)
Pressure work is done only in the implicit Lagrangian phase.	Pressure work is done in both the explicit and implicit Lagrangian phases.
Control volumes are (1) computational cells and (2) volumes centered on vertices.	Control volumes are (1) computational cells and (2) volumes centered on cell faces.
Vertex motion algorithm	Vertices stay fixed.
Arbitrary hexahedral cells	Parallelepiped cells
Algorithm for cell volumes	Volume calculations are straightforward.
Face fluxing in rezone phase (face-fluxing u must be computed from vertex u)	x -, y -, and z -face fluxing in rezone phase
	Linearized volume treatment in implicit Lagrangian phase

Figure 3-2. A 2D mesh slice showing the u and v staggered momentum control volumes associated with cell (i, j, k) .

momentum equations. A momentum control volume, V_m , is defined as half of each of the two cells sharing a common face (Figure 3-2). In this sense, we say that momentum control volumes are "face-centered," although this is strictly true only if both cells are the same size. A momentum control volume for the east face of cell (i, j, k) is $V_m = (V_{i,j,k} + V_{i+1,j,k})/2$. A similar definition is made for the momentum control volumes that straddle the north and top faces.

Because we are interested only in the Eulerian solution of the flow equations, a full continuous rezone always will be applied (see Section 3.4, Phase C: Rezone Phase), with the Lagrangian phase being only an intermediate step toward the full solution.

Each fluid dynamics time step is broken into three phases as described below and is followed by turbulent transport calculations.

3.1 Beginning of Time Cycle Initialization

GASFLOW allows the user to compute molecular transport properties by a number of methods. The first and simplest is a "nonmechanistic" calculation using constant default or input variables such as kinematic viscosity, thermal conductivity, binary mass diffusion coefficient, and the nondimensional Prandtl and Schmidt numbers. These options are discussed in detail in the User's Manual. Based upon the gas composition of each finite control volume, the mixture transport properties are updated by the procedures outlined in Section 2.5.1.2 (Transport Properties).

If the user has specified a turbulence model, then the molecular transport coefficients are updated to the apparent or turbulent values using the methodology described in Section 2.7.3 (Turbulence Effects on the Transport Coefficients).

3.2 Phase A: Explicit Lagrangian Phase for the Multidimensional Finite Control Volumes

In this phase, the densities, velocities, and specific internal energy fields are updated by the effects of all chemical and physical processes. These effects include combustion, catalytic recombination, heat transfer, phase change between liquid film on structural surfaces and within the fluid mixture, body forces, and turbulence effects.

3.2.1 Volume Equation

The change in each computational cell volume associated with the scalar variable, V_s , is calculated from the discrete approximation to Equation (2-5) with $\Phi = 1$ and application of the divergence theorem (Appendix A):

$$\frac{V^A - V^n}{\Delta t} = \sum_f (uA)_f^n \Delta S_f \quad (3-1)$$

Superscript A denotes the Lagrangian Phase A, and n denotes the beginning of computation cycle time-level, while subscript f denotes the cell faces of the appropriate control volume.

3.2.2 Momentum Equations

The components of the velocity field then can be found from the discrete approximation of Equation (2-13):

$$\frac{\rho_m^A \mathbf{u}^A V_m^A - \rho_m^n \mathbf{u}^n V_m^n}{\Delta t} = - \sum_f (p)_f^n \mathbf{S}_f + \rho_m^n \mathbf{g} V_m^n - \sum_f (\tau A)_f^n \Delta S_f - \sum_f (\mathbf{D}_d A)_f^A \Delta S_f \quad (3-2)$$

In addition to the resistance to flow through reduced flow areas, areas that are smaller than the computational cell-face area, the structural drag vector, $\mathbf{D}_d$, can represent the resistance of internal structures such as pipes, I-beams, catwalks, and such configurations that are impossible to resolve on any practical mesh. These internal structures play an important role as heat sinks and, to a lesser degree, as momentum sinks. However, we do attempt to model their momentum effects by the expression

$$\mathbf{D}_d = \frac{1}{2} \mathbf{C}_D (\rho_m \mathbf{u})^A |\mathbf{u}^n| \quad (3-3)$$

where the subscript m refers to the staggered momentum control volumes associated with the velocity field. Note that fractional A is dependent on the orientation of the structures. For example, there is little resistance to flows parallel to the gratings of the catwalks but quite a different resistance to flows normal to the gratings. The drag coefficient, C_D , for reduced area flows is computed from an orifice correlation (Ref. 3-8).

$$C_D = \left[1 + 0.707 \cdot (1 - A)^{\frac{1}{2}} - A \right]^2, \quad (3-4)$$

or can be determined empirically or selected from tables of drag coefficients of common shapes.

Equation (3-2) with Equation (3-3) can be solved for the advanced time-level "A" momenta as

$$\rho_m^A \mathbf{u}^A = \frac{\rho_m^n \mathbf{u}^n V_m^n - \Delta t \left[\sum_f (p)_f^n S_f - \rho_m^n \mathbf{g} V_m^n + \sum_f (\tau A)_f^n \Delta S_f \right]}{V_m^A + \Delta t A \frac{1}{2} C_D |\mathbf{u}^n| S_f}, \quad (3-5)$$

which provides a computationally fast, local implicitness that provides additional robustness to Phase A and the GASFLOW algorithm. When the mixture density field is updated to the same time-level, as will be shown below, the velocity field can be determined.

3.2.3 Mixture and Species Mass Equations

The mass change for each species because of combustion, phase change, and inter-species diffusion is calculated as follows:

$$\begin{aligned} \frac{\rho_\alpha^A V^A - \rho_\alpha^n V^n}{\Delta t} = & - \sum_f (JA)_f^n \Delta S_f + S_{\rho, \alpha, recombination}^A V^n + \\ & S_{\rho, \alpha, combustion}^A V^n + S_{\rho, h_2o, mixture}^A V^n + S_{\rho, h_2o, condensation/vaporization}^A V^n + S_{\rho, h_2ol, rainout}^A V^n. \end{aligned} \quad (3-6)$$

When Equations (3-2) is summed over all species, we derive the Phase A mixture mass equation:

$$\frac{\rho^A V^A - \rho^n V^n}{\Delta t} = S_{\rho, h_2o, condensation/vaporization}^A V^n + S_{\rho, h_2ol, rainout}^A V^n. \quad (3-7)$$

The "A" time-level on the various source and sink terms will become evident as those models are developed in the sections below.

3.2.4 Internal Energy Equation

The change in the total internal energy can be written from Equation (2-14) as

$$\begin{aligned} \frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = & -p^n \sum_f (\mathbf{u} \cdot \mathbf{A})_f^n \Delta S_f + S_{I, \text{recombination}}^A V^n + \\ & \Re_{h_2o} T^A (S_{p, h_2o, \text{condensation/vaporization}}^A + S_{p, h_2o, \text{mixture}}^A) V^n - \sum_f (\mathbf{q} \cdot \mathbf{A})_f^n \Delta S_f + \\ & S_{I, \text{convection}}^A V^n + S_{I, \text{combustion}}^A V^n + S_{I, \text{condensation/vaporization}}^A V^n + S_{I, \text{rainout}}^A V^n \end{aligned} \quad (3-8)$$

All source terms will be derived and discussed in subsequent sections.

3.2.5 Gas Mixture Temperature

The gas-mixture temperature, T^A , is computed by inverting a polynomial of up to the 4th degree, which is similar to Equation (2-18) but cast in a slightly different form

$$A_0 + T^A A_1 + (T^A)^2 A_2 + (T^A)^3 A_3 + (T^A)^4 A_4 = 0 \quad (3-9)$$

such that the polynomial coefficients contain all the know quantities from Equations (3-6) and (3-8). These coefficients will become evident in later developments. The user specifies in the input the degree of the polynomial, from linear to quartic. Our development here will assume the quartic because it contains all the ingredients of the lesser degree polynomials.

3.2.6 Equation of State

Finally, the updated pressure is determined from the equation of state [Equation (2-25)] as follows:

$$p^A = \frac{T^A \sum_{\alpha \neq h_2ol} R_\alpha \rho_\alpha^A}{1 - \theta_{h_2ol}^n} \quad (3-10)$$

where the gas volume fraction is

$$\theta_{h_2ol}^n = 1 - \frac{\rho_{h_2ol}^n}{\rho_{h_2ol}^{thermo}} \quad (3-11)$$

3.2.7 Structural Heat Conduction

A heat conducting solid of depth x_D is discretized by N heat conducting elements ($1 \leq j \leq N$). Material properties (ρ , c_p , and κ) are independent of temperature in these derivations but thermal conductivity can be different in each element (composite layer). Nodes, also numbered 1 through N , are located on the positive side of the conducting elements. Node zero denotes the surface node on the negative side; node N denotes the surface node on the positive side as shown in Figure 3-3.

Figure 3-3. Geometry for 1D structural heat conduction

For purposes of problem definition, heat conducting structures are divided into three categories: slabs, sinks, and walls. *Slabs* and *sinks* have only one element in contact with fluid (element No. 1). More accurate spatial resolution of temperatures is generally wanted near the fluid/structure interface; hence, the smallest element is normally element 1 with increasing element sizes away from the interface. *Walls* have both surfaces in contact with a fluid. Comparable discretization of each structural type is shown in Figures 3-4 and 3-5.

Figure 3-4. Slab and sink discretization

Figure 3-5. Wall discretization

New time-level temperatures at all but the boundary nodes are computed from an implicit finite-difference approximation to Equation (2-52). Details are presented in Appendix B in the following equation:

$$\frac{V\rho c_p}{\Delta t}(T_j^{n+1} - T_j^n) = A \left[\begin{aligned} & \left((1-\Theta)(T_{j+1}^n - T_j^n) + \Theta(T_{j+1}^{n+1} - T_j^{n+1}) \right) k_{j+1} / \Delta x_e \\ & - \left((1-\Theta)(T_j^n - T_{j-1}^n) + \Theta(T_j^{n+1} - T_{j-1}^{n+1}) \right) k_j / \Delta x_w \end{aligned} \right] \quad (3-12)$$

Three methods are provided for the evaluation of this equation: (1) the temporal fully implicit first-order backward Euler method ($\Theta = 1$), (2) the temporal unconditionally stable second-order Crank-Nicholson method ($\Theta = \frac{1}{2}$), and (3) the temporal fully explicit first-order backward Euler method ($\Theta = 0$). The explicit method is not recommended for containment analyses in which many temporal and spatial scales are encountered.

Different boundary conditions, including specified temperature, specified heat flux, as well as an adiabatic surface, are provided in the solution of Equation (3-12). These details are discussed in Appendix B.

Equation (3-12) and two boundary-condition-dependent equations for nodes 0 and N are a linear system of N equations for the unknown temperatures T_i^{n+1} that are found from a tridiagonal matrix solution algorithm.

3.2.8 Mass and Energy Transfer

3.2.8.1 Structural Convective Heat Transfer

Whenever the temperatures of structural surfaces and the adjacent gas differ there will be heat exchange by convection. In the case when neither water component is included in the calculation, all species densities remain unchanged during this calculation. The resulting change in energy of the gas appears as source terms in the Phase A energy Equation (3-8) with Equation (2-27),

$$\frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = S_{I,convection}^A V^n = \sum_s h_s A_s (T_s^n - T^A) \quad , \quad (3-13)$$

and as a heat flux boundary condition in the structural heat conduction Equation (3-12). The uncorrected (there is no water component in this case) heat transfer coefficient is computed from Equation (2-29). Making use of Equation (2-18) gives a polynomial of up to degree 4,

$$\left[\sum_{\alpha} (\rho_{\alpha}^A a_{\alpha}) - \rho^n I^n \frac{V^n}{V^A} - \frac{\Delta t}{V^A} \sum_s h_s A_s T_s^n \right] + T^A \left[\sum_{\alpha} (\rho_{\alpha}^A b_{\alpha}) + \frac{\Delta t}{V^A} \sum_s h_s A_s \right] + (T^A)^2 \sum_{\alpha} (\rho_{\alpha}^A c_{\alpha}) + (T^A)^3 \sum_{\alpha} (\rho_{\alpha}^A d_{\alpha}) + (T^A)^4 \sum_{\alpha} (\rho_{\alpha}^A e_{\alpha}) = 0 \quad , \quad (3-14)$$

which must be inverted to find the new mixture temperature. This equation demonstrates the combination of terms that make up the coefficients presented in Equation (3-9). Once the mixture temperature is found the source term in the energy equation can be computed from

$$S_{I,convection}^A V^n = \sum_s h_s A_s (T_s^n - T^A) \quad , \quad (3-15)$$

and, therefore, the energy convected to or from any given surface is

$$q_{s,total} = q_{s,convection} = h_s A_s (T^A - T_s^n) \quad . \quad (3-16)$$

3.2.8.2 Structural Convective Heat and Mass Transfer

When the water vapor component is specified with user input, phase change on structural surfaces may occur. In this case, the water vapor species mass Equation (3-6) with Equation (2-42) is

$$\frac{\rho_{h_2o}^A V^A - \rho_{h_2o}^n V^n}{\Delta t} = S_{\rho,h_2o,condensation/vaporization}^A V^n = - \sum_s \max \left[- \frac{\delta_s^n A_s \rho_{h_2o}^{thermo}}{2 \Delta t}, h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \quad , \quad (3-17)$$

and the energy Equation (3-8) with Equations (2-27) and (2-44) becomes

$$\frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = \Re_{h_2o} T^A S_{\rho,h_2o,condensation/vaporization}^A V^n + S_{I,convection}^A V^n + S_{I,condensation/vaporization}^A V^n =$$

$$\mathcal{R}_{h_2o} T^A S_{\rho, h_2o, condensation/vaporization}^A V^n + \sum_s h_s A_s (T_s^n - T^A) +$$

$$- \sum_s \max \left[\begin{array}{l} -\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2 \Delta t} I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o}^A - \rho_{s, saturation}) I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o}^A - \rho_{s, saturation}) I_{h_2o}(T^A) \end{array} \right] . \quad (3-18)$$

The enhanced or corrected heat and mass transfer coefficients are computed as described in Sections 2.6.1 and 2.6.2, and the surface saturation density is evaluated by the formulation given in Section 2.6.2.

The solution procedure for Equations (3-17) and (3-18) requires several passes through the mesh. For example, the term on the right-hand side of Equation (3-17) checks to see if surface dryout occurs (the liquid film is depleted); this must be determined without knowing the advanced time-level water vapor density. One could employ a iterative scheme, but we have found a much faster solution procedure: we make a predictive pass through the mesh and then, based upon the predictive information, a correction pass is performed.

First, a fully local implicit evaluation of Equation (3-17) is executed without regard to surface dryout to find a predicted density, $\rho_{h_2o}^p$, by reducing Equation (3-17) to

$$\frac{\rho_{h_2o}^p V^A - \rho_{h_2o}^n V^n}{\Delta t} = - \sum_s h_d^* A_s (\rho_{h_2o}^p - \rho_{s, saturation}) . \quad (3-19)$$

The solution for the predictor water vapor density, $\rho_{h_2o}^p$, is

$$\rho_{h_2o}^p = \frac{\rho_{h_2o}^n V^n + \Delta t \sum_s h_d^* A_s \rho_{s, saturation}}{V^A + \Delta t \sum_s h_d^* A_s} . \quad (3-20)$$

The corrective step makes use of the predicted density, $\rho_{h_2o}^p$, in the following way:

$$\frac{\rho_{h_2o}^A V^A - \rho_{h_2o}^n V^n}{\Delta t} =$$

$$\begin{aligned}
& - \sum_s^{\text{evaporation}} \left[1 - H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{\text{thermo}}}{2 \Delta t}, \right. \\
& \left. - \sum_s^{\text{condensation}} H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) \cdot \max \left[0, \right. \right. \\
& \left. \left. h_d^* A_s (\rho_{h_2o}^A - \rho_{s,\text{saturation}}) \right] \right] , \quad (3-21)
\end{aligned}$$

where $H(\rho_{h_2o}^p - \rho_{s,\text{saturation}})$ is the usual Heaviside function

$$H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) = \begin{cases} 0; \rho_{h_2o}^p - \rho_{s,\text{saturation}} < 0 \\ 1; \rho_{h_2o}^p - \rho_{s,\text{saturation}} > 0 \end{cases} . \quad (3-22)$$

Note that the first term on the right-hand side of the equation acts as a source of water vapor because evaporation of the liquid film is occurring, whereas the second term on the right-hand side is a loss of water vapor mass due to condensation of water vapor in the mixture. Since the second term could result in negative water vapor density, it can be treated implicitly with the water vapor source term being treated as a constant. The corrected water vapor density is then computed as follows:

$$\rho_{h_2o}^A = \frac{\rho_{h_2o}^n V^n - \Delta t \left\{ \begin{aligned} & \sum_s^{\text{evaporation}} \left[1 - H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{\text{thermo}}}{2 \Delta t}, \right. \\ & \left. - \sum_s^{\text{condensation}} H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) \cdot h_d^* A_s \rho_{s,\text{saturation}} \right] \end{aligned} \right\}}{V^A + \Delta t \sum_s^{\text{condensation}} H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) \cdot h_d^* A_s} . \quad (3-23)$$

The actual source term is then computed as follows:

$$S_{\rho, h_2o, \text{condensation/vaporization}}^A V^n =$$

$$\begin{aligned}
& - \sum_s^{\text{evaporation}} \left[1 - H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{\text{thermo}}}{2 \Delta t}, \right. \\
& \left. - \sum_s^{\text{condensation}} H(\rho_{h_2o}^p - \rho_{s,\text{saturation}}) \cdot \max \left[0, \right. \right. \\
& \left. \left. h_d^* A_s (\rho_{h_2o}^A - \rho_{s,\text{saturation}}) \right] \right] , \quad (3-24)
\end{aligned}$$

where the mass transfer for each surface is

$$\begin{aligned} \dot{m}_s = & \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2 \Delta t}, \right. \\ & \left. h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \right] \\ & + H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \\ & \left. h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \end{aligned} \quad (3-25)$$

The liquid film thickness, δ_s^A , for each surface is finally updated using the mass transfer computed by Equation (3-25):

$$\delta_s^A = \delta_s^n + \frac{\dot{m}_s \Delta t}{A_s \rho_{h_2ol}^{thermo}} \quad (3-26)$$

The energy equation (3-18) can be evaluated to determine the mixture temperature by inverting the following equation:

$$\begin{aligned} & \left\{ \sum_{\alpha} (\rho_{\alpha}^A a_{\alpha}) - \frac{1}{V^A} \rho^n T^n V^n - \frac{\Delta t}{V^A} \sum_s h_s A_s T_s^n + \right. \\ & \left. \frac{\Delta t}{V^A} \sum_s \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2 \Delta t} I_{h_2o}(T_s), \right. \right. \\ & \left. \left. h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) I_{h_2o}(T_s) \right] \right\} + \\ & \left\{ \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \right. \\ & \left. \left. a_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \right\} \\ & T^A \left\{ \sum_{\alpha} (\rho_{\alpha}^A b_{\alpha}) - \frac{\Delta t}{V^A} R_{h_2o} S_{\rho, h_2o, condensation/vaporization}^A V^n + \frac{\Delta t}{V^A} \sum_s h_s A_s + \right. \\ & \left. \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \right. \\ & \left. \left. b_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \right\} + \\ & (T^A)^2 \left\{ \sum_{\alpha} (\rho_{\alpha}^A c_{\alpha}) + \right. \\ & \left. \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \right. \\ & \left. \left. c_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \right\} + \end{aligned}$$

$$\begin{aligned}
& (T^A)^3 \left\{ \sum_{\alpha} (\rho_{\alpha}^A d_{\alpha}) + \right. \\
& \left. \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \right. \\
& \left. \left. d_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \right\} + \\
& (T^A)^4 \left\{ \sum_{\alpha} (\rho_{\alpha}^A e_{\alpha}) + \right. \\
& \left. \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \right. \\
& \left. \left. e_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \right\} = 0 \quad (3-27)
\end{aligned}$$

Once the mixture density and temperature are found, we can determine each of the energy source terms found in Equation (3-18) as follows:

$$\begin{aligned}
& R_{h_2o} T^A S_{\rho, h_2o, condensation/vaporization}^A V^n = \\
& -R_{h_2o} T^A \left\{ \begin{aligned} & \sum_s^{evaporation} [1 - H(\rho_{h_2o}^p - \rho_{s,saturation})] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2\Delta t}, \right. \\ & \left. h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \right] \\ & + \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \\ & \left. h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \end{aligned} \right\} \quad (3-28)
\end{aligned}$$

$$S_{I, convection}^A V^n = \sum_s h_s A_s (T_s^n - T^A) \quad (3-29)$$

$$\begin{aligned}
& S_{I, condensation/vaporization}^A V^n = \\
& - \sum_s^{evaporation} [1 - H(\rho_{h_2o}^p - \rho_{s,saturation})] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2\Delta t}, \right. \\
& \left. h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \right] \\
& - \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \\
& \left. h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \quad (3-30)
\end{aligned}$$

The total energy, $q_{s,total}$, delivered to a given surface is

$$q_{s,total} = q_{s,convection} + q_{s,condensation/vaporization} =$$

$$\begin{aligned}
& h_s A_s (T^A - T_s^n) + \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \left\{ \max \left[\begin{aligned} & -\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2\Delta t}, \\ & h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \end{aligned} \right] \right. \\
& \left. \left[h_{fg} + I_{h_2o}(T_s^n) \right] \right\} \\
& + H(\rho_{h_2o}^p - \rho_{s,saturation}) \left\{ \max \left[\begin{aligned} & 0, \\ & h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \end{aligned} \right] \right. \\
& \left. \left[h_{fg} + I_{h_2o}(T^A) - I_{h_2o}(T_s^n) \right] \right\} . \quad (3-31)
\end{aligned}$$

3.2.8.3 Structural Convective Heat and Mass Transfer with Phase Change in the Fluid Mixture – HEM

When the water vapor and liquid components are specified with user input, phase change on structural surfaces may occur plus phase change with the fluid mixture may also occur. In this case, the water vapor species mass Equation (3-6) with Equations (2-42) and (2-45) is

$$\begin{aligned}
\frac{\rho_{h_2o}^A V^A - \rho_{h_2o}^n V^n}{\Delta t} &= S_{\rho, h_2o, condensation/vaporization}^A V^n + S_{\rho, h_2o, mixture}^A V^n = \\
& - \sum_s \max \left[-\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2\Delta t}, h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \\
& - V^n C \cdot \max \left[\begin{aligned} & -\rho_{h_2ol}^n / 2, \\ & \rho_{h_2o}^A - \rho_{saturation}(T, p_{saturation}) \end{aligned} \right] , \quad (3-32)
\end{aligned}$$

the water liquid species mass Equation (3-6) is

$$\begin{aligned}
\frac{\rho_{h_2ol}^A V^A - \rho_{h_2ol}^n V^n}{\Delta t} &= S_{\rho, h_2ol, fluid}^A V^n = -S_{\rho, h_2o, mixture}^A V^n = \\
& + V^n C \cdot \max \left[\begin{aligned} & -\rho_{h_2ol}^n / 2, \\ & \rho_{h_2o}^A - \rho_{saturation}(T, p_{saturation}) \end{aligned} \right] , \quad (3-33)
\end{aligned}$$

and the energy Equation (3-8) with Equations (2-27), (2-44), and (2-49) is

$$\frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = \mathfrak{R}_{h_2o} T^A (S_{\rho, h_2o, condensation/vaporization}^A + S_{\rho, h_2o, mixture}^A) V^n +$$

$$\begin{aligned}
& S_{I,condensation/vaporization}^A V^n + S_{I,convection}^A V^n + \\
& R_{h_2o} T^A \left(S_{\rho,h_2o,condensation/vaporization}^A + S_{\rho,h_2o,mixture}^A \right) V^n + \sum_s h_s A_s (T_s^n - T^A) + \\
& - \sum_s \max \left[\begin{array}{l} -\frac{\delta_s^n A_s \rho_{h_2o}^{thermo}}{2 \Delta t} I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) I_{h_2o}(T_s), \\ h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) I_{h_2o}(T^A) \end{array} \right] . \quad (3-34)
\end{aligned}$$

A limiter of 1/2 is invoked in the right most term in Equation (3-32) and (3-33) to prevent the liquid density from going negative. The enhanced or corrected heat and mass transfer coefficients are computed as described in Sections 2.6.1 and 2.6.2, the surface saturation density is evaluated by the formulation given in Section 2.6.2, and the saturation density in the fluid mixture is computed from Equation (2-48) in Section 2.6.3.

The solution procedure for Equation (3-32) is very similar to the solution procedure shown in the previous section which required several passes through the mesh. For example, the first term on the right-hand side of Equation (3-32) checks to see if surface dryout occurs (the liquid film is depleted), whereas the second term accounts for phase change within the fluid mixture. We again implement a procedure to make a predictive pass through the mesh, and then, based upon the predictive information, a correction pass is performed.

First, a fully local implicit evaluation of Equation (3-32) is executed without regard to surface dryout to find a predicted density, $\rho_{h_2o}^p$, by reducing Equation (3-32) to the following:

$$\begin{aligned}
& \frac{\rho_{h_2o}^p V^A - \rho_{h_2o}^n V^n}{\Delta t} = \\
& - \sum_s h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) - V^n C [\rho_{h_2o}^p - \rho_{saturation}(T, p_{saturation})] . \quad (3-35)
\end{aligned}$$

The solution to this equation is

$$\rho_{h_2o}^p = \frac{\rho_{h_2o}^n V^n + \Delta t \left\{ \sum_s h_d^* A_s \rho_{s,saturation} + V^n C \rho_{saturation}(T, p_{saturation}) \right\}}{V^A + \Delta t \left\{ \sum_s h_d^* A_s + V^n C \right\}} . \quad (3-36)$$

The corrective step makes use of the predicted density, $\rho_{h_2o}^p$, in the following way:

$$\begin{aligned}
 \frac{\rho_{h_2o}^A V^A - \rho_{h_2o}^n V^n}{\Delta t} = & \\
 & - \sum_s^{evaporation} \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2 \Delta t}, \right. \\
 & \left. h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \right] \\
 & - \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \right. \\
 & \left. h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \\
 & - V^n C \left\{ \left[1 - H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat})) \right] \cdot \max \left[\frac{-\rho_{h_2ol}^n / 10,}{\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat})} \right] \right. \\
 & \left. + H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat})) \cdot \max \left[0, \right. \right. \\
 & \left. \left. \rho_{h_2o}^A - \rho_{sat}(T^n, p_{sat}) \right] \right\} . \tag{3-37}
 \end{aligned}$$

Using the same reasoning as in the previous section, we note that the first term on the right-hand side of the equation acts as a source of water vapor because evaporation of the liquid film is occurring, whereas the second term on the right-hand side is a loss of water vapor mass due to condensation of water vapor from the mixture. The third term is the exchange of mass between the liquid and vapor phases, which can be either a source or sink in this equation. Since the second and third terms could result in negative water vapor density, they can be treated implicitly with the water vapor source term being treated as a constant.

Solving Equation (3-35) for $\rho_{h_2o}^A$ yields

$$\rho_{h_2o}^A = \frac{\rho_{h_2o}^n V^n - \Delta t \left\{ \begin{aligned} & V^n C \cdot [1 - H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat}))] \cdot \max \left[\begin{aligned} & -\rho_{h_2ol}^n / 10, \\ & \rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat}) \end{aligned} \right] \\ & + \sum_s^{evaporation} [1 - H(\rho_{h_2o}^p - \rho_{s,sat})] \cdot \max \left[\begin{aligned} & \frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2\Delta t}, \\ & h_d^* A_s (\rho_{h_2o}^p - \rho_{s,sat}) \end{aligned} \right] \\ & - \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot h_d^* A_s \rho_{s,saturation} \end{aligned} \right\}}{V^A + \Delta t \left(V^n C \cdot [1 - H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat}))] + \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot h_d^* A_s \right)} \quad (3-38)$$

The actual source terms are then computed as follows:

$$\begin{aligned} S_{\rho, h_2o, condensation/vaporization}^A V^n = & \\ & - \sum_s^{evaporation} [1 - H(\rho_{h_2o}^p - \rho_{s,saturation})] \cdot \max \left[\begin{aligned} & \frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2\Delta t}, \\ & h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \end{aligned} \right] \\ & - \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[\begin{aligned} & 0, \\ & h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \end{aligned} \right] \end{aligned} \quad (3-39)$$

The mass transfer between phases in the mixture is

$$S_{\rho, h_2o, mixture}^A V^n = -V^n C \left\{ \begin{aligned} & [1 - H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat}))] \cdot \max \left[\begin{aligned} & -\rho_{h_2ol}^n / 10, \\ & \rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat}) \end{aligned} \right] \\ & + H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat})) \cdot \max \left[\begin{aligned} & 0, \\ & \rho_{h_2o}^A - \rho_{sat}(T^n, p_{sat}) \end{aligned} \right] \end{aligned} \right\} \quad (3-40)$$

Just as in the previous section, the actual mass transfer to or from any given surface is

$$\dot{m}_s = [1 - H(\rho_{h_2o}^p - \rho_{s,saturation})] \cdot \max \left[\begin{aligned} & \frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2\Delta t}, \\ & h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \end{aligned} \right]$$

$$+H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \quad (3-41)$$

The liquid film thickness, δ_s^A , for each surface is finally updated using the mass transfer computed by Equation (3-41):

$$\delta_s^A = \delta_s^n + \frac{\dot{m}_s \Delta t}{A_s \rho_{h_2o}^{thermo}} \quad (3-42)$$

The energy Equation (3-34) can be evaluated to determine the mixture temperature by inverting the following equation:

$$\left\{ \begin{aligned} & \sum_{\alpha} (\rho_{\alpha}^A a_{\alpha}) - \frac{1}{V^A} \rho^n I^n V^n - \frac{\Delta t}{V^A} \sum_s h_s A_s T_s^n + \\ & \frac{\Delta t}{V^A} \sum_s \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \cdot \max \left[\begin{aligned} & -\frac{\delta A_s \rho_{h_2o}^{thermo}}{2 \Delta t} I_{h_2o}(T_s), \\ & h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) I_{h_2o}(T_s) \end{aligned} \right] + \\ & \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, a_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \end{aligned} \right\} + \\ T^A \left\{ \begin{aligned} & \sum_{\alpha} (\rho_{\alpha}^A b_{\alpha}) - \frac{\Delta t}{V^A} R_{h_2o} (S_{\rho,h_2o,condensation/vaporization}^A + S_{\rho,h_2o,mixture}^A) V^n + \\ & \frac{\Delta t}{V^A} \sum_s h_s A_s + \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, b_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \end{aligned} \right\} + \\ (T^A)^2 \left\{ \begin{aligned} & \sum_{\alpha} (\rho_{\alpha}^A c_{\alpha}) + \\ & \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, c_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \end{aligned} \right\} + \\ (T^A)^3 \left\{ \begin{aligned} & \sum_{\alpha} (\rho_{\alpha}^A d_{\alpha}) + \\ & \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, d_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \right] \end{aligned} \right\} +$$

$$(T^A)^4 \left\{ \sum_{\alpha} (\rho_{\alpha}^A e_{\alpha}) + \frac{\Delta t}{V^A} \sum_s H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \frac{e_{h_2o} h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation})}{2 \Delta t} \right] \right\} = 0 \quad (3-43)$$

Once the mixture density and temperature are found, we can determine each of the energy source terms found in Equation (3-34) as follows:

$$R_{h_2o} T^A (S_{\rho, h_2o, condensation/vaporization}^A + S_{\rho, h_2o, mixture}^A) V^n = -R_{h_2o} T^A \left\{ \begin{aligned} & \sum_s^{evaporation} \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2 \Delta t}, \frac{h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation})}{2 \Delta t} \right] + \\ & \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \frac{h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation})}{2 \Delta t} \right] + \\ & V^n C \left\{ \begin{aligned} & \left[1 - H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat})) \right] \cdot \max \left[\frac{-\rho_{h_2ol}^n / 10, \rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat})}{2 \Delta t} \right] \\ & + H(\rho_{h_2o}^p - \rho_{sat}(T^n, p_{sat})) \cdot \max \left[0, \frac{\rho_{h_2o}^A - \rho_{sat}(T^n, p_{sat})}{2 \Delta t} \right] \end{aligned} \right\} \end{aligned} \right\} \quad (3-44)$$

$$S_{I, convection}^A V^n = \sum_s h_s A_s (T_s^n - T^A) \quad (3-45)$$

$$S_{I, condensation/vaporization}^A V^n = - \sum_s^{evaporation} \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \cdot \max \left[\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2 \Delta t}, \frac{h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation})}{2 \Delta t} \right] - \sum_s^{condensation} H(\rho_{h_2o}^p - \rho_{s,saturation}) \cdot \max \left[0, \frac{h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation})}{2 \Delta t} \right] \quad (3-46)$$

The total energy, $q_{s, total}$, delivered to a given surface is

$$q_{s, total} = q_{s, convection} + q_{s, condensation/vaporization} =$$

$$\begin{aligned}
& h_s A_s (T^A - T_s^n) + \left[1 - H(\rho_{h_2o}^p - \rho_{s,saturation}) \right] \left\{ \max \left[\begin{aligned} & -\frac{\delta_s^n A_s \rho_{h_2ol}^{thermo}}{2 \Delta t}, \\ & h_d^* A_s (\rho_{h_2o}^p - \rho_{s,saturation}) \end{aligned} \right] \right\} \\
& + H(\rho_{h_2o}^p - \rho_{s,saturation}) \left\{ \max \left[\begin{aligned} & 0, \\ & h_d^* A_s (\rho_{h_2o}^A - \rho_{s,saturation}) \end{aligned} \right] \right\} \\
& \left\{ \begin{aligned} & [h_{fg} + I_{h_2o}(T_s^n)] \\ & [h_{fg} + I_{h_2o}(T^A) - I_{h_2o}(T_s^n)] \end{aligned} \right\} . \quad (3-47)
\end{aligned}$$

3.2.9 Liquid Droplet Depletion or "Rainout"

When the water liquid component is specified with user input, water droplets may be allowed to rain out if the accumulation of liquid water mass exceeds a specified loading value. The liquid water species mass Equation (3-6) with Equation (2-50) is

$$\begin{aligned}
& \frac{\rho_{h_2ol}^A V^A - \rho_{h_2ol}^n V^n}{\Delta t} = S_{\rho,h_2ol,rainout}^A V^n = \\
& + V^n C_{h_2ol,mixture} \cdot \min \left[\begin{aligned} & 0, \\ & (\rho_{h_2ol,max} - \rho_{h_2ol}^A) \end{aligned} \right] , \quad (3-48)
\end{aligned}$$

and the energy Equation (3-8) with Equation (2-51) is

$$\begin{aligned}
& \frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = S_{I,rainout}^A V^n = \\
& V^n C_{h_2ol,mixture} \cdot \min \left[\begin{aligned} & 0, \\ & (\rho_{h_2ol,max} - \rho_{h_2ol}^A) \end{aligned} \right] \cdot I(T^A) . \quad (3-49)
\end{aligned}$$

Equation (3-48) is only solved if the liquid density exceeds a specified value. If that should be true, then the advanced time-level liquid water density is

$$\rho_{h_2ol}^A = \frac{\rho_{h_2ol}^n V^n + \Delta t V^n C_{h_2ol,mixture} \rho_{h_2ol,max}}{V^A + \Delta t V^n C_{h_2ol,mixture}} , \quad (3-50)$$

which allows an easy evaluation of the rainout mass term

$$S_{\rho, h_{2ol}, rainout}^A V^n = V^n C_{h_{2ol}, mixture} \cdot \min \left[0, \left(\rho_{h_{2ol}, max} - \rho_{h_{2ol}}^A \right) \right] \quad (3-51)$$

The time-advanced mixture temperature is computed from Equation (3-49) as

$$\begin{aligned} & \text{EMBED "Equation" * mergeformat} \\ & \left[\sum_{\alpha} \rho_{\alpha}^A a_{\alpha} - \rho^n I^n \frac{V^n}{V^A} - \Delta t \frac{V^n}{V^A} C_{h_{2ol}, mixture} \cdot \left(\rho_{h_{2ol}, max} - \rho_{h_{2ol}}^A \right) a_{h_{2ol}} \right] \\ & + (T^A) \left[\sum_{\alpha} \rho_{\alpha}^A b_{\alpha} - \Delta t \frac{V^n}{V^A} C_{h_{2ol}, mixture} \cdot \left(\rho_{h_{2ol}, max} - \rho_{h_{2ol}}^A \right) b_{h_{2ol}} \right] \\ & + (T^A)^2 \left[\sum_{\alpha} \rho_{\alpha}^A c_{\alpha} - \Delta t \frac{V^n}{V^A} C_{h_{2ol}, mixture} \cdot \left(\rho_{h_{2ol}, max} - \rho_{h_{2ol}}^A \right) c_{h_{2ol}} \right] \\ & + (T^A)^3 \left[\sum_{\alpha} \rho_{\alpha}^A d_{\alpha} - \Delta t \frac{V^n}{V^A} C_{h_{2ol}, mixture} \cdot \left(\rho_{h_{2ol}, max} - \rho_{h_{2ol}}^A \right) d_{h_{2ol}} \right] \\ & + (T^A)^4 \left[\sum_{\alpha} \rho_{\alpha}^A e_{\alpha} - \Delta t \frac{V^n}{V^A} C_{h_{2ol}, mixture} \cdot \left(\rho_{h_{2ol}, max} - \rho_{h_{2ol}}^A \right) e_{h_{2ol}} \right] = 0 \quad , \end{aligned} \quad (3-52)$$

which allows a straight forward evaluation of the rainout energy term

$$S_{I, rainout}^A V^n = V^n C_{h_{2ol}, mixture} \cdot \left(\rho_{h_{2ol}, max} - \rho_{h_{2ol}}^A \right) \cdot I(T^A) \quad (3-53)$$

3.2.10 Hydrogen Combustion

3.2.10.1 One-Step Model

For the current one-step chemical kinetics model [Equation (2-74)], we see that three species—hydrogen, oxygen, and water vapor—are involved in this fundamental chemical balance. The mass Equation (3-6) for each of these species is

$$\begin{aligned} \frac{\rho_{h_2}^A V^A - \rho_{h_2}^n V^n}{\Delta t} &= S_{\rho, h_2, combustion}^A V^n \\ \frac{\rho_{o_2}^A V^A - \rho_{o_2}^n V^n}{\Delta t} &= S_{\rho, o_2, combustion}^A V^n \\ \frac{\rho_{o_2}^A V^A - \rho_{o_2}^n V^n}{\Delta t} &= S_{\rho, h_2 o, combustion}^A V^n \end{aligned} \quad (3-54)$$

and the Energy equation (3-8) is

$$\frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = S_{I, combustion}^A V^n \quad (3-55)$$

We use Equations (2-75), (2-78), (2-80), and (2-84) to obtain the right-hand sides of the above equations, with

$$\frac{d\rho_\alpha}{dt} = M_\alpha \frac{dc_\alpha}{dt} \quad (3-56)$$

If the mixture is fuel lean, $c_{h_2} < 2 \cdot c_{o_2}$, we solve Equation (2-82) and arrive at

$$\frac{1}{2} \frac{c_{h_2}^A - c_{h_2}^n}{\Delta t} = \dot{\omega} = \frac{k(T) c_{o_2}^n c_{h_2}^n}{1 + 2\Delta t k(T) c_{o_2}^n} \quad (3-57)$$

and if the mixture is fuel rich, $c_{h_2} > 2 \cdot c_{o_2}$, we solve Equation (2-83) and arrive at

$$-\frac{c_{o_2}^A - c_{o_2}^n}{\Delta t} = \dot{\omega} = \frac{k(T) c_{o_2}^n c_{h_2}^n}{1 + \Delta t k(T) c_{h_2}^n} \quad (3-58)$$

which gives the mass source terms for Equation (3-54)

$$\begin{aligned} S_{\rho, h_2, combustion}^A &= -2M_{h_2} \dot{\omega} \\ S_{\rho, o_2, combustion}^A &= -M_{o_2} \dot{\omega} \\ S_{\rho, h_2 o, combustion}^A &= -2M_{h_2 o} \dot{\omega} \end{aligned} \quad (3-59)$$

and the energy source term

$$S_{I, combustion}^A = C_c \cdot \dot{\omega} \quad (3-60)$$

Note that the solutions for the reaction rate, $\dot{\omega}$, in both Equations (3-57) and (3-58) contain the rate constant described by Equation (2-80), which is only a function of the mixture temperature. When computing the chemical kinetics of this model, the temperature is held constant, but it is this rate constant that provides the key to modeling ignitors. When an ignitor is activated, Equation (2-111) in Section 2.10 is evaluated with a temperature of 2000K, which effectively ignites the flammable mixture.

3.2.10.2 Two-Step Model

For this model, as for the one-step model, the three species hydrogen, oxygen, and water vapor are involved in the chemical balance. The mass equation [Equation (36)] for each of these species is

$$\begin{aligned}\frac{\rho_{h_2}^A V^A - \rho_{h_2}^n V^n}{\Delta t} &= S_{\rho, h_2, combustion}^A V^n \\ \frac{\rho_{o_2}^A V^A - \rho_{o_2}^n V^n}{\Delta t} &= S_{\rho, o_2, combustion}^A V^n \\ \frac{\rho_{h_2 o}^A V^A - \rho_{h_2 o}^n V^n}{\Delta t} &= S_{\rho, h_2 o, combustion}^A V^n\end{aligned}\quad (3-61)$$

and the energy equation [Equation (3-8)] is

$$\frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = S_{I, combustion}^A V^n \quad (3-62)$$

When the induction parameter is greater than 1, meaning that energy is released, the mass source term for Equation (3-54) for hydrogen is calculated in two different ways depending on the regime the combustion is in.

If the local turbulent Reynolds number is smaller than a critical value, the combustion takes place in a quasi-laminar regime. Hydrogen is burned in a stepwise linear way. The rate depends on the energy release time and the subcycle time step:

$$-\frac{c_{h_2}^A - c_{h_2}^n}{\Delta t_{sub}} = \dot{\omega} = \frac{c_{h_2, before combustion}}{t_{rel}} \quad (3-63)$$

If the local turbulent Reynolds number is greater than a critical value, the combustion takes place in a fully turbulent regime. Assuming the Damkoehler number (ratio of induction time to turbulent time) is greater than the ignition/extinction criterion, the mass source term for hydrogen is calculated as follows:

$$-(c_{h_2}^A - c_{h_2}^n) = \frac{2 \cdot A}{\tau_i} \cdot c_{lim}^n \quad (3-64)$$

The resulting mass source terms for oxygen and water vapor are

$$\begin{aligned}
S_{\rho, O_2, combustion}^A &= -\frac{1}{2} M_{O_2} \dot{\omega} \\
S_{\rho, H_2O, combustion}^A &= -M_{H_2O} \dot{\omega}
\end{aligned}
\tag{3-65}$$

and the energy source term

$$S_{I, combustion}^A = C_c \dot{\omega} \tag{3-66}$$

In case the Damkoehler number is smaller than Di_e , no hydrogen is burned, so the mass and energy source terms are zero.

If the energy is released in a quasi-laminar regime in a stepwise linear way, the combustion time step is determined by dividing the minimum value of the energy release time by the number of time steps used for energy release:

$$\Delta t_{combustion} = \frac{t_{rel, min}}{relstep} \tag{3-67}$$

The value of *relstep* can be input by the user; the default is 1.

If the combustion time step is very small and would determine the time step of the next cycle, the combustion will be subcycled with this time step to allow for a larger time step in the fluid dynamics routines.

3.2.11 Hydrogen Recombination

For the hydrogen recombination chemical kinetics, three species—hydrogen, oxygen, and water vapor—are involved in the fundamental chemical balance. The mass Equation (3-6) for each of these species is

$$\begin{aligned}
\frac{\rho_{H_2}^A V^A - \rho_{H_2}^n V^n}{\Delta t} &= S_{\rho, H_2, recombination}^A V^n \\
\frac{\rho_{O_2}^A V^A - \rho_{O_2}^n V^n}{\Delta t} &= S_{\rho, O_2, recombination}^A V^n \\
\frac{\rho_{H_2O}^A V^A - \rho_{H_2O}^n V^n}{\Delta t} &= S_{\rho, H_2O, recombination}^A V^n
\end{aligned}
\tag{3-68}$$

and the energy Equation (3-8) is

$$\frac{\rho^A I^A V^A - \rho^n I^n V^n}{\Delta t} = S_{I, recombination}^A V^n \tag{3-69}$$

Each of the recombiner models currently modeled in GASFLOW are described in Section 2.9 [Equations (2-94), (2-99), (2-106), and (1-109), where a reaction rate $\dot{\omega}$, was developed for the consumption of hydrogen.

In each of these cases, the change of hydrogen concentration is computed from Equation (3-57) in the form

$$-\frac{1}{2} \frac{c_{h_2}^A - c_{h_2}^n}{\Delta t} = \dot{\omega} \quad (3-70)$$

or the recombination source terms for the species mass equations

$$\begin{aligned} S_{\rho, h_2, recombination}^A &= -2M_{h_2} \dot{\omega} \\ S_{\rho, o_2, recombination}^A &= -M_{o_2} \dot{\omega} \\ S_{\rho, h_2 o, recombination}^A &= -2M_{h_2 o} \dot{\omega} \end{aligned} \quad (3-71)$$

and the energy source term

$$S_{I, recombination}^A = C_c \dot{\omega} \quad (3-72)$$

3.2.12 Ventilation System

The 1D duct Phase A solution is the same as the multidimensional Phase A solution for a finite control volume as described above, with the following exceptions:

- (1) each 1D duct cell has two neighboring cells, so the summation over cell faces for a 1D duct cell is over the left and right cell face;
- (2) junction cells can have from one to six cell faces, and therefore the summation over cell faces is over the number of ducts connected to the junction cell;
- (3) inclusion of wall shear into the momentum equation;
- (4) inclusion of the change in elevation to appropriately account for the change in the gravity body force between the 1D duct and junction cells,
- (5) inclusion of flow loss coefficients (i.e., user provided flow loss coefficients, filter model flow loss coefficients, damper model flow loss coefficients, area change loss coefficients, and curved duct loss coefficients);
- (6) inclusion of momentum source term to represent the blower/fan performance; and

- (7) incorporation of the momentum flux terms for 1D ducts and junctions into the Phase A solution to improve computational stability.

The finite control volume equations are consistent between the 3D and 1D solutions in GASFLOW. The turbulent loss coefficients and wall shear loss coefficient in the 1D duct models are combined into a single total loss coefficient and included into the momentum equation using Equation (3-5) with C_D replaced with the total loss coefficient. The total loss coefficient is given as,

$$K_t = K_d + K_l + K_{ft} + K_a + K_c + \frac{fL}{D_h} \quad , \quad (3-73)$$

where K_d is the damper loss coefficient, K_a is the user input loss coefficient, K_{ft} is the filter turbulent loss coefficient, K_a is the loss coefficient associated with an area change, K_c is the loss coefficient associated with a curved duct, f is the friction factor, L is the length of the control volume and D_h is the hydraulic diameter. The filter laminar loss coefficient (K_l) is proportional to the velocity as compared to the turbulent loss coefficients which are proportional to velocity squared; therefore, the filter laminar loss is included in the Phase A solution as an explicit momentum sink.

The gravity body force term in the 1D equations is written as

$$\rho_m^n g_c \cos \vartheta V_m^n \quad , \quad (3-74)$$

where $\cos \vartheta$ is the change in elevation for the momentum control volume divided by the length of the control volume and g_c is the acceleration of the gravity constant.

The Phase A momentum equation with all relevant terms for 1D ducts is as follows:

$$\rho_m^A \mathbf{u}^A = \frac{\rho_m^n \mathbf{u}^n V_m^n - \Delta t \left[\sum_f (p)_f^n S_f - \rho_m^n g_c \cos \vartheta V_m^n - \frac{K_t \rho_m^n \mathbf{u}^n A}{D_h} + \sum_f (\tau A)_f^n \Delta S_f + \rho_m^n g_c H_b A - \sum_f (\rho A \mathbf{u} \mathbf{u})_f^n \Delta S_f \right]}{V_m^A + \Delta t A \frac{1}{2} K_t |\mathbf{u}^n| S_f} \quad . \quad (3-75)$$

The Phase A momentum equation includes a momentum source term that represents blower operation. In the equation given above, H_b is the head in centimeters developed by the operation of the blower, and

$$\rho_m^n g_c H_b A \quad (3-76)$$

is the momentum source term associated with the operation of the blower.

In addition, the change in momentum flux term was moved from the Phase C solution to the Phase A solution to improve the stability of the 1D numerics for calculations involving abrupt area changes. In the phase A momentum equation given above, the momentum flux term is the last term in the numerator.

3.3 Phase B: Implicit Pressure Iteration Phase

3.3.1 Three-Dimensional Developments

In this phase, an implicit evaluation of the time-advanced densities, velocities, pressure, and specific internal energy fields is achieved. The purpose of this phase is to compute time-advanced pressures to allow calculations of low-speed (low-Mach-number) flows without any time-step restrictions from the fluid sound speeds. The following argument (Ref. 3-1) explains the need for this step.

In an explicit method, pressure forces can be transmitted only one cell each time step, that is, cells exert pressure forces only on neighboring cells. When the time step is chosen so large that sound waves should travel more than one cell, the one cell limitation is clearly inaccurate and a catastrophic instability develops. The instability arises because the explicit pressure gradients lead to excessive cell compressions or expansions when multiplied by too large a time step. This then leads to larger pressure gradients the next cycle, which try to reverse the previous excesses, but since the time step is too large the reversal is also too large and the process repeats itself with a rapidly increasing amplitude. The over response to pressure gradients in this fashion is eliminated by using time-advanced pressure gradients, for then cells cannot compress or expand to the point where gradients are reversed.

In this phase, the mixture differential equations for cell volume [Equation (2-8)], mass [Equation (2-7)], momentum [Equation (2-13)], and energy [Equation (2-14)] are

$$\frac{V^B - V^A}{\Delta t} = V^n \nabla \cdot [(A\mathbf{u})^B - (A\mathbf{u})^n] \quad , \quad (3-77)$$

$$\frac{\rho^B V^B - \rho^A V^A}{\Delta t} = 0 \quad , \quad (3-78)$$

$$\frac{\rho_m^B V_m^B \mathbf{u}^B - \rho_m^A V_m^A \mathbf{u}^A}{\Delta t} = V_m^n [-\nabla(p^B - p^n) - (AD^B - AD^A)] \quad , \quad (3-79)$$

and

$$\frac{\rho^B V^B I^B - \rho^A V^A I^A}{\Delta t} = -V^n p^n \nabla \cdot [(\mathbf{A}\mathbf{u})^B - (\mathbf{A}\mathbf{u})^n] \quad (3-80)$$

The equation of state for the mixture [Equation (2-25)] may be written as

$$T^B = \frac{\theta^B p^B V^B}{\rho^B V^B \sum_{\alpha} x_{\alpha}^B R_{\alpha}} \quad (3-81)$$

and with the approximation for the mixture specific heat at constant volume

$$c_v(T^A) \equiv \frac{(I^B - I^A)}{(T^B - T^A)} \quad (3-82)$$

we present an equation set, Equations (3-77) through (3-82), that is coupled with seven linear and one nonlinear [Equation (3-81)] algebraic equation in eight unknowns (V^B , ρ^B , u_x^B , u_y^B , u_z^B , p^B , I^B , and T^B). We are able to reduce this equation set to a single Poisson equation involving the pressure change as the dependent variable.

The Poisson equation is solved for the change in the pressure field, and from the pressure change, the volume, velocity, density, and internal energy fields are found by back substitution.

The Poisson equation is derived as follows:

(1) The left-hand side of the conservation of energy Equation (3-80) is manipulated using the conservation of mass Equation (3-78), the equation of state (3-81), and the specific heat approximation (3-82) to yield

$$\frac{\theta^A c_v(T^A) (p^B V^B - p^A V^A)}{\Delta t \sum_{\alpha} x_{\alpha}^A R_{\alpha}} = -V^n p^n \nabla \cdot [(\mathbf{A}\mathbf{u})^B - (\mathbf{A}\mathbf{u})^n] \quad (3-83)$$

(2) The right-hand side of Equation (3-83) can be modified using the conservation of volume Equation (3-77); and, in addition, $p^A V^B$ is subtracted and added to the numerator of the left-hand side to give

$$\frac{\theta^A c_v(T^A) (p^B V^B - p^A V^B + p^A V^B - p^A V^A)}{\sum_{\alpha} x_{\alpha}^A R_{\alpha}} = -p^n (V^B - V^A) \quad (3-84)$$

(3) Rearranging Equation (3-84) yields the following:

$$p^B - p^A = - \left[\frac{p^n \sum_{\alpha}^{\alpha \neq h_2 ol} x_{\alpha}^A R_{\alpha}}{\theta^A c_v(T^A)} + p^A \right] \frac{(V^B - V^A)}{V^B} \quad (3-85)$$

(4) This equation can be linearized by rearranging $(V_s^B - V_s^A)/V_s^B$ and then applying a binomial series to obtain

$$\frac{(V^B - V^A)}{V^B} \cong \frac{(V^B - V^A)}{V^A} \quad , \quad (3-86)$$

provided $\frac{(V^B - V^A)}{V^A} \ll 1$, to produce

$$p^B - p^A = - \left[\frac{p^n \sum_{\alpha}^{\alpha \neq h_2 ol} x_{\alpha}^A R_{\alpha}}{\theta^A c_v(T^A)} + p^A \right] \frac{(V^B - V^A)}{V^A} \quad (3-87)$$

(5) Adding and subtracting $(Au)^A$ inside the divergence operator in Equation (3-77) yields

$$V^B - V^A = \Delta t V^n \nabla \cdot [(Au)^B - (Au)^A + (Au)^A - (Au)^n] \quad (3-88)$$

(6) Equation (3-88) can be substituted into Equation (3-87) and, after some algebra, yields

$$\frac{V^A}{\Delta t} (p^B - p^A) = -V^n \{ \} \left[\nabla \cdot [(Au)^B - (Au)^A] + \nabla \cdot [(Au)^A - (Au)^n] \right] \quad , \quad (3-89)$$

where

$$\{ \} = \left[\frac{p^n \sum_{\alpha}^{\alpha \neq h_2 ol} x_{\alpha}^A R_{\alpha}}{\theta^A c_v(T^A)} + p^A \right] \quad .$$

(7) Making use of Equation (3-78), Equation (3-79) can be cast into the following form:

$$(\mathbf{Au})^B - (\mathbf{Au})^A = -\frac{\mathbf{A}\Delta t V_m^n \nabla(p^B - p^n)}{\langle \rangle} , \quad (3-90)$$

where

$$\langle \rangle = \rho_m^A V_m^A \left(1 + \frac{\Delta t C |\mathbf{u}^n|}{2\Delta x} \right) .$$

(8) Introducing $\delta p = p^B - p^n$ into Equations (3-89) and (3-90) and eliminating $(\mathbf{Au})^B - (\mathbf{Au})^A$ between the two equations yields

$$\begin{aligned} \Delta t^2 \nabla \cdot \left[\frac{\mathbf{A} V_m^n \nabla \delta p}{\langle \rangle} \right] - \frac{V^A}{V^n \{ \}} \delta p = \\ \frac{V^A}{V^n \{ \}} (p^n - p^A) + \Delta t \nabla \cdot [(\mathbf{Au})^B - (\mathbf{Au})^n] , \end{aligned} \quad (3-91)$$

which is second order and linear in δp . To solve this Poisson pressure change equation, we use the Preconditioned Conjugate Residual (PCR) method that is described in Appendix C.

This implicit solution of the pressure equation allows for greater efficiency than a purely explicit calculation with reduced time steps. The numerical stability achieved permits pressure waves to traverse more than one computational cell in a time step.

In practice, after solving Equation (3-91) for the pressure change, δp , we evaluate $\mathbf{u}^B$ from Equation (3-90), since $\delta p = p^B - p^n$, V^B from Equation (3-77), the time-advanced density ρ^B from Equation (3-78), ρ_α^B from

$$\frac{\rho_\alpha^B V^B - \rho_\alpha^A V^A}{\Delta t} = 0 , \quad (3-92)$$

p^B from Equation (3-85), T^B from Equation (3-81), and finally I^B from a direct evaluation of Equations (2-19) as

$$\begin{aligned} I^B = \sum_\alpha \left(\frac{\rho_\alpha^B}{\rho^B} a_\alpha \right) + \\ T^B \left\langle \sum_\alpha \left(\frac{\rho_\alpha^B}{\rho^B} b_\alpha \right) + T^B \left\{ \sum_\alpha \left(\frac{\rho_\alpha^B}{\rho^B} c_\alpha \right) + T^B \left[\sum_\alpha \left(\frac{\rho_\alpha^B}{\rho^B} d_\alpha \right) + T^B \sum_\alpha \left(\frac{\rho_\alpha^B}{\rho^B} e_\alpha \right) \right] \right\} \right\rangle . \end{aligned} \quad (3-93)$$

3.3.2 Ventilation System Developments

The 1D duct Phase B solution is the same as the Phase B solution used for 3D blocks, except for the inclusion of the momentum source terms for the blower operation and the change in momentum flux. These two momentum source terms are included in Equation (3-94) as explicit source terms, which are differences between Phase A and Phase B.

$$\frac{\rho_m^B V_m^B \mathbf{u}^B - \rho_m^A V_m^A \mathbf{u}^A}{\Delta t} = V_m^n \left[-\nabla(p^B - p^n) - (A\mathbf{D}^B - A\mathbf{D}^A) + \rho_m^n g_c H_b A - \sum_f (\rho A \mathbf{u} \mathbf{u})_f^n \Delta S_f \right] \quad (3-94)$$

In addition, the total flow loss, included in the Phase B solution, is consistent with the internal structure drag for the 3D blocks. With these two modifications, the development of the Phase B pressure equation for 1D ducts follows the Phase B development of the pressure equation for 3D blocks.

3.4 Phase C: Rezone Phase

3.4.1 Multidimensional Developments

The third phase explicitly performs all the advective flux calculations, repartitioning the dependent variables onto the original mesh. The superscript $n+1$ (and not C) is used to indicate that this Eulerian rezone phase completes the spatiotemporal integration of the equations of motion from time-level n to time-level $n+1$.

Recognizing that $V_s^{n+1} = V_s^n$ because of the exact remap of the Lagrangian mesh onto the original Eulerian mesh, we provide the finite volume equations for mass, momentum, and energy advection, respectively, as follows:

$$\frac{\rho_\alpha^{n+1} V^n - \rho_\alpha^B V^B}{\Delta t} = - \sum_f (\rho_\alpha A \mathbf{u})_f^B \Delta S_f \quad (3-95)$$

$$\frac{\rho_m^{n+1} V_m^n \mathbf{u}^{n+1} - \rho_m^B V_m^B \mathbf{u}^B}{\Delta t} = - \sum_f (\rho A \mathbf{u} \mathbf{u})_f^B \Delta S_f - \sum_f (\mathbf{D}_d \mathbf{A})_f^{n+1} \Delta S_f \quad (3-96)$$

and

$$\frac{\rho^{n+1} V^n I^{n+1} - \rho^B V^B I^B}{\Delta t} = - \sum_f (\rho I A \mathbf{u})_f^B \Delta S_f \quad (3-97)$$

Decoupling the rezoning step from the rest of the physics computations facilitates the implementation of different numerical advection algorithms. We have implemented both a first-order donor cell algorithm and a second order van Leer with limiting (Ref. 3-9) to evaluate the right-hand sides of Equations (3-95) through (3-97).

To illustrate the van Leer algorithm, we first expand the right-hand side of the species mass, momenta, or energy in Equations (3-95) through (3-97) over the finite-volume control surfaces as

$$\sum_f (\phi Au)_f^B \Delta S_f = \begin{cases} \langle \phi Au \rangle_E^B \delta y \delta z - \langle \phi Au \rangle_W^B \delta y \delta z + \\ \langle \phi Av \rangle_N^B \delta x \delta z - \langle \phi Av \rangle_S^B \delta x \delta z + \\ \langle \phi Aw \rangle_T^B \delta x \delta y - \langle \phi Aw \rangle_B^B \delta x \delta y \end{cases}, \quad (3-98)$$

where ϕ is, respectively, ρ_α , $\rho \mathbf{u}$, and ρI . We remind the reader that A is the fractional area open for flow on that particular surface.

The East (E) surface of computation volume (I, J, K) corresponding with the mass and energy equations coincides with the indexing notation of $i+1/2$, where the special notation $\langle \rangle$ is defined:

$$\langle \phi Au \rangle_{i+1/2}^B = \begin{cases} A_{i+1/2} u_{i+1/2}^B \left\{ \phi_i^B + \frac{1}{2} \left[\delta x_i - u_{i+1/2}^B \delta t \right] \left(\frac{\partial \phi^B}{\partial x} \right)_i \right\}; u_{i+1/2}^B \geq 0 \\ A_{i+1/2} u_{i+1/2}^B \left\{ \phi_{i+1}^B + \frac{1}{2} \left[\delta x_{i+1} + u_{i+1/2}^B \delta t \right] \left(\frac{\partial \phi^B}{\partial x} \right)_{i+1} \right\}; u_{i+1/2}^B < 0 \end{cases} \quad (3-99)$$

We make use of central differencing to evaluate the average slope in Equation (3-99) when the fluid velocity at face $i+1/2$ is positive as

$$\left(\frac{\partial \phi^B}{\partial x} \right)_i = \bar{S}_i \equiv \frac{\phi_{i+1}^B - \phi_{i-1}^B}{\delta x_{i+1/2} + \delta x_{i-1/2}}, \quad (3-100)$$

which is interpreted schematically in Figure 3-6.

Figure 3-6. Schematic diagram of van Leer second-order advection algorithm when face velocity is positive

When the fluid velocity at face $i+1/2$ is negative, the average slope in Equation (3-99) is given by

$$\left(\frac{\partial \phi^B}{\partial x} \right)_{i+1} = \overline{S_{i+1}} \equiv \frac{\phi_{i+2}^B - \phi_i^B}{\delta x_{i+3/2} + \delta x_{i+1/2}}, \quad (3-101)$$

which is interpreted schematically in Figure 3-7.

Figure 3-7. Schematic diagram of van Leer second-order advection algorithm when face velocity is negative

Note that when the average slope in Equation (3-99) is identically zero, the algorithm reduces to the classical first-order donor cell or Godunov's first-order scheme:

$$\langle \phi A u \rangle_{i+1/2}^B = \begin{cases} A_{i+1/2} u_{i+1/2}^B \phi_i^B; u_{i+1/2}^B \geq 0 \\ A_{i+1/2} u_{i+1/2}^B \phi_{i+1}^B; u_{i+1/2}^B < 0 \end{cases} \quad (3-102)$$

By limiting the value of the slope in various situations (which we will discuss below) we can impose the monotonicity condition. Basically, the monotonicity condition states that when the initial conditions for a particular variable are monotone, the time-advanced values are also monotone. In other words, if ϕ_i^B lies between ϕ_{i+1}^B and ϕ_{i-1}^B , then ϕ_i^{n+1} must lie between ϕ_{i+1}^{n+1} and ϕ_{i-1}^{n+1} .

The idea of limiting the slope is shown in Figures 3-8a, 3-8b, and 3-8c, which show the slope distribution of ϕ . In Figure 3-8a, the slope of the variable between $i-1/2$ and $i+1/2$ lies outside the zero slope values for $i-1$ and $i+1$. We limit the value of the slope in this case so that the actual slope used when computing Equation 3-99 is the heavy dark slope shown for i in Figure 3-8a. In Figure 3-8b, the mesh value at i

reaches an extreme; in this case, the slope is reduced to zero. Also, if the slope at i doesn't agree with the trend of the adjacent slopes as shown in Figure 3-8c, the slope is reduced to zero.

Based upon this limiter model, we retain or reduce the slope as computed by Equation (3-100) for positive fluid velocity at $i+1/2$ by

$$(\overline{S}_i)_{monotone} = \left\{ \begin{array}{l} \left[\begin{array}{l} \text{sign}(\phi_{i+1}^B - \phi_{i-1}^B) \cdot \min \left(\left| \frac{\phi_i^B - \phi_{i-1}^B}{\delta x_{i-\frac{1}{2}}} \right|, \left| \frac{\phi_{i+1}^B - \phi_{i-1}^B}{\delta x_{i+\frac{1}{2}} + \delta x_{i-\frac{1}{2}}} \right|, \left| \frac{\phi_{i+1}^B - \phi_i^B}{\delta x_{i+\frac{1}{2}}} \right| \right) \\ \text{if: } \text{sign}(\phi_i^B - \phi_{i-1}^B) = \text{sign}(\phi_{i+1}^B - \phi_{i-1}^B) = \\ \text{sign}(\phi_{i+1}^B - \phi_i^B) \\ 0; \text{otherwise} \end{array} \right] \end{array} \right. \quad (3-103)$$

and Equation (3-101) for negative fluid velocity at $i+1/2$ by

$$(\overline{S}_{i+1})_{monotone} = \left\{ \begin{array}{l} \left[\begin{array}{l} \text{sign}(\phi_{i+2}^B - \phi_i^B) \cdot \min \left(\left| \frac{\phi_{i+1}^B - \phi_i^B}{\delta x_{i+\frac{1}{2}}} \right|, \left| \frac{\phi_{i+2}^B - \phi_i^B}{\delta x_{i+\frac{3}{2}} + \delta x_{i+\frac{1}{2}}} \right|, \left| \frac{\phi_{i+2}^B - \phi_{i+1}^B}{\delta x_{i+\frac{3}{2}}} \right| \right) \\ \text{if: } \text{sign}(\phi_{i+1}^B - \phi_i^B) = \text{sign}(\phi_{i+2}^B - \phi_i^B) = \\ \text{sign}(\phi_{i+2}^B - \phi_{i+1}^B) \\ 0; \text{otherwise} \end{array} \right] \end{array} \right. \quad (3-104)$$

Figure 3-8a. A monotonicity condition shown by plotting the slope distribution of ϕ (slope of i lies outside the zero slope values for $i - 1$ and $i + 1$).

Figure 3-8b. A monotonicity condition shown by plotting the slope distribution of ϕ (slope of i is reduced to zero when its mesh value reaches an extreme)

Figure 3-8c. A monotonicity condition shown by plotting the slope distribution of ϕ (slope of i is reduced to zero when it doesn't agree with the trend of the adjacent slopes)

The actual implemented advection algorithm is therefore

$$\langle \phi A u \rangle_{i+1/2}^B = \begin{cases} A_{i+1/2} u_{i+1/2}^B \left\{ \phi_i^B + \frac{1}{2} \left[\delta x_i - u_{i+1/2}^B \delta t \right] (\bar{S}_i)_{monotone} \right\}; u_{i+1/2}^B \geq 0 \\ A_{i+1/2} u_{i+1/2}^B \left\{ \phi_{i+1}^B + \frac{1}{2} \left[\delta x_{i+1} + u_{i+1/2}^B \delta t \right] (\bar{S}_{i+1})_{monotone} \right\}; u_{i+1/2}^B < 0 \end{cases} \quad (3-105)$$

Equation (3-95) can be solved using the structural drag function Equation (3-3) to yield

$$(\rho_m \mathbf{u})^{n+1} = \frac{\rho_m^B V_m^B \mathbf{u}^B - \Delta t \sum_f (\rho A \mathbf{u} \mathbf{u})_f^B \Delta S_f}{V_m^n + \Delta t A \frac{1}{2} C_D |\mathbf{u}^B| S_f} \quad (3-106)$$

Phase C is completed by computing the total density ρ^{n+1} from

$$\rho^{n+1} = \sum_{\alpha} \rho_{\alpha}^{n+1} \quad (3-107)$$

the temperature T^{n+1} from inverting the polynomial of up to 4th degree in

$$\left(\sum_{\alpha} \rho_{\alpha}^{n+1} a_{\alpha} - \rho^{n+1} I^{n+1} \right) + (T^{n+1}) \sum_{\alpha} \rho_{\alpha}^{n+1} b_{\alpha} +$$

$$(T^{n+1})^2 \sum_{\alpha} \rho_{\alpha}^{n+1} c_{\alpha} + (T^{n+1})^3 \sum_{\alpha} \rho_{\alpha}^{n+1} d_{\alpha} + (T^{n+1})^4 \sum_{\alpha} \rho_{\alpha}^{n+1} e_{\alpha} = 0 \quad , \quad (3-108)$$

and the pressure p^{n+1} from

$$p^{n+1} = \frac{T^{n+1} \sum_{\alpha} R_{\alpha} \rho_{\alpha}^{n+1}}{\theta^{n+1}} \quad (3-109)$$

with

$$\theta^{n+1} = 1 - \frac{\rho_{h_2ol}^{n+1}}{\rho_{h_2ol}^{thermo}} \quad . \quad (3-110)$$

3.4.2 Ventilation System Developments

Again, the 1D duct Phase C solution is the same as the 3D Phase C solution with the following exception. Since the change in momentum flux for the 1D ducts is included in the Phase A and Phase B solutions for 1D ducts, there is no Phase C momentum equation solution for 1D ducts. The velocity obtained from the Phase B solution for 1D ducts is the new time velocity, which is not modified in Phase C. The mass and energy equations for Phase C for 1D ducts are the same as those for the 3D blocks.

3.5 Turbulence Transport

The final fluid dynamics task in each computational cycle is the explicit updating of turbulence variables.

3.5.1 Algebraic Model

The new time-level turbulent viscosity follows directly from Equation (2-65):

$$\mu^{n+1} = C_{\mu} \rho^{n+1} \left\{ 0.1 \cdot \frac{1}{2} \left[(u^{n+1})^2 + (v^{n+1})^2 + (w^{n+1})^2 \right] \right\}^{1/2} \quad . \quad (3-111)$$

3.5.2 κ - ϵ Model

The new time-level products $\rho\kappa$ and $\rho\epsilon$ are computed from the discrete versions of Equations (2-68) and (2-69):

$$\frac{(\rho\kappa)^{n+1}V^n - (\rho\kappa)^nV^n}{\Delta t} = \sum_f \left[\begin{array}{c} -\rho\kappa\mathbf{u} + \\ \left(\frac{\mu}{\sigma_\kappa} \nabla\kappa \right) + \\ \tau:\nabla\mathbf{u} \end{array} \right]_f A_f \Delta S_f + V^n [\mu\alpha\mathbf{g} \cdot \nabla T - \rho\varepsilon + \kappa S_\kappa]^n \quad (3-112)$$

and

$$\begin{aligned} \frac{(\rho\varepsilon)^{n+1}V^n - (\rho\varepsilon)^nV^n}{\Delta t} = & \sum_f \left[\begin{array}{c} -\rho\varepsilon\mathbf{u} + \\ \left(\frac{\mu}{\sigma_\varepsilon} \nabla\varepsilon \right) + \\ C_1 \frac{\varepsilon}{\kappa} \tau:\nabla\mathbf{u} \end{array} \right]_f A_f \Delta S_f + \\ & V^n \left[C_1 \frac{\varepsilon}{\kappa} \mu\alpha\mathbf{g} \cdot \nabla T - C_1 \rho \frac{\varepsilon^2}{\kappa} + \varepsilon S_\varepsilon \right]^n . \end{aligned} \quad (3-113)$$

The turbulent viscosity then is computed from Equation (2-70):

$$\mu^{n+1} = \frac{C_\mu \rho^{n+1} (\kappa^{n+1})^2}{\varepsilon^{n+1}} . \quad (3-114)$$

3.6 Time-Step Controls

The new time step is controlled by checking the entire computational mesh for a material velocity Courant condition, the diffusion stability limit, the ignition of hydrogen, the pressure iteration count, and the maximum time step allowed by input.

3.6.1 Courant Condition for Material Velocity

The Courant material velocity time-step limitation is computed as the minimum limit on the entire computational mesh by

$$\delta t_{convection} = \frac{1}{4 \cdot \max \left\{ \frac{|u_i|}{\delta x_i}, \frac{|v_j|}{\delta y_j}, \frac{|w_k|}{\delta z_k}, \varepsilon_{convection} \right\}} , \quad (3-115)$$

where $\varepsilon_{convection} = 10^{-10}$. Note that for a zero velocity field, the convective time-step limit is roughly the reciprocal of $\varepsilon_{convection}$, which is a large value. The coefficient 4

effectively limits material convection to one-fourth of the smallest computational cell in the mesh. We have experimented with this coefficient by relaxing its value to nearly 1. The solution remained very stable; however, for accuracy considerations we recommend the default value of 4.

3.6.2 Diffusional Condition for Mass, Momentum, and Energy

The diffusional time-step limitation is calculated every time step for the minimum values on the computational mesh by

$$\delta t_{diffusion} = \frac{1}{4 \cdot \lambda_{i,j,k} \cdot \left(\frac{1}{\delta x_i^2} + \frac{1}{\delta y_j^2} + \frac{1}{\delta z_k^2} \right)}, \quad (3-116)$$

where

$$\lambda_{i,j,k} = \max \left[\left(D_{apparent} \right)_{i,j,k}, \left(\frac{\mu_{apparent}}{\rho} \right)_{i,j,k}, \left(\frac{\phi_{apparent}}{\rho \cdot c_p} \right)_{i,j,k}, \varepsilon_{diffusion} \right] \quad (3-117)$$

and $\varepsilon_{diffusion} = 10^{-10}$. Formally, the coefficient 4 in Equation (3-115) can be relaxed to 2, but we have chosen to be conservative in this calculation.

3.6.3 Ignition Conditions

When an ignition occurs, the energy of combustion dominates the internal energy Equation (3-8). We have determined an empirical relationship to limit the time step at ignition periods. Our calculation of the ignition time step is based upon the change of energy during ignition:

$$\delta t_{combustion} = \max \left[5 \cdot 10^{-4}, \frac{5 \cdot 10^{-5} \cdot I^n}{(I^A - I^n)} \right]. \quad (3-118)$$

3.6.4 Pressure Iteration Considerations

The user can define a range for the target pressure iteration variable (see Reference 3-10) with the user input for itupdt, itdowndt, and itmax. This iteration time-step control is formulated as

$$\begin{aligned} \delta t_{iteration} &= 1.02 \cdot \delta t \text{ if iteration} < \text{itupdt} \\ \delta t_{iteration} &= 0.98 \cdot \delta t \text{ if iteration} > \text{itdowndt} \\ \delta t_{iteration} &= 0.90 \cdot \delta t \text{ if iteration} > \text{itmax} \end{aligned} \quad (3-119)$$

This time-step control allows the time step to target a range for the pressure iteration value by either increasing or decreasing the time step by 2% so that the iteration performance of the Poisson equation solver reaches a specified range of pressure iterations (i.e., between $itupdt$ and $itdowndt$). If the pressure iteration goes above $itmax$, then the time step size for the next time step is reduced by 10%.

3.6.5 Maximum Time Step

The user can also define the maximum time step, $\delta t_{\text{maximum}}$, allowed for a particular calculation (default value: $\text{deltmax} = 10^{30}$). Based upon the above time-step considerations, the next computational GASFLOW time step is

$$\delta t = \min(\delta t_{\text{convection}}, \delta t_{\text{diffusion}}, \delta t_{\text{combustion}}, \delta t_{\text{iteration}}, \delta t_{\text{maximum}}) \quad (3-120)$$

3.7 Particle Computational Model

The particle transport, deposition, and entrainment governing equations are solved independently of the fluid-flow equations. In this one-way coupled particle model, the particle/fluid volume ratio is small enough that it is assumed that the presence of the particles has no effect on the conveying gas. The particle behavior is governed by the local gas velocity field that exists after the final fluid dynamics task is performed in each computational cycle.

Each computational aerosol particle is initialized at specific physical mesh coordinates in the computational domain. The particle size and material properties are assigned to each particle. A location (x_p, y_p, z_p) , velocity (u_p, v_p, w_p) , diameter (d_p) , and density (ρ_p) are stored for each particle.

3.7.1 Particle Equations of Motion

The fluid velocity components (u_g, v_g, w_g) at the particle location are computed from the fluid velocity components on the six faces of the cell that contains the particle. A linear interpolation is used in each direction, that is, a tri-linear interpolation. The equations of motion for a particle are as follows:

$$\begin{aligned} \frac{dx_p}{dt} &= u_p \\ \frac{dy_p}{dt} &= v_p \\ \frac{dz_p}{dt} &= w_p \end{aligned} \quad (3-121)$$

$$\begin{aligned}
\frac{du_p}{dt} &= \frac{3}{4} C_D \frac{\rho_g}{\rho_p} \frac{(u_g - u_p)|u_g - u_p|}{d_p} + \frac{\xi}{x_p} (v_p)^2 + g_x \\
\frac{dv_p}{dt} &= \frac{3}{4} C_D \frac{\rho_g}{\rho_p} \frac{(v_g - v_p)|v_g - v_p|}{d_p} - \frac{\xi u_p v_p}{x_p} + g_y \\
\frac{dw_p}{dt} &= \frac{3}{4} C_D \frac{\rho_g}{\rho_p} \frac{(w_g - w_p)|w_g - w_p|}{d_p} + g_z,
\end{aligned} \tag{3-122}$$

where ξ is a geometry factor ($\xi = 0$ for Cartesian coordinates and $\xi = 1$ for cylindrical coordinates) and C_D , the drag coefficient, is

$$C_D = 0.4 + \frac{24}{\text{Re}_p} + \frac{6}{(1 + \sqrt{\text{Re}_p})}, \tag{3-123}$$

where Re_p , the particle Reynolds number, is

$$\text{Re}_p = \frac{d_p |\mathbf{U}_g - \mathbf{U}_p|}{\nu}. \tag{3-124}$$

The term $\frac{d}{dt}$ is the Lagrangian time derivative along the trajectory of the particle, and ρ_g is the conveying gas density. The first term on the right of each Equation (3-122) is the acceleration resulting from fluid drag forces. The second term in the first two equations accounts for inertial accelerations in a cylindrical coordinate system. The third term in each equation is the acceleration caused by body forces.

3.7.2 Particle Diffusion

Turbulent particle diffusion is modeled by a stochastic scheme developed by Hotchkiss and Hirt (Ref. 3-11). The discrete particle is considered to be a point source that diffuses in all directions and forms a conceptual cloud with a Gaussian mass distribution in each direction. The particle is to remain a point, so the Gaussian function is interpreted as a probability distribution function for the moving particle. A new location for the particle is selected using a random number generator to calculate the probability of its location corresponding to the mass distribution within the conceptual cloud. In this way, a Monte Carlo approximation is generated for the local diffusion of each particle. A velocity is computed for the new location and added to the conveying gas velocity corresponding to the location of that particle.

Three random numbers are selected for each particle to compute shifts in each of the three coordinate directions. The random number generator used in the code is based on a uniform distribution in the interval (0,1). This number, x , is transformed to a uniform distribution in the interval (-1,1) by the arithmetic operation $2x-1$; an inverse error function then must be computed to get the desired Gaussian distribution.

For computer time efficiency, we use a table of inverse error functions with 101 entries covering the error function argument from 0 to WMAX, which is an input number that has a default value of 2.0. Experience has shown this approach to be sufficiently accurate for most applications. In the particle diffusion subroutine PARTDIFF, this table is interpolated for the inverse error function for each random number, which requires much less time than the more accurate system routine for inverse error functions. A call is made to a system clock at the beginning of subroutine RPARTS, which initializes the random number generator. This procedure ensures a new random number sequence with each new calculation.

3.7.3 Deposition/Rebound

When particle velocity components have been computed, the particle is moved in each of the coordinate directions. Particles hitting a solid boundary are specularly reflected or deposited on the surface.

A class of particles may all adhere, they may all bounce, or their behavior may be determined by the deposition/rebound model. The value of the input parameter IPDEP makes this determination. If the behavior of the particle is to be determined by the deposition/rebound model, the subroutine PARTBNC determines the particle threshold bounce velocity, U_i^* , above which the particle may rebound:

$$U_i^* = \left[\frac{2E}{m} \left(\frac{1-e^2}{e^2} \right) \right]^{\frac{1}{2}}, \quad (3-125)$$

where

$$E = \left(\frac{Ad}{12z_0} \right) \left[1 + \left(\frac{A^2 K^2 d}{72z_0^7} \right) + \left(\frac{A^4 K^4 d^2}{72^2 z_0^{14}} \right) \right] + \left(\frac{4\sqrt{2}d}{15K} \right) \left(\frac{A^2 K^2 d}{72z_0^6} \right)^{\frac{5}{2}},$$

and A is the Hamaker constant, z_0 is the equilibrium separation between the particle sphere and a surface, d is the particle diameter, and K is a function of mechanical properties.

The critical rebound velocity, U_i^* , is the value of velocity for a 50% probability of bounce. The incident velocity window outside of which the particle either adheres

or bounces is somewhat arbitrary, but plus or minus 50% of U_i^* is a reasonable assumption for this; that is, for $U_i < U_i^*(0.5)$ the particle always adheres, and for $U_i > U_i^*(1.5)$ the particle always bounces. When the velocity is in the range $0.5 U_i^* < U_i < 1.5 U_i^*$ the determination of whether or not specific particles will bounce or adhere is made by generating a random number, α , with a value between 0 and 1, and testing for α as follows:

$$\alpha \leq \left[\frac{(-0.5U_i^* + U_i)}{U_i^*} \right]. \quad (3-126)$$

When this condition is met, the particle bounces.

The experimentally observed trend is for the coefficient of restitution, e , to reach a maximum value at the threshold bounce velocity, and almost immediately the ratio of rebound velocity to incident velocity begins to decrease as the incident velocity increases. The following equation is used to model this behavior:

$$e = e_0(0.60)^{\text{exp}}, \quad (3-127)$$

where

$$\text{exp} = \frac{U_i - U_i^*}{10.0U_i^*},$$

and e_0 is the coefficient of restitution, the input parameter CORE, at the threshold bounce velocity.

Deposition is, in a real sense, a stochastic process that follows the general trend of the theoretical and empirical models developed and compared with available experimental data. Because of this, it is a reasonable assumption that some small, unknown percentage of the particles that impact a surface will adhere. To account for this, a percentage of all particles that impact a surface adheres. The percentage is chosen by the input parameter DEPPERC, which has a default value of 5%. The specific particles that adhere are randomly chosen, using the random number generator.

3.7.4 Entrainment

A single particle deposited on a surface will begin to move when the forces acting in the direction parallel to the surface are zero. These opposing forces are typically the fluid-drag force and the frictional force, which is the product of the normal forces and the coefficient of friction. For a horizontal surface, the particle forces normal to

the surface are adhesion, gravitational, buoyant and lift forces; for vertical surfaces the gravitational and buoyant forces are tangential to the surface. A force balance equation of these surface and aerodynamic forces is iteratively solved by a Newton-Raphson method to determine the minimum pickup velocity of each particle. This equation is

$$C_D U_{gcp}^2 = f_s \left[\frac{4}{3} d_p \frac{(\rho_p - \rho_g)}{\rho_g} g - \frac{A d_p}{12 z_0^2} \left(1 + \frac{A^2 K^2 d_p}{108 z_0^7} \right) \frac{1}{0.3927 \rho_g d_p^2} + 4.11 \sqrt{v} \sqrt{\frac{\partial U_g}{\partial y} U_{gcp}} \right] \quad (3-128)$$

where the drag coefficient is

$$C_D = 0.4 + \frac{24}{Re_p} + \frac{6}{(1 + \sqrt{Re_p})}$$

and the particle Reynolds number is

$$Re_p = \frac{d_p U_{gcp}}{v}$$

The vector U_{gcp} is the velocity of the gas at the center of the particle and is the computed particle threshold gas pickup velocity, U_{gpu0} . Particle suspension is initiated when the velocity of the fluid flowing around the particle equals or exceeds this particle threshold suspension velocity.

This model uses a force balance approach modified by the experimental data of Cabrejos and Klinzing.* After the threshold suspension velocity in each coordinate direction for each particle is computed, these velocities are adjusted by the experimental data to obtain a semi-empirical threshold velocity. The correlation is

$$U_{gpu} = \left(1.27 Ar^{\frac{1}{3}} + 0.036 Ar^{\frac{1}{3}} + 0.45 \right) \left(0.70 Ar^{\frac{1}{5}} + 1.0 \right) U_{gpu0} \quad (3-129)$$

where the Archimedes number is

$$Ar = \frac{g (\rho_p - \rho_g)}{v^2 \rho_g} d_p^3$$

* Francisco J. Cabrejos and George E. Klinzing, "Incipient Motion of Solid Particles in Horizontal Pneumatic Conveying," Dept. of Mech. Engr., University of Pittsburgh, unpublished paper (1991).

The semi-empirical threshold velocity component is computed for each particle for each coordinate direction.

The semi-empirical threshold velocity is used to test for particle entrainment. The orientation of the solid boundary on which the particle is located in the computational mesh has been determined, and the information is stored in the array MPAC for each deposited particle. In addition, the velocity in each coordinate direction at the particle location has been computed and is stored. The determination of these velocities uses the law-of-the-wall equation, as discussed in Section 2.9.3.1, to estimate these velocities at the particles, which are typically embedded in the viscous, inner sublayer of the boundary layer. Again considering the stochastic behavior of particles, a probability of entrainment is computed. This is not based on experimental data but is solely an artifice to broaden the critical velocity at which particles will be suspended. When $0.8U_{gpu} \leq U_{gcp} < U_{gpu}$, the probability of entrainment is

$$PRB_{ntrn} = 4.0 \left(\frac{U_{gcp} - 0.8U_{gpu}}{U_{gpu}} \right). \quad (3-130)$$

When $U_{gcp} \geq U_{gpu}$,

$$PRB_{ntrn} = 0.8 + \left(\frac{U_{gcp} - U_{gpu}}{U_{gpu}} \right). \quad (3-131)$$

This gives an 80% probability of entrainment when the gas velocity at the particle location, U_{gcp} , is equal to the semi-empirical threshold velocity, U_{gpu} , and a 100% probability of entrainment when the velocity at the particle location is equal to or greater than 1.2 times the semi-empirical threshold velocity. The particle is never entrained when the gas velocity at the particle location is less than or equal to 0.8 times the semi-empirical threshold velocity. A random number, α , is generated and used to determine if the particle is actually entrained. When $PRB_{ntrn} \geq \alpha$, the particle is entrained. In this case, the particle is assigned the local fluid velocity components parallel to the surface. The particle velocity component normal to the surface is set to zero. The particle is also moved to a point directly out from (normal to) the surface where the specific particle was located. The distance from the surface at which the particle is set is between one-half and one computational cell dimension. The exact location in this range is randomly chosen.

3.7.5 Numerical Solution Method

The basic procedure for advancing the particle transport solution through one increment of time, Δt , consists of four steps for each particle.

- (1) Compute the fluid velocity at the particle location. This local fluid velocity, which is used to calculate the fluid drag force, has two parts: the velocity interpolated from the computed velocity field (Section 3.4) and a diffusion velocity computed from a Monte-Carlo method (Section 3.7.2).
- (2) Compute intermediate particle velocities from explicit approximations of the momentum Equation (3-121) without fluid drag forces.
- (3) Compute a new time-level particle velocity by iteratively adjusting the intermediate particle velocities to include the effects of the particle fluid drag forces.
- (4) Move the particles to a new location using the average particle velocity for the time increment, Δt .

Following the transport of the particles, two additional phenomena are modeled.

- (1) Deposit particles impacting a rigid surface, if criteria discussed in Section 3.7.3 are met.
- (2) Entrain particles deposited on surfaces, if criteria discussed in Section 3.7.4 are met.

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4 SUMMARY

In this report we have described the theory behind the GASFLOW computer code and the computational model used to numerically integrate the governing equations in time and space.

The core of the code is based on the conservation laws for mass, momentum, and energy, which were presented in integral form to more closely mirror the finite volume formulation for the discrete equations. The basic fluid dynamics equations are supplemented with relations for multiple gas species, heat transfer, structural condensation and vaporization of liquid films, a two-phase homogeneous equilibrium model for the fluid mixture, a parametric droplet depletion or rainout model, turbulence transport, a simple finite-rate global chemical kinetics model for combustion, an ignitor model for both spark- and glow-plug-type ignitors, recombiner box models for the NIS and Siemens devices, and a discrete particle model for transport, deposition, and entrainment.

An ICE'd-ALE numerical method, adapted to fixed geometry, is used to solve the equations of motion. Each time step is split into three phases: (1) an explicit Lagrangian phase in which most of the physics and chemistry is evaluated, (2) an implicit Lagrangian phase in which time-advanced pressure, velocity, density, and energy are computed together, and (3) a rezone phase in which problem variables are repartitioned or rezoned onto the original mesh. Turbulence quantities and a computational time-step stability analysis then complete the time step.

Using the above field equation model coupled with finite-rate global chemical kinetics, we have successfully analyzed the hydrogen transport, mixing, and combustion and mitigating measures with recombiners and ignitors in a nuclear reactor containment under accident conditions. The reader is referred to the GASFLOW Assessment Manual for more details.

APPENDIX A. THE GAUSS DIVERGENCE THEOREM

The divergence of a continuously differentiable vector Φ integrated over a finite volume V may be written as

$$\int_V \nabla \cdot \Phi dV .$$

Using the Gauss Divergence Theorem, this may be expressed as a surface integral

$$\int_V \nabla \cdot \Phi dV = \int_S \Phi \cdot n dA . \quad (A-1)$$

A rigorous development of Equation (A-1) may be found in most advanced calculus texts; for example, see Apostol (Ref. A-1).

A discrete approximation to the surface integral, which is applied to hexahedral control volumes, is obtained by summing the individual contributions from each face, f , as follows:

$$\int_S \Phi \cdot n dA \approx \sum_f \Phi_f dA_f , \quad (A-2)$$

where Φ_f is the outward face-normal component of Φ , and dA_f is the face area. For the regular parallelepiped cells used in GASFLOW, the sum is over the west, east, south, north, bottom, and top faces (abbreviated as W, E, S, N, B, and T, respectively).

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APPENDIX B. STRUCTURAL HEAT-CONDUCTION ALGORITHM

1 INTEGRAL FORMULATION

The equation of change in integral form for heat stored in a solid volume is

$$\frac{d}{dt} \int_V q \, dV = - \int_V \nabla \cdot \mathbf{q} \, ds + \int_V q^* \, dV \quad (\text{B-1})$$

or

$$\frac{d}{dt} \int_V q \, dV = - \oint_S \mathbf{q} \cdot \mathbf{n} \, ds + \int_V q^* \, dV \quad (\text{B-2})$$

which in one dimension may be expressed as

$$\frac{d}{dt} \int_V q \, dV = \oint_S k \frac{\partial T}{\partial x} \, ds + \int_V q^* \, dV \quad (\text{B-3})$$

We neglect here any volumetric heat sources; thus, the second term on the right-hand side of Equation (B-3) is set to zero, yielding the following equation:

$$\frac{d}{dt} \int_V q \, dV = \int_S k \frac{\partial T}{\partial x} \, ds \quad (\text{B-4})$$

In the GASFLOW model for structural heat conduction, these equations are solved one dimensionally in Cartesian or cylindrical coordinates.

2 STRUCTURES

A heat conducting solid of depth x_D is discretized by N heat-conducting elements ($1 \leq j \leq N$). Material properties (ρ , C_p , and k) are independent of temperature in these derivations, but thermal conductivity can be different in each element (composite layer). Nodes, also numbered 1 through N , as shown in Figure B-1, are located on the positive side of the conducting elements. Node zero denotes the surface node on the negative side; node N denotes the surface node on the positive side.

Structures. For purposes of problem definition, heat-conducting structures are divided into three categories: *slabs*, *sinks*, and *walls*. *Slabs* and *sinks* have only one element in contact with fluid (element No. 1). More accurate spatial resolution of temperatures is generally wanted near the fluid-structure interface; hence, the smallest element is normally element 1 with increasing element sizes away from the interface. *Walls* have both surfaces in contact with a fluid. Comparable discretization of each structural type is shown in Figures B-2 and B-3.

Figure B-1. Diagram of structural heat conductor elements and nodes

Figure B-2. Slab and sink discretization

Figure B-3. Wall discretization

The user has the option to specify the size of the surface node for slabs and sinks. The user enters `dxslabc` for concrete slabs, `dxslabs` for steel slabs, `sinkdef(13,*)` for sink surface nodes, and `walldef(5,*)` for the surface node thickness that applies on both sides of the walls. A dynamic mesh expansion is then automatically applied that divides the structure thickness x_D into the specified number of elements (`nhteslab`, `nhtesink`, `nhtewall`). If these numbers are left blank or set to zero, an equidistant mesh is applied (see the User's Manual).

3 CARTESIAN COORDINATES

3.1 Interior Elements

Consider a planar heat-conducting element $V = \Delta x \Delta y \Delta z$ where Δx is the region around the node j , $x_w \leq x \leq x_e$, as shown in Figure B-4.

Figure B-4. Planar heat conducting element

The change of heat energy stored in element V over the region Δx is calculated from the following expression:

$$V\rho C_p(T_j^{n+1} - T_j^n)/\Delta t \quad (B-5)$$

The heat flux passing through the surface at x_w is calculated from the following terms:

$$-k_j A \left((1 - \Theta)(T_j^n - T_{j-1}^n) + \Theta(T_j^{n+1} - T_{j-1}^{n+1}) \right) / \Delta x_w \quad (B-6)$$

A numerical multiplier Θ is used to weight information from the beginning of a time step T^n and from the end of a time step T^{n+1} . Here, the numerical multiplier Θ distinguishes between the backward Euler and Crank Nicholson integration schemes with

$$\Theta = \begin{cases} 1 & \text{for backward Euler} \\ \frac{1}{2} & \text{for Crank Nicholson} \end{cases} \quad (B-7)$$

The heat flux passing through the surface at x_e is calculated from the following terms:

$$k_{j+1}A\left((1-\Theta)(T_{j+1}^n - T_j^n) + \Theta(T_{j+1}^{n+1} - T_j^{n+1})\right)/\Delta x_e \quad (B-8)$$

Thus, the equation of change for heat stored in the region Δx around node j is

$$\frac{V\rho\overline{C_p}}{\Delta t}(T_j^{n+1} - T_j^n) = A \left[\begin{aligned} & \left((1-\Theta)(T_{j+1}^n - T_j^n) + \Theta(T_{j+1}^{n+1} - T_j^{n+1})\right)k_{j+1}/\Delta x_e \\ & - \left((1-\Theta)(T_j^n - T_{j-1}^n) + \Theta(T_j^{n+1} - T_{j-1}^{n+1})\right)k_j/\Delta x_w \end{aligned} \right] , \text{ or} \quad (B-9)$$

$$\frac{\Delta x \Delta y \Delta z \overline{\rho C_p}}{\Delta t}(T_j^{n+1} - T_j^n) = \Delta y \Delta z \left[\begin{aligned} & \left((1-\Theta)(T_{j+1}^n - T_j^n) + \Theta(T_{j+1}^{n+1} - T_j^{n+1})\right)k_{j+1}/\Delta x_e \\ & - \left((1-\Theta)(T_j^n - T_{j-1}^n) + \Theta(T_j^{n+1} - T_{j-1}^{n+1})\right)k_j/\Delta x_w \end{aligned} \right] , \text{ or} \quad (B-10)$$

$$\frac{\Delta x \overline{\rho C_p}}{\Delta t}(T_j^{n+1} - T_j^n) = \left[\begin{aligned} & \left((1-\Theta)(T_{j+1}^n - T_j^n) + \Theta(T_{j+1}^{n+1} - T_j^{n+1})\right)k_{j+1}/\Delta x_e \\ & - \left((1-\Theta)(T_j^n - T_{j-1}^n) + \Theta(T_j^{n+1} - T_{j-1}^{n+1})\right)k_j/\Delta x_w \end{aligned} \right] . \quad (B-11)$$

The coefficients can be ordered according to the temperature indices, which yields the general equation:

$$\Theta\Lambda_w T_{j-1}^{n+1} - (1 + \Theta(\Lambda_w + \Lambda_e))T_j^{n+1} + \Theta\Lambda_e T_{j+1}^{n+1} = \left[\begin{aligned} & -(1-\Theta)\Lambda_w T_{j-1}^n \\ & + ((1-\Theta)(\Lambda_w + \Lambda_e) - 1)T_j^n \\ & -(1-\Theta)\Lambda_e T_{j+1}^n \end{aligned} \right] , \quad (B-12)$$

where

$$\eta = \frac{\Delta t}{\Delta x \overline{\rho C_p}}, \quad \Lambda_w = \frac{k_j \eta}{\Delta x_w}, \quad \Lambda_e = \frac{k_{j+1} \eta}{\Delta x_e} , \quad (B-13)$$

and

$$\Delta x = \frac{(x_{j+1} - x_{j-1})}{2}, \Delta x_w = (x_j - x_{j-1}), \Delta x_e = (x_{j+1} - x_j) , \quad (B-14)$$

and

$$\overline{\rho C_p} = \frac{((\rho C_p)_j \Delta x_w + (\rho C_p)_{j+1} \Delta x_e)}{2\Delta x} . \quad (B-15)$$

3.2 Boundary Conditions

3.2.1 General. A wall with its thickness along the x coordinate has two boundaries: a front (or west) boundary at node 0 and a back (or east) boundary at node N , as shown in Figure B-5. The fluid temperatures at the boundaries are described in GASFLOW as being at the west or east sides, i.e., T_{fw} or T_{fe} .

Figure B-5. Configuration for a wall, or two-sided heat-conduction problem

The heat balance for the front boundary element Δx for $j=0$ is

$$\frac{\Delta x (\rho C_p)_1}{\Delta t} (T_0^{n+1} - T_0^n) = \left[\begin{aligned} &((1 - \Theta)(T_1^n - T_0^n) + \Theta(T_1^{n+1} - T_0^{n+1}))k_1/\Delta x_e \\ &- h_w(\Theta T_0^{n+1} + (1 - \Theta)T_0^n - T_{fw}) + q_{cw} \end{aligned} \right] \quad (B-16)$$

This yields the following matrix coefficients for the surface temperature node 0:

$$-(1 + \Theta(\Lambda_e + \eta h_w))T_0^{n+1} + \Theta \Lambda_e T_1^{n+1} = \left[\begin{aligned} &+ ((1 - \Theta)(\Lambda_e + \eta h_w) - 1)T_0^n \\ &- (1 - \Theta)\Lambda_e T_1^n - \eta(h_w T_{fw} + q_{cw}) \end{aligned} \right] \quad (B-17)$$

with

$$\eta = \frac{\Delta t}{\Delta x (\rho C_p)_1}, \quad \Lambda_e = \frac{k_1 \eta}{\Delta x_e}, \quad \Delta x = \frac{(x_1 - x_0)}{2}, \quad \Delta x_e = (x_1 - x_0) \quad (B-18)$$

The heat balance for the back boundary element Δx for $j = N$ is

$$\frac{\Delta x (\rho C_p)_N}{\Delta t} (T_N^{n+1} - T_N^n) = \left[\begin{aligned} &((1 - \Theta)(T_{N-1}^n - T_N^n) + \Theta(T_{N-1}^{n+1} - T_N^{n+1}))k_N/\Delta x_w \\ &- h_e(\Theta T_N^{n+1} + (1 - \Theta)T_N^n - T_{fe}) + q_{ce} \end{aligned} \right] \quad (B-19)$$

This yields the equation for the back boundary temperature in a mirrored form to Equation (B-17):

$$\Theta \Lambda_w T_{N-1}^{n+1} - (1 + \Theta(\Lambda_w + \eta h_e)) T_N^{n+1} = \left[\begin{array}{l} + ((1 - \Theta)(\Lambda_w + \eta h_e) - 1) T_N^n \\ - (1 - \Theta) \Lambda_w T_{N-1}^n - \eta (h_e T_{fe} + q_{ce}) \end{array} \right] \quad (B-20)$$

with

$$\eta = \frac{\Delta t}{\Delta x (\rho C_p)_N}, \quad \Lambda_w = \frac{k_N \eta}{\Delta x_w}, \quad \Delta x = \frac{(x_N - x_{N-1})}{2}, \quad \Delta x_w = (x_N - x_{N-1}) \quad (B-21)$$

3.2.2 Specified Heat Flux. Instead of using the fluid temperature with a heat-transfer coefficient h and the condensation/vaporization heat flux q_c , one could also solve for the boundary temperature with a specified total heat flux. The specified total heat flux would be q_w on the west surface and q_e on the east surface. The heat flux may be specified on one or both surfaces. For specified heat fluxes at both boundaries, Equations (B-17) and (B-20) are written with the heat-transfer coefficient h set to zero and with the condensation heat flux q_{cw} and q_{ce} replaced by the total heat fluxes q_w and q_e , respectively. The total heat flux is supplied as input with a positive value on either structure surface denoting an energy addition. The total heat flux may be specified on one or both surfaces.

3.2.3 Adiabatic. For an adiabatic boundary condition, no heat flows across the surface. A zero temperature gradient then exists at the surface. For adiabatic boundary conditions on both surfaces, Equations (B-17) and (B-20) are written without any heat transfer from the fluid side by zeroing both surface values:

$$q_{cw} = h = 0 \quad (B-22)$$

Adiabatic boundary conditions may be specified on one or both surfaces.

3.2.4 Specified Surface Temperature. When using specified surface temperatures at both surfaces, one applies directly the input surface temperatures T_{sw} and T_{se} , and Equations (B-17) and (B-20) are replaced by the following:

$$T_0^{n+1} = T_{sw} = \text{input for west surface}, \quad T_N^{n+1} = T_{se} = \text{input for east surface} \quad (B-23)$$

Surface temperatures may be specified on one or both surfaces.

4 CYLINDRICAL COORDINATES

4.1 Interior Elements

Structures in radial direction are considered as cylindrical when applying cylindrical coordinates in GASFLOW. We then solve for the radial heat conduction consistently in cylindrical geometry. For the azimuthal and the axial heat conduction we continue to simulate 1D heat conduction through Cartesian structures. Radial energy balance is made for the cylindrical heat-conducting element. Figure B-6 shows the configuration of this element. The convention is that the west wall is on the inside and the east wall is on the outside of the cylinder.

Figure B-6. Configuration for a cylindrical heat-conducting element

The heat balance for the region Δr around node j , centered at r_j , is

$$\frac{V \rho C_p}{\Delta t} (T_j^{n+1} - T_j^n) = \left[\begin{aligned} & \left((1 - \Theta)(T_{j+1}^n - T_j^n) + \Theta(T_{j+1}^{n+1} - T_j^{n+1}) \right) k_{j+1} A_e / \Delta r_e \\ & - \left((1 - \Theta)(T_j^n - T_{j-1}^n) + \Theta(T_j^{n+1} - T_{j-1}^{n+1}) \right) k_j A_w / \Delta r_w \end{aligned} \right] \quad (B-24)$$

or

$$\frac{\bar{r} \Delta r \rho C_p}{\Delta t} (T_j^{n+1} - T_j^n) = \left[\begin{aligned} & \left((1 - \Theta)(T_{j+1}^n - T_j^n) + \Theta(T_{j+1}^{n+1} - T_j^{n+1}) \right) k_{j+1} r_e / \Delta r_e \\ & - \left((1 - \Theta)(T_j^n - T_{j-1}^n) + \Theta(T_j^{n+1} - T_{j-1}^{n+1}) \right) k_j r_w / \Delta r_w \end{aligned} \right] \quad (B-25)$$

This gives the same form of the equation for the internal temperatures at node j as Equation (B-17):

$$\Theta \Lambda_w T_{j-1}^{n+1} - (1 + \Theta(\Lambda_w + \Lambda_e)) T_j^{n+1} + \Theta \Lambda_e T_{j+1}^{n+1} = \begin{bmatrix} -(1 - \Theta) \Lambda_w T_{j-1}^n \\ + ((1 - \Theta)(\Lambda_w + \Lambda_e) - 1) T_j^n \\ -(1 - \Theta) \Lambda_e T_{j+1}^n \end{bmatrix} . \quad (\text{B-26})$$

The coefficients in cylindrical coordinates are the following:

$$\eta = \frac{\Delta t}{\bar{r} \Delta r \rho C_p}, \quad \Lambda_w = \frac{k_j \eta r_w}{\Delta r_w}, \quad \Lambda_e = \frac{k_{j+1} \eta r_e}{\Delta r_e} \quad (\text{B-27})$$

with

$$\bar{r} = \frac{r_w + r_e}{2}, \quad r_w = \frac{r_{j-1} + r_j}{2}, \quad r_e = \frac{r_j + r_{j+1}}{2}, \quad \Delta r = |r_e - r_w|, \quad (\text{B-28})$$

$$\Delta r_w = |r_j - r_{j-1}|, \quad \Delta r_e = |r_{j+1} - r_j|, \quad \text{and} \quad (\text{B-29})$$

$$\bar{\rho C_p} = \frac{\left(r_w \frac{\Delta r_w}{2} (\rho C_p)_j + r_e \frac{\Delta r_e}{2} (\rho C_p)_{j+1} \right)}{\left(r_w \frac{\Delta r_w}{2} + r_e \frac{\Delta r_e}{2} \right)} . \quad (\text{B-30})$$

The absolute values for Δr in Equations (B-28) and (B-29) allow one to simulate with the same equations the conditions in which the radius at the west side of the structure is larger than at the east side, i.e., for convex slabs.

4.2 Boundary Conditions

4.2.1 General. In cylindrical coordinates, a wall has two boundaries: the front (or west) is the inside surface, and the back (or east) is the outside surface, as shown in Figure B-7. The solid surface element at either boundary is Δr thick, where $\Delta r = r_N - r_e$ on the east side and $\Delta r = r_e - r_0$ on the west side. The fluid temperatures at the boundaries are T_{fe} on the east side and T_{fw} on the west side.

Figure B-7. Configuration for a two-sided cylindrical heat-conducting element

The heat balance for the west (front) boundary element at $j=0$ yields

$$\frac{\bar{r}\Delta r(\rho C_p)_1}{\Delta t}(T_0^{n+1} - T_0^n) = \left[\begin{aligned} &((1-\Theta)(T_1^n - T_0^n) + \Theta(T_1^{n+1} - T_0^{n+1}))k_1 r_e / \Delta r_e \\ &- (h_w(\Theta T_0^{n+1} + (1-\Theta)T_0^n - T_{fw}) + q_{cw})r_0 \end{aligned} \right] \quad (B-31)$$

This gives the following linear equation for the boundary temperature T_0

$$-(1 + \Theta(\Lambda_e + \eta h_w r_0))T_0^{n+1} + \Theta \Lambda_e T_1^{n+1} = \left[\begin{aligned} &+ ((1-\Theta)(\Lambda_e + \eta h_w r_0) - 1)T_0^n \\ &- (1-\Theta)\Lambda_e T_1^n - \eta r_0(h_w T_{fw} + q_{cw}) \end{aligned} \right] \quad (B-32)$$

with

$$\eta = \frac{\Delta t}{\bar{r}\Delta r(\rho C_p)_1}, \quad \Lambda_e = \frac{k_1 \eta r_e}{\Delta r_e}, \quad \text{and} \quad (B-33)$$

$$\Delta r = \frac{\Delta r_e}{2}, \quad \Delta r_e = |r_1 - r_0|, \quad r_e = \frac{(r_1 + r_0)}{2}, \quad \bar{r} = \frac{(r_e + r_0)}{2} \quad (B-34)$$

The heat balance for the east (back) boundary element at $j = N$ yields

$$\frac{\bar{r}\Delta r(\rho C_p)_N}{\Delta t}(T_N^{n+1} - T_N^n) = \left[\begin{aligned} &((1-\Theta)(T_{N-1}^n - T_N^n) + \Theta(T_{N-1}^{n+1} - T_N^{n+1}))k_N r_w / \Delta r_w \\ &- (h_e(\Theta T_N^{n+1} + (1-\Theta)T_N^n - T_{fe}) + q_{ce})r_N \end{aligned} \right], \quad (B-35)$$

which results in the linear equation for the boundary temperature T_N that is the mirrored form of Equation (B-32), shown as

$$\Theta \Lambda_w T_{N-1}^{n+1} - (1 + \Theta(\Lambda_w + \eta h_e r_N))T_N^{n+1} = \left[\begin{aligned} &+ ((1-\Theta)(\Lambda_w + \eta h_e r_N) - 1)T_N^n \\ &- (1-\Theta)\Lambda_w T_{N-1}^n - \eta r_N (h_e T_{fe} + q_{ce}) \end{aligned} \right], \quad (B-36)$$

with

$$\eta = \frac{\Delta t}{\bar{r}\Delta r(\rho C_p)_N}, \quad \Lambda_w = \frac{k_N \eta r_w}{\Delta r_w}, \quad \text{and} \quad (B-37)$$

$$\Delta r = \frac{\Delta r_w}{2}, \quad \Delta r_w = |(r_N - r_{N-1})|, \quad r_w = \frac{(r_N + r_{N-1})}{2}, \quad \bar{r} = \frac{(r_w + r_N)}{2}. \quad (B-38)$$

4.2.2 Specified Heat Flux. Instead of using the fluid temperature with a heat-transfer coefficient h and the condensation/vaporization heat flux q_c , one could also solve for the boundary temperature with a specified total heat flux. The specified total heat flux would be q_w on the west surface and q_e on the east surface. The heat flux may be specified on one or both surfaces. For specified heat fluxes at both boundaries, Equations (B-32) and (B-36) are written with the heat-transfer coefficient h set to zero and with the condensation heat flux q_{cw} and q_{ce} replaced by the total heat fluxes q_w and q_e , respectively. The total heat flux is supplied as input with a positive value on either structure surface, denoting an energy addition. The total heat flux may be specified on one or both surfaces.

4.2.3 Adiabatic. For an adiabatic boundary condition, no heat flows across the surface. A zero temperature gradient then exists at the surface. For adiabatic boundary conditions on both surfaces, Equations (B-32) and (B-36) are written without any heat transfer from the fluid side by zeroing both surface values:

$$q_{cw} = h = 0. \quad (B-39)$$

Adiabatic boundary conditions may be specified on one or both surfaces.

4.2.4 Specified Surface Temperature. When using specified surface temperatures at both surfaces, one applies directly the input surface temperatures T_{sw} and T_{se} , and Equations (B-32) and (B-36) are replaced by the following:

$$T_0^{n+1} = T_{sw} = \text{input for west surface}, \quad T_N^{n+1} = T_{se} = \text{input for east surface} \quad (B-40)$$

Surface temperatures may be specified on one or both surfaces.

5 SUMMARY OF NUMERICAL EQUATIONS

GASFLOW solves the 1D structural heat-conduction equations by using a variable mesh Crank Nicholson method. The numerical equations described above may be cast in the form of the following equation to solve for temperatures T^{n+1} at the end of time step, given temperatures T^n at the beginning of the time step for all nodes j from 1 to N , per the following equation:

$$aT_{j-1}^n + bT_j^n + cT_{j+1}^n = r \quad . \quad (B-41)$$

Equations for nine cases are cast into Equation (B-41): interior nodes; and boundary nodes at the east and west surfaces for general, specified heat flux, specified temperature, and adiabatic boundary conditions. The coefficients a , b , and c , and the terms on the right hand side, designated by r , in Equation (B-41) are summarized in Table B-1 for nodes 1 through N .

Table B-1. Coefficients and Terms for Heat-Conduction Algorithm

Case	j	a	b	c	r
Interior	1 to N-1	$\Theta\Lambda_w$	$-(1+\Theta(\Lambda_w+\Lambda_e))$	$\Theta\Lambda_e$	$\begin{bmatrix} -(1-\Theta)\Lambda_w T_{j-1}^n - (1-\Theta)\Lambda_e T_{j+1}^n \\ + ((1-\Theta)(\Lambda_w + \Lambda_e) - 1)T_j^n \end{bmatrix}$
General	0	0	$-\left(1 + \frac{\Theta(\Lambda_e + \eta h_w \phi_0)}{\Theta(\Lambda_e + \eta h_w \phi_0)}\right)$	$\Theta\Lambda_e$	$\begin{aligned} & ((1-\Theta)(\Lambda_e + \eta h_w \phi_0) - 1)T_0^n \\ & -(1-\Theta)\Lambda_e T_1^n - \eta\phi_0(h_w T_{fw} + q_{cw}) \end{aligned}$
Specified q	0	0	$(1+\Theta\Lambda_e)$	$\Theta\Lambda_e$	$\begin{aligned} & ((1-\Theta)\Lambda_e - 1)T_0^n \\ & -(1-\Theta)\Lambda_e T_1^n - \eta\phi_0 q_w \end{aligned}$
Adiabatic	0	0	$(1+\Theta\Lambda_e)$	$\Theta\Lambda_e$	$\begin{aligned} & ((1-\Theta)\Lambda_e - 1)T_0^n \\ & -(1-\Theta)\Lambda_e T_1^n - \eta\phi_0 q_w \end{aligned}$
Specified T	0	0	1	0	T_{sw}
General	N	$\Theta\Lambda_w$	$-\left(1 + \frac{\Theta(\Lambda_w + \eta h_e \phi_N)}{\Theta(\Lambda_w + \eta h_e \phi_N)}\right)$	0	$\begin{aligned} & ((1-\Theta)(\Lambda_w + \eta h_e \phi_N) - 1)T_N^n \\ & -(1-\Theta)\Lambda_w T_{N-1}^n - \eta\phi_N(h_e T_{fc} + q_{cc}) \end{aligned}$
Specified q	N	$\Theta\Lambda_w$	$-(1+\Theta\Lambda_w)$	0	$\begin{aligned} & ((1-\Theta)\Lambda_w - 1)T_N^n \\ & -(1-\Theta)\Lambda_w T_{N-1}^n - \eta\phi_N q_e \end{aligned}$
Adiabatic	N	$\Theta\Lambda_w$	$-(1+\Theta\Lambda_w)$	0	$\begin{aligned} & ((1-\Theta)\Lambda_w - 1)T_N^n \\ & -(1-\Theta)\Lambda_w T_{N-1}^n - \eta\phi_N q_e \end{aligned}$
Specified T	N	0	1	0	T_{se}

Expressions for expanding parameters used in the coefficients in Equation (B-41) into primary variables are listed below:

Cartesian Coordinates

$$\eta = \frac{\Delta t}{\Delta x \rho C_p}, \quad \Lambda_w = \frac{k_j \eta}{\Delta x_w}, \quad \Lambda_e = \frac{k_{j+1} \eta}{\Delta x_e}, \quad \phi_0 = \phi_N = 1$$

$$\Delta x = \frac{1}{2} \begin{cases} x_1 - x_0 & \text{for } j=0 \\ x_{j+1} - x_{j-1} & \text{for } j=1, N-1 \\ x_N - x_{N-1} & \text{for } j=N \end{cases}, \quad \overline{\rho C_p} = \begin{cases} (r C_p)_1 & \text{for } j=0 \\ \left(\frac{(\rho C_p)_j \Delta x_w + (\rho C_p)_{j+1} \Delta x_e}{2 \Delta x} \right) & \text{for } j=1, N-1 \\ (\rho C_p)_N & \text{for } j=N \end{cases}$$

$$\Delta x_w = x_j - x_{j-1}, \quad \Delta x_e = x_{j+1} - x_j$$

Cylindrical Coordinates

$$\eta = \frac{\Delta t}{\bar{r} \Delta r \rho C_p}, \quad \Lambda_w = \frac{k_j r_w \eta}{\Delta r_w}, \quad \Lambda_e = \frac{k_{j+1} r_e \eta}{\Delta r_e}, \quad \phi_0 = r_0, \quad \phi_N = r_N$$

$$\Delta r = \frac{1}{2} \begin{cases} (r_1 - r_0) & \text{for } j=0 \\ (r_{j+1} - r_{j-1}) & \text{for } j=1, N-1 \\ (r_N - r_{N-1}) & \text{for } j=N \end{cases}, \quad \bar{r} = \frac{1}{2} \begin{cases} (r_w + r_0) & \text{for } j=0 \\ (r_w + r_e) & \text{for } j=1, N-1 \\ (r_N + r_e) & \text{for } j=N \end{cases}$$

$$r_w = \left(\frac{r_{j-1} + r_j}{2} \right), \quad r_e = \left(\frac{r_j + r_{j+1}}{2} \right), \quad \Delta r_w = |r_j - r_{j-1}|, \quad \Delta r_e = |r_{j+1} - r_j|$$

$$\overline{\rho C_p} = \begin{cases} (\rho C_p)_1 & \text{for } j=0 \\ \left(\frac{r_w \frac{\Delta r_w}{2} (\rho C_p)_j + r_e \frac{\Delta r_e}{2} (\rho C_p)_{j+1}}{r_w \frac{\Delta r_w}{2} + r_e \frac{\Delta r_e}{2}} \right) & \text{for } j=1, N-1 \\ (\rho C_p)_N & \text{for } j=N \end{cases}$$

APPENDIX C. PRECONDITIONED CONJUGATE RESIDUAL ALGORITHM

1 INTRODUCTION

The pressure equation [Equation (3-91), Section 3.3] is solved by the preconditioned conjugate residual (PCR) method described in this section. Consider the linear system

$$Az = b, \quad (C-1)$$

where A is an n by n symmetric positive definite (SPD) matrix, z is a solution vector, and b is known. The residual vector $r \equiv b - Ax$, a measure of error of any vector x from the exact solution given in Equation (C-1), is the focus of the development that follows. Variable definitions that are applicable only in this appendix are listed in Section 2 below.

2 DEFINITION OF VARIABLES

A	n -by- n SPD coefficient matrix
b	Right-hand side vector
B	Diagonal of matrix A
D	Diagonal of matrix M
k	Iteration count
L	Strictly lower triangular part of A
M	n -by- n SPD preconditioning matrix
n	Number of equations to be solved
p	Search vector
Q	Nonsingular matrix such that $M = QQ^T$
q	Working array
$\hat{r}$	Residual vector for preconditioned system
r	Residual vector ($r \equiv b - Ax$)
U	Strictly upper triangular part of A
V	Cell volume
x	Solution vector estimate
z	Solution vector for $Az = b$
a_k	Step length
b_k	Orthogonalization coefficient
e	Global convergence criteria
λ	Eigenvalue

3 MOTIVATION

The guiding philosophy behind the PCR method can be shown by first considering the functional $E_m(x)$ defined as

$$E_\mu(x) \equiv \frac{1}{2}((x-z), A^\mu(x-z)) \quad , \quad (C-2)$$

where (v, w) denotes an inner product for vectors v and w . For example, $(x, Ax) \equiv x^T Ax$. $E_m(x)$ is defined as the error functional and is equal to one-half the square of the A^m norm of $(x - z)$. The exponent μ takes on positive integer values; $\mu = 1$ for conjugate gradient minimization, and $\mu = 2$ for conjugate residual minimization (the choice made here). Recalling $r = b - Ax = -A(x - z)$, we write $E_2(x)$ as

$$E_2(x) \equiv \frac{1}{2}(A(x-z), A(x-z)) = \frac{1}{2}(r, r) \quad . \quad (C-3)$$

It follows that the minimum of $E(x)$ as x varies over R^n is

$$\frac{\partial E_2(x)}{\partial x} \equiv A(Ax - b) = -Ar \quad . \quad (C-4)$$

Hence, the problem of minimizing the quadratic error functional $E_2(x)$ is seen to be equivalent to solving the original linear system [Equation (C-1)] with the solution being $x = z$ in each case.

The goal of the PCR procedure is to successively calculate improved estimates for the solution vector x_k ,

$$x_k = x_{k-1} + a_k p_k, \quad (C-5)$$

by minimizing $E(x)$ along yet-to-be-determined search directions, p_k , where a_k and b_k are constants. Substituting Equation (C-5) into Equation (C-3) gives

$$E_2(x_k) \equiv \frac{1}{2}(A(x_{k-1} + \alpha_k p_k - z), A(x_{k-1} + \alpha_k p_k - z)) \quad . \quad (C-6)$$

The optimum value of a_k minimizes $E_2(x)$ with respect to a_k

$$\frac{\partial E_2(x_k)}{\partial \alpha_k} = \alpha_k (Ap_k, Ap_k) - (r_{k-1}, Ap_k) = 0 \quad (C-7)$$

or

$$\alpha_k = (r_{k-1}, Ap_k) / (Ap_k, Ap_k) \quad . \quad (C-8)$$

Because constant values of $E(x)$ correspond to level surfaces (hyper ellipsoids) in R^n , it is natural to select the negative gradient of $E(x)$ [Equation (C-3)] as the search

direction, with $-E(x_k)$ being the direction of most rapid change at x . This is equivalent to using r as the search direction vector p in Equation (C-5) and is known as the method of steepest descent. The set of residual vectors r_i ($i = 0, k$) in the steepest descent method is not usually linearly independent, and if the condition number of A , $k(A) = l_{\max}/l_{\min}$, is large (corresponding to highly elongated ellipsoids), the convergence can be slow. Instead, we compute p_k as follows:

$$p_k = r_{k-1} + b_k p_{k-1} \quad (C-9)$$

subject to the requirement

$$(p_i, Ap_j) = 0 \text{ for } i \neq j \leq n \quad (C-10)$$

Computed this way, the search directions, p_i , are *A-conjugate* (or *A-orthogonal*) to all other directions p_j , and the solution vector x_k computed from Equation (C-5) will minimize $E_2(x_k)$ over the span $\{p_0, p_1, \dots, p_k\}$ (Ref. C-1). Chandra (Ref. C-2) shows that the family of conjugate direction methods (which includes the conjugate residual method) are optimal among all linear iterative methods with respect to $E_m(x)$.

The orthogonalization coefficient b_k is found by substituting Equation (C-9) into Equation (C-10)

$$\beta_k = -(r_{k-1}, Ap_{k-1}) / (p_{k-1}, Ap_{k-1}) \quad (C-11)$$

4 PRECONDITIONING

The solution to Equation (C-1) can be obtained more rapidly if we precondition the system $Ax = b$. Instead, we solve

$$A'x' = b' \quad (C-12)$$

where $A' = Q^{-1}AQ^{-T}$, $x' = Q^T x$, $b' = Q^{-1}b$, and Q is a nonsingular matrix. If $Q^{-1}AQ^{-T} \approx I$, then $k(A')$ is small and $A' \approx Q^{-1}Q^{-T}$. Defining $M \approx Q^{-1}Q^{-T}$ as the preconditioning matrix, we use the factorization of Dupont, Kendall, and Rachford (Ref. C-3) for M ,

$$M = (L + D)D^{-1}(D + U) \quad (C-13)$$

to solve a system of the form $Mu = v$, which may be inverted rapidly by an LU decomposition. (LU refers to a matrix procedure operating on the Lower and Upper off-diagonal terms.) The additional effort required to solve for u is more than offset by the faster convergence of the PCR algorithm presented in the next section.

5 THE NUMERICAL PCR ALGORITHM

The solution to the linear system [Equation (C-1)] is obtained from the following version of the PCR method and closely follows the algorithm of Chandra (Ref. C-2, Section 5.4).

Step 1. Initialization

$$\text{Choose } x_0 \quad (C-14a)$$

$$r_0 = b - Ax_0 \quad (C-14b)$$

$$\text{Solve: } M\hat{r}_0 = r_0 \text{ for } \hat{r}_0 \quad (C-14c)$$

$$p_0 = \hat{r}_0 \quad (C-14d)$$

$$\text{If } [r_0/V]_m < e \text{ for } 1 \leq m \leq n, \text{ quit (solution is already converged).} \quad (C-14e)$$

$$q_0 = 0 \quad (C-14f)$$

Step 2. Compute new search, solution, and residual vectors

For $k = 1, 2, \dots, n$

$$\beta_k = -(\hat{r}_{k-1}, q_{k-1}) / (q_{k-1}, Ap_{k-1}) \quad (C-15a)$$

$$p_k = \hat{r}_{k-1} + \beta_k p_{k-1} \quad (C-15b)$$

$$\text{Solve: } Mq_k = Ap_k \text{ for } q_k \quad (C-15c)$$

$$\alpha_k = (\hat{r}_{k-1}, Ar_{k-1}) / (q_k, Ap_k) \quad (C-15d)$$

$$x_k = x_{k-1} + \alpha_k p_k \quad (C-15e)$$

$$\hat{r}_k = \hat{r}_{k-1} - \alpha_k q_k \quad (C-15f)$$

Step 3. Has solution converged?

$$r_k = r_{k-1} - \alpha_k Ap_k \quad (C-16a)$$

$$\text{If } [r_k/V]_m < e \text{ for } 1 \leq m \leq n, \text{ quit; otherwise go to step 2.} \quad (C-16b)$$

REFERENCES

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