Theoretical and Computational Models of the GASFLOW-II Code

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ABSTRACT
GASFLOW-II is a finite-volume computer code that solves the time-dependent compressible Navier-Stokes equations for multiple gas species in a dispersed liquid water two-phase medium. The fluid-dynamics algorithm is coupled to the chemical kinetics of combusting gases to simulate diffusion or propagating flames in complex geometries of nuclear containments. GASFLOW-II is therefore able to predict gaseous distributions and thermal and pressure loads on containment structures and safety related equipment in the event combustion occurs. Current developments of GASFLOW-II are focused on hydrogen distribution, mitigation measures including carbon dioxide inerting, and possible combustion events in nuclear reactor containments. Fluid turbulence is calculated to enhance the transport and mixing of gases in rooms and volumes that may be connected by a ventilation system. Condensation, vaporization, and heat transfer to walls, floors, ceilings, internal structures, and within the fluid are calculated to model the appropriate mass and energy sinks.

I. INTRODUCTION

The potential for the occurrence of severe accidents in nuclear reactor systems has motivated research activities to model hydrogen transport, mixing, distribution, and possible combustion phenomena in these systems. Additional research of certain mitigation measures involving recombiners and inerting concepts is being conducted. As a logical and natural consequence of the complete analysis, the analysis tool should predict gaseous stratification without simplifying assumptions and provide a means to demonstrate possibilities of preventing combustible mixtures of gases accumulating. In the event that hydrogen distributions reach flammable mixtures, it is important to analyze entire facilities to determine the transient pressure and possible heating loads that may result from combustion events on the containment or ventilation structures and safety-related equipment. These analyses are also needed to plan emergency evacuation, to validate existing safety measures or programs or suggested changes, and to integrate the effects of hydrogen events with other safety analysis requirements.

II. 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, condensation, vaporization, 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) and temperature (T). As suggested by the "ALE" name, GASFLOW-II (Ref. 1) uses both the
Lagrangian and Eulerian viewpoints. The Lagrangian (or material) specification considers specific elements of matter and describes the motion as functions of space (x) and time (t). This viewpoint 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 parallelepipeds Eulerian volumes (cells) in either Cartesian or cylindrical geometry, it is natural to present the continuous equations in integral form (Refs. 2 and 3). This makes it easier to see how the integration of continuous volume and surface integrals are approximated by the discrete or finite-volume equations.

II.A. The Generalized Conservation Equation
The conservation of any arbitrary extensive variable (for example, mass, momentum, or energy) is

$$\frac{d}{dt} \int_V \Phi dV = \int_V S_\Phi dV$$  \hspace{1cm} (1)

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

$$\int_V \frac{\partial \Phi}{\partial t} dV = \oint_S \Phi(u \cdot A) dS + \int_V S_\Phi dV$$  \hspace{1cm} (2)

where $u(x, t)$ is the fluid velocity and $A$ 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. 4) 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. 3) (not necessarily a material volume) enclosed by surface $S^*$ gives

$$\frac{d}{dt} \int_{V^*} \Phi dV = \oint_{S^*} \frac{\partial \Phi}{\partial t} dV + \oint_{S^*} \Phi(b \cdot A) dS + \int_{V^*} S_\Phi dV$$  \hspace{1cm} (3)

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

$$\frac{d}{dt} \int_{V^*} \Phi dV = \oint_{S^*} \Phi(b - u) \cdot A dS + \int_{V^*} S_\Phi dV$$  \hspace{1cm} (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 $\Phi$ in an arbitrary control volume $V^*$ (left side) is equal to the inflow of $\Phi$ through the boundary plus the source term (right side). The term $b - u$ is the relative velocity between the control surface and the fluid. When $b = u$, we recover the Lagrangian form [Eq. (1)]. For a control volume that is fixed with respect to the coordinate axes, $b = 0$ and we recover the Eulerian form

$$\frac{d}{dt} \int_{V^*} \Phi dV = \oint_{S^*} \Phi(u \cdot A) dS + \int_{V^*} S_\Phi dV$$  \hspace{1cm} (5)

or

XI-158
\[ \int \frac{\partial \Phi}{\partial t} dV = -\int \Phi (\mathbf{u} \cdot \mathbf{n}) dA + \int S_{\rho} dV \quad (6) \]

II.B. The Mass Conservation Equations
The mixture mass conservation equation follows directly from Eq. (4) by letting \( \Phi = \rho \)

\[ \frac{d}{dt} \int \rho dV = \oint \rho (\mathbf{b} - \mathbf{u}) \cdot \mathbf{A} dS + \int S_{\rho} dV \quad (7) \]

where \( \rho \) is the mixture density or the sum of the macroscopic densities for each individual species, \( \mathbf{u} \) is the mass-average velocity vector, and \( S_{\rho} \) is the mass loss or gain (condensation/vaporization) per unit volume and time. Similarly, setting \( \Phi = 1 \) in Eq. (4) gives an expression for the change in volume

\[ \frac{dV}{dt} = \oint b \cdot \mathbf{A} dS \quad (8) \]

The transport equation for individual species is given by

\[ \frac{d}{dt} \int \rho_{\alpha} dV = \oint \rho_{\alpha} (\mathbf{b} - \mathbf{u}) \cdot \mathbf{A} dS - \oint (J_{\alpha} \cdot \mathbf{A}) dS + \int S_{\rho,\alpha} dV \quad (9) \]

where \( \alpha \) denotes the gas species, \( \rho_{\alpha} \) is the mass per unit volume (macroscopic density), \( J_{\alpha} \cdot \mathbf{A} \) is the mass diffusion flux vector with Cartesian geometry components \( \{A_x, J_{\alpha, x}, A_y, J_{\alpha, y}, A_z, J_{\alpha, z} \} \), 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 \( \alpha \) is represented by the second integral on the right side of Eq. (9), which is often reported in the literature (Refs. 5 and 6) as

\[ J_{\alpha} \cdot \mathbf{A} = \begin{bmatrix} -A_x \rho D_{\alpha, mix} \frac{\partial}{\partial x} \left( \frac{\rho_{\alpha}}{\rho} \right) \\ -A_y \rho D_{\alpha, mix} \frac{\partial}{\partial y} \left( \frac{\rho_{\alpha}}{\rho} \right) \\ -A_z \rho D_{\alpha, mix} \frac{\partial}{\partial z} \left( \frac{\rho_{\alpha}}{\rho} \right) \end{bmatrix} \quad (10) \]

for Cartesian geometry, where \( D_{\alpha, mix} \) is the "apparent" or "turbulent" mass diffusion coefficient of species \( \alpha \) into the gaseous mixture. It is essential that the diffusion fluxes identically sum to zero, so Eq. (10) is

\[ \sum_{\alpha} J_{\alpha} \cdot \mathbf{A} = \sum_{\alpha} J_{\alpha} \equiv 0 \quad (11) \]

As pointed out by Ramshaw (Ref. 7), the condition of Eq. (11) is only exact for Eq. (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. 7), so a correction to Eq. (10) is incorporated that properly reflects the physical content of Eq. (10) while providing full symmetry in all species:

\[
J_{\alpha} \cdot \mathbf{A} = \begin{cases} 
-A_x \left[ c M_{\alpha} D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial x} \left( \frac{c_{\alpha}}{\rho} \right) - \left( \frac{c_{\alpha}}{\rho} \right) \sum_{\beta} M_{\beta} D_{\beta \rightarrow \text{mix}} \frac{\partial}{\partial x} \left( \frac{c_{\beta}}{c} \right) \right], \\
-A_y \left[ c M_{\alpha} D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial y} \left( \frac{c_{\alpha}}{\rho} \right) - \left( \frac{c_{\alpha}}{\rho} \right) \sum_{\beta} M_{\beta} D_{\beta \rightarrow \text{mix}} \frac{\partial}{\partial y} \left( \frac{c_{\beta}}{c} \right) \right], \\
-A_z \left[ c M_{\alpha} D_{\alpha \rightarrow \text{mix}} \frac{\partial}{\partial z} \left( \frac{c_{\alpha}}{\rho} \right) - \left( \frac{c_{\alpha}}{\rho} \right) \sum_{\beta} M_{\beta} D_{\beta \rightarrow \text{mix}} \frac{\partial}{\partial z} \left( \frac{c_{\beta}}{c} \right) \right]
\end{cases}
\]  
(12)

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

II.C. The Momentum Transport Equations
The mixture-momentum conservation equations are given by

\[
\frac{d}{dt} \int_V \rho u dV = \int_V \rho u (b - u) \cdot dS - \int_V \rho g dV - \int_V \tau \cdot dS - \int_V (u \cdot D) dS + \int_V S_u dV
\]
(13)

where \(\rho\) is the pressure, \(\tau\) is the viscous stress tensor, \(g\) is the gravitational vector, and \(D\) is the internal structural drag vector. 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; and fluid drag forces acting on structural surfaces; and any additional momentum sources. The viscous stress tensor is modeled by the usual Newtonian one, where the coefficient of viscosity, \(\mu\), is interpreted as an apparent viscosity. Here we have used the second viscosity coefficient, \(\lambda = -2\mu/3\), which is equivalent to assuming the bulk viscosity to be zero.

II.D. The Internal Energy Transport Equation
The equation of change for total internal energy is

\[
\frac{d}{dt} \int_V \rho I dV = \int_V \rho I (b - u) \cdot dS - \int_V \rho u \frac{\partial (H_{\text{int}})}{\partial t} dV - \int_V (q \cdot \mathbf{A}) dS + \int_V S_i dV
\]
(14)

where \(I\) is the mixture specific internal energy and \(Q\) is the energy source or sink per unit volume and time as a result of combustion, condensation, vaporization, and energy exchange with internal structures, floors, ceilings, and walls. Because phase change effects can dominate the \(P V \mathbf{u}\) work term, we must account for the remaining gas in a computational cell expanding or compressing into the volume change associated with phase change. We account for this effect by using the ideal gas equation of state to arrive at

\[
\frac{P}{V} \frac{\partial V_{h_{\text{int}}}}{\partial t} = -R_{h_{\text{int}}} TS_{p,h_{\text{int}}},
\]

XI-160
where \( R_{g,\alpha} \) is the gas constant for steam, \( T \) is the gas mixture temperature, \( V_{b,\alpha} \) is the steam volume, and \( S_{b,\alpha} \) 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 \( S_{b,\alpha} \) is the same mass source per unit volume and time as Eq. (7), i.e., the water vapor component conservation equation. The energy flux vector \( \mathbf{q} \) is given by

\[
\mathbf{q} \cdot \mathbf{A} = \begin{cases} 
-A_z \left[ \phi_j \frac{\partial T}{\partial x} - \sum_\alpha h_{\alpha,j,x} J_{\alpha,x} \right] \\
-A_y \left[ \phi_j \frac{\partial T}{\partial y} - \sum_\alpha h_{\alpha,j,y} J_{\alpha,y} \right] \\
-A_z \left[ \phi_j \frac{\partial T}{\partial z} - \sum_\alpha h_{\alpha,j,z} J_{\alpha,z} \right]
\end{cases}
\]  

(15)

where \( \phi_j \) is the apparent conductivity and \( h_{\alpha} \) is the enthalpy for species \( \alpha \).

II.E. Constitutive Relationships

The specific internal energy of species \( \alpha \) is related to the temperature by

\[
I_{\alpha} = (I_{\alpha})_0 + \int_{T_0}^{T} (C_v)_\alpha \, dt
\]  

(16)

For the species in which we are most interested [CO, CO\(_2\), H\(_2\), H\(_2\)O (both vapor and liquid droplets), N\(_2\), O\(_2\), air, and He], we can approximate the specific heats by

\[
(C_v)_\alpha = a_0 + a_1 T + a_2 T^2 + a_3 T^3
\]  

(17)

where the \( a_i \)'s are species-dependent coefficients (Ref. 8). After integrating Eq. (16), the specific internal energy as a function of temperature is approximated with the quartic function

\[
I_{\alpha} = A_0 + A_1 T + A_2 T^2 + A_3 T^3 + A_4 T^4
\]  

(18)

over the temperature range 200–2500 K. The total specific internal energy then is given by

\[
I = \sum_\alpha x_{\alpha} I_{\alpha}
\]  

(19)

where \( x_{\alpha} \) is the mass fraction for species \( \alpha \). The pressure, \( p \), is obtained by applying the Gibbs-Dalton law of partial pressures to an ideal gas mixture

\[
p = \frac{T \sum_\alpha R_{\alpha} \rho_{\alpha}}{\theta} = \frac{\rho T \sum_\alpha x_{\alpha} R_{\alpha}}{\theta}
\]  

(20)

where \( R_{\alpha} \) is the gas constant for species \( \alpha \) and the gas volume fraction \( \theta \) is defined by.
\[ \theta = \frac{\rho_0}{\rho_s} = \left(1 - \frac{\rho_s}{\rho_0}\right) \]  

where the microscopic or thermodynamic density for the gas and liquid is given by \( \rho_0 \) and \( \rho_s \), respectively. The constant-pressure specific heats are calculated by

\[ (C_v)_a = R_a + (C_v)_a \]  

(22)

### III. Computational Model

The solution procedure of the governing equations is a modified Los Alamos ICE’d-ALE methodology (Ref. 9) for solving multidimensional, time-dependent fluid flow equations. An efficient semi-implicit algorithm is implemented that exploits the vector processing capability of the CRAY J-90 and Fujitsu VPP300 architectures. The Appendix presents the GASFLOW integration scheme.

In the ALE method, the computational time cycle consists of three steps. Phase A is the explicit Lagrangian phase. In this phase, the density, velocity, and specific internal energy fields are updated by the effects of all chemical and physical processes which have been evaluated as source terms before entering this phase. These include combustion, heat transfer and two-phase processes, body forces, and diffusional (both laminar and turbulence) effects. Phase B is the implicit Lagrangian phase, where a semi-implicit solution of the mass, momentum, and energy equations in terms of the time-advanced densities, pressures, velocities and internal energies is obtained. This allows the propagation of pressure waves through the computational domain without time-step restrictions. The iteration scheme used to solve this set of equations is the preconditioned conjugate residual method that closely follows the algorithm proposed by Chandra (Ref. 10). The final phase, Phase C, is a rezone or remapping phase in which all the advective flux calculations, repartitioning of the dependent variables onto the mesh, are explicitly performed. In the general ALE formulation, the mesh may move with the fluid (Lagrangian), remain fixed (Eulerian), or move in any arbitrarily prescribed manner. In the GASFLOW code, the mesh usually remains fixed and the remapping translates to rezoning to the original mesh.

### IV. Summary

In this report we have described the theory of the GASFLOW computer code and the computational model used to numerically integrate the governing equations in time and space.

The time-dependent, three-dimensional, compressible Navier-Stokes equations are the field equation set that determines fluid motion for GASFLOW. Two-phase dynamics is computed through a Homogeneous Equilibrium Model (HEM) assumption where the dispersed phase of water droplets is considered incompressible. An internal energy transport equation relates the internal energy, density, pressure and velocity fields with the exchange of heat and mass (condensation and evaporation). Multiple species transport equations model the transport of individual species through the gas mixture. The sum of the species transport equations is the total fluid density conservation equation. These equations, the Navier-Stokes equations, the internal energy equations, and the summed species transport equations, express the conservation of momentum, energy, and mass, respectively. They relate the dynamics of the fluid to temporal and spatial influences, such as, viscous stress, body force, turbulence, structural resistance, heat transfer, condensation, vaporization, and combustion. Fluid turbulence is simulated by an algebraic mixing model, a \( k-\varepsilon \) turbulence or \( k-\omega \) turbulence model with buoyancy production terms.
Heat transfer and two-phase processes on walls and surfaces, such as internal structures, are calculated to model appropriate energy sinks. A modified Reynolds analogy for heat and mass transport to walls and structures accounts for the influence the thermal boundary layer has on the rates of heat transfer and condensation. A library of more than 25 gas species with transport properties and temperature dependent specific heat capacities and internal energies has been developed to address accident issues in Light Water Reactors.

Finite rate chemical kinetics models for combustion simulate diffusion and propagating flames in complex geometries. A one-step, global chemical kinetics model is often used for diffusion flames involving hydrogen or hydrocarbon fuels. This simplifies the actual chemical processes, which has many more elementary reaction steps and intermediate chemical species. The chemical reaction time scale is, however, very short compared with fluid dynamic motions and meaningful calculations can be accomplished using this simplified chemical kinetics mechanism. The reaction rate in the finite-rate chemical kinetics equations is modeled by a modified Arrhenius law that accounts for both fuel lean or fuel rich mixtures. Modeling recombiner follow a similar methodology where the combustion effects are restricted to computational cells adjacent to recombiner surfaces.

Appendix
GASFLOW-II: Arbitrary Lagrangian Eulerian (ALE) Integration Scheme

Compute Source Terms & Fluid Properties
Molecular Transport Properties
- Species diffusion coefficients (species & energy)
- Binary coefficients and Mixture coefficients
- Mixture viscosity (momentum)
- Mixture thermal conductivity (energy)
Heat Transfer and Phase Change
- Convection (energy)
- Bulk phase change (species & energy)
- Phase change with structures (species, mass & energy)
- Diffusion in structures (energy)
Laminar & Turbulent Diffusion Processes
- Species (species & energy)
- Viscous stress tensor (momentum)
- Structural Drag (momentum)
- External Body Forces (momentum)
- Thermal (energy)
Combustion/Recombination
- Species destruction & production (species)
- Energy of combustion (energy)

PHASE A: Explicit Lagrangian Phase (including Source Terms)
\[
\frac{m^A_{\alpha} - m^n_{\alpha}}{dt} = S_{\alpha}
\]

PHASE B: Linearized Implicit Lagrangian Phase (pressure iteration)
\[
\frac{m^B_{\alpha} - m^A_{\alpha}}{dt} = 0 \quad \nabla \cdot (\Psi \nabla \delta p) = \Omega
\]

PHASE C: Rezone Phase
\[
\frac{m^{n+1}_{\alpha} - m^B_{\alpha}}{dt} = -\nabla \cdot (\rho_{\alpha} \overline{u})^B
\]

XI-163
Calculate Turbulent Transport Coefficients
Algebraic Model
Sub-grid Scale model
k-ε Model

Determine New Time Step & Update End of Time-Step Information
Transport Conditions
Material Velocity Condition and Diffusion Criterion
Energy Considerations
Pressure-Volume Work and Combustion

Output
2-D Scalar Variable Contours and Velocity Vectors
1-D Scalar Variable, Velocity Vector, and Structural Temperature Profiles
Time History Plots
Scalar variables
Velocities
Mass fluxes
Mass flow rates
Volumetric flow rates
Structure surface temperature
Pressure gradients
Saturation pressure and temperature
Computational domain
Mass conservation, Species conservation,
Internal energy conservation, Kinetic energy conservation, and
Total energy conservation.

REFERENCES

XI-164