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**FUSION TECHNOLOGY AND CHARGED PARTICLE RESEARCH
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**STUDY OF HIGH GAIN SPHERICAL SHELL ICF TARGETS CONTAINING
UNIFORM LAYERS OF LIQUID DEUTERIUM TRITIUM FUEL**

**Subtitle:
A Numerical Model for Analyzing Thermal Layering of
Liquid Mixtures of Hydrogen Isotopes Inside
a Spherical inertial Confinement Fusion Target**

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by

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ABSTRACT

A numerical model has been developed to describe the thermally induced behavior of a liquid layer of hydrogen isotopes inside a spherical Inertial Confinement Fusion (ICF) target and to calculate the far-field temperature gradient which will sustain a uniform liquid layer. This method is much faster than the trial-and-error method previously employed. The governing equations are the equations of continuity, momentum, energy, mass diffusion-convection, and conservation of the individual isotopic species. Ordinary and thermal diffusion equations for the diffusion of fluxes of the species are included. These coupled equations are solved by a finite-difference method using upwind schemes, variable mesh, and rigorous boundary conditions. The solution methodology unique to the present problem is discussed in detail. In particular, the significance of the surface tension gradient driven flows (also called Marangoni flows) in forming uniform liquid layers inside ICF targets is demonstrated. Using the theoretical model, the values of the externally applied thermal gradients that give rise to uniform liquid layers of hydrogen inside a cryogenic spherical-shell ICF target are calculated, and the results compared with the existing experimental data.

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NOMENCLATURE

Except where otherwise noted, the following notations will be used.

a	=	vapor bubble radius
A, B	=	coefficients in the definition of pure-component surface tension
b	=	SGS inner radius
c	=	SGS outer radius
c_1, c_2, c_3	=	coefficients in the energy equation
c_{pi}	=	specific heats of individual components
$\bar{c}_p$	=	mean specific heat
C	=	number of components
d	=	outer radius of helium region
D_1 to D_6	=	coefficients in the discretized governing equations
D_i^T	=	thermal diffusion coefficients
D_{ij}	=	multicomponent diffusion coefficients
$\bar{e}$	=	energy flux
F	=	degrees of freedom
F_z	=	total upward force on the vapor bubble
g	=	acceleration due to gravity
h_i	=	enthalpy of the individual species in liquid and vapor
k	=	thermal conductivity
Le_1 to Le_4	=	Lewis numbers
M_l, M_v	=	mean molecular weights of liquid and vapor
M_1, M_2, M_3	=	component molecular weights
Ma_T	=	thermal Marangoni number

Ma_{c1}, Ma_{c2}	=	concentration Marangoni numbers
$\bar{n}$	=	mass flux
p	=	pressure
P	=	number of phases
Pr	=	Prandtl number
Q	=	generic quantity
r	=	radial coordinate
SGS	=	Spherical Glass Shell
TDN_1, TDN_2	=	Thermal Diffusion Numbers
T	=	temperature in Kelvin
T_m	=	mean temperature of the target in Kelvin
u	=	radial velocity
v	=	tangential velocity
$\vec{v}$	=	total velocity vector, $u\hat{e}_r + v\hat{e}_\theta$
x_1, x_2, x_3	=	mole fractions
x, y, z	=	Cartesian coordinates

Greek symbols

α	=	thermal diffusivity
α_T	=	thermal diffusion ratio in vapor
β	=	mesh expansion ratio
γ	=	surface tension
$\Delta\eta$	=	nondimensional radial mesh size
θ	=	angular coordinate, angle
η	=	nondimensional radial coordinate
μ	=	dynamic viscosity

ν	=	kinematic viscosity
ρ	=	density
τ	=	shear stress
Ψ	=	stream function
$\omega_1, \omega_2, \omega_3$	=	mass fractions
ω	=	relaxation parameter
Ω	=	modified vorticity

Subscripts

1, 2, 3	=	components 1, 2 and 3
C1, C2	=	concentration Marangoni numbers due to components 1 and 2
h	=	helium
i	=	i-th node in the radial direction, i-th component or fluid
j	=	j-th node in the tangential direction
ℓ	=	liquid
m	=	mean value
r	=	radial direction
s	=	solid, SGS
s1, s2, s3	=	saturation pressures
t	=	total pressure
T	=	thermal Marangoni number
v	=	vapor
z	=	upward vertical direction
∞	=	far-field, outer surface of the helium region

Superscripts

' , "	=	first and second derivatives
k	=	k-th iteration
T	=	thermal diffusion

CHAPTER 1

INTRODUCTION

As population increases, demands for energy - particularly electrical energy - will also increase. Because reserves of fossil fuel are limited, society cannot continue to rely on this traditional energy source. Even if fossil fuels existed in abundance, their continued use would severely pollute the environment. Nonfossil fuel energy sources such as water power, solar heat, geothermal energy, and wind power offer alternative sources of electricity. However, they can be considered as secondary power sources only because of their intrinsic limitations. While nuclear fission energy is reliable and relatively inexpensive, it should not be considered the sole energy source for the future. As the resources of fossil fuels and fissile material are depleted, other potential fuel resources will be required to meet the ever growing demands for energy.

Nuclear fusion has been regarded as the most promising choice for the future energy source. While fusion fuel is not inexhaustible, it is abundant. This form of energy is released when two light nuclei are brought together to form a heavier nucleus. Nuclear fusion is possible only at very high temperatures. Such temperatures are maintained continuously in the stars, and fusion reactions account for the majority of energies radiated into space. They are briefly attained in the hydrogen bomb,¹ triggered by the initial explosion of a fission bomb.

One of the major problems in controlling nuclear fusion is how to handle the super hot fusion fuel. The temperature of the fuel must be high because the reaction rate of fusion fuel, in general, will not be significant until its temperature reaches 10^7 K (about 1 keV). For instance, the deuterium-tritium (D-T) reaction,

which has the highest reaction rate among all of the fusion fuels, will not be at the peak level until its temperature reaches 7×10^8 K (about 60 keV).²

Two approaches have been adopted to confine such high-temperature fuel. The first approach is based on magnetic confinement of the plasma. Under the action of an external magnetic field, the nuclei in the deuterium-tritium mixture are directed into helical paths around the magnetic lines of force and are confined. The second approach is inertial confinement in which fuel is compressed and confined by the inertia of matter. The goal is to reach a point at which the released fusion energy is greater than or equal to the energy needed to start the reaction. This critical point is proportional to the product of the density and confinement time of the fuel at a given temperature, and was first derived by Lawson.³ For a fuel containing D-T, the product is about 10^{14} ions/cm³ at a temperature of 10 keV.⁴

In inertial confinement fusion (ICF), the fusion fuel is put inside a spherical shell (called a target), which is illuminated by energetic laser or ion beams from all directions. The outer portion of the target is then heated up and blasted off, and the fuel in the middle of the target is compressed according to Newton's laws. While the fuel at the center is compressed and raised to high temperatures, a series of fusion reactions take place. A sudden release of a large amount of energy at the center of the target then forces the target to explode. After the target is disintegrated, the fusion reaction is also stopped. The confinement time in this case is therefore very short; its typical value is about 10^{-10} second. Because of this limitation in the confinement time, the fuel has to be compressed to high density in order to have a high fusion yield, and to reach or exceed the critical point derived by Lawson.

It has been theoretically determined that a higher-density compression can be achieved if the D-T is in the condensed state rather than the gaseous state of room temperature.⁵ Additional studies have shown that indeed the fusion yield is enhanced when spherical microshells containing uniform cryogenic layers of fusion fuel are used.⁶⁻⁸ For this reason, the fusion fuel target typically takes the form of a thin, spherically symmetric coating of liquid on the inside of a microshell which is cooled till the D-T condenses.

The remaining question is how to fabricate such a high-gain target. The formation of simple cryogenic targets which are spherical glass or plastic shells containing a uniform layer of fusion fuel has been experimentally studied.⁹⁻¹⁸ Thin uniform layers of fusion fuel can be formed by a rapid isothermal refreeze technique;^{11,12} but uniformly thick layers of fuel cannot be easily formed due to the gravity-induced sagging of the liquid layer during the freezing period. Hence, the key issue here is to find a method to create and maintain thick uniform liquid layers inside a spherical microshell.

The basic physical issues of the uniform liquid layer formation inside the microshells are as follows. The liquid layer of hydrogen isotopes inside the ICF target completely covers the target interior due to its excellent wetting characteristics. The equilibrium profile of the liquid layer is nonuniform because of the sagging of the liquid due to its weight. The liquid layer inside the target coexists with its vapor at the cryogenic temperature of interest. The formation of a liquid layer in dynamic situations can be analyzed by modeling the motion of the vapor bubble inside the finite-thickness liquid layer which itself is contained within the spherical ICF target.

The earliest analysis of motion of gas bubbles, or in general, a fluid sphere in an isothermal liquid bath was done independently by Rybczinski and

Hadamard.^{19,20} More recently, Haberman and Sayre²¹ studied the effect of the container wall on the bubble motion for the particular case in which a fluid sphere is initially at a position concentric with a spherical-shell container. Further studies and comparison with experiments pertaining to the motion of fluid spheres in infinite medium are reported in Refs. 22-25. A thermal gradient in the liquid has been shown to induce an interfacial tension gradient on the gas bubble surface, and the resulting bubble motion has been theoretically and experimentally studied by Young, Goldstein, and Block²⁶ for a bubble in an infinite medium. The presence of impurities and the motion of bubbles inside liquid droplets has been investigated in Ref. 27. The relevant problem of the motion of the bubble contained by successive layers of liquid and uniform spherical shell and subject to external thermal gradient has been reported in Refs. 28-30. Therein, the velocity of the pure-component bubble at the center of the target due to imposition of a vertical linear thermal gradient on the target has been derived analytically using a low Reynolds number model; hence, the thermal gradient that makes the velocity of the concentric bubble zero and holds it stationary can be estimated.²⁹

The physical mechanism underlying the formation of a uniform layer, owing to the external thermal gradient on the target, is the combined effect of the induced surface-tension gradients and the mass transfer due to the phase change at the liquid-vapor interface. The surface tension at the liquid-vapor interface is temperature and composition dependent, and the temperature and concentration gradients induced at the liquid-vapor interface result in surface-tension gradients. The presence of the concentration gradient along the liquid-vapor interface is due to the tendency of the components to separate into differing levels around the mean once there are thermal and pressure gradients

along the interface. The surface-tension-generated flows are normally referred to as capillary flows. Depending upon the dominance of the temperature-gradient-induced or the concentration-gradient-induced surface-tension gradients, the flows can be referred to, respectively, as thermocapillary flows or as concentration flows. The capillary flows are also referred to as Marangoni flows.

With reference to ICF target research, it is required to model the multicomponent hydrogen isotopic fluids inside the target. Though efforts in that direction have been partially attempted in Refs. 28-30, a complete analytical solution of the multicomponent system has been stymied by the necessity to solve the fully nonlinear diffusion-convection equations, including the body forces, which can be accomplished only numerically. The fundamental equations for incompressible flow of a Newtonian fluid with constant properties are the momentum equations (Navier-Stokes) and the continuity equation. These equations are written in the primitive variables of velocity components, pressure and the fluid properties of mass density and kinematic viscosity. Although it is possible to obtain numerical solutions from these equations, the vorticity-stream function approach has been used in this work. A finite difference scheme is employed to solve the resulting equations. Chapter 2 details the basic assumptions, constraints, and the boundary conditions. The mesh geometry, discretization procedure and general iteration scheme are discussed in Chapter 3. Chapter 4. discusses the results of the computations using the model. The summary and the concluding remarks are presented in Chapter 5. Derivations of some of the important relations can be found in the appendices.

CHAPTER 2

THEORETICAL MODEL

Because of the extremely good wetting capability of liquid hydrogen isotopes and the small size of the target, a spherical-shell ICF target containing hydrogen isotopes will have its inner surface completely covered with a layer of liquid hydrogen, when it is cooled below the liquefaction point. In an isothermal situation, the resultant liquid layer is not uniform, but thicker at the bottom due to gravity-induced sagging. In a nonisothermal situation, the resultant liquid-layer configuration depends on whether the ICF target contains a single hydrogen isotope (single-component) or a mixture of hydrogen isotopes (multicomponent).

Previous experiments have shown that a vertical temperature gradient can create a uniform liquid layer inside an ICF target.^{15,31-34} Several models have been developed that try to quantitatively describe how a nonuniform temperature field affects liquid hydrogen inside a spherical microshell.^{17,35} Analytical expressions for the temperature gradient required to form a uniform liquid hydrogen isotope layer inside a spherical-shell ICF target have been derived for targets containing single-component layers.³⁵ In their paper, Mok et al.²⁸ calculated the values of the temperature gradient necessary to form and maintain a uniform liquid layer. Two models were analyzed. In the first, Model I, it was assumed that the liquid hydrogen surface-tension gradient is the only effect caused by the temperature gradient. Model II is an extension of Model I and includes mass transfer due to evaporation and condensation. These two models are for targets containing single-component layers.

Temperature gradient effects in a target containing a mixture of hydrogen isotopes are quite different from those for a single-component target due to

component separation. For targets containing multicomponent layers, an analytical expression is not possible due to the nonlinearity of the calculations. A model has been developed describing the behavior of a two-component target.³⁵ This model includes the effects of the temperature-induced liquid-vapor interfacial tension gradient, which is common to both the single-component and multicomponent liquid layers and the concentration-induced tension gradient due to component separation, which is exclusively for multicomponent liquid layers.

To study the equilibrium of the ternary mixture vapor bubble at the center of the ICF target, one has to consider the coupled equations of energy, momentum, and mass diffusion-convection in a multiregion configuration. To compare the experimental data with the theoretical prediction, the exterior region of the stationary helium envelope is also included in the analysis. The concentric spherical system considered in the analysis is shown in Figure 2.1. The basic assumptions, the governing equations, and the associated boundary conditions are discussed, respectively, in Sections 2.1, 2.2, and 2.3. The condition of force balance on the concentric vapor bubble is formulated in Section 2.4.

2.1 Basic Assumptions

The governing equations are highly nonlinear and coupled. Some assumptions have to be made to solve the problem efficiently. The assumptions are made in such a way that they do not introduce large errors into the calculation. Therefore, they should not change the results beyond a specified limit, which depends on the problem and the accuracy desired. Thus the assumptions are made only when the errors resulting from them are negligible and the calculation becomes simplified. Care is taken to make assumptions that

Figure 2.1 Geometry of the spherical ICF target and the enclosing helium region used in numerical computations.

do not give cumulative errors. The assumptions adopted for the present problem are as follows:

- (i) The flow field can be considered to be azimuthally symmetric about the vertical center line owing to the imposition of the external thermal gradient symmetrically about the vertical center line. This assumption eliminates the need for the azimuthal coordinate, and hence r and θ are the only coordinate variables. The angular coordinate is measured from the top vertical in the clockwise direction. It is enough to consider the region $0 \leq \theta \leq \pi$, because of azimuthal symmetry.
- (ii) It is assumed that the liquid-bearing spherical ICF target is cooled by an envelope of quiescent helium gas and that the heat transport in this region is predominantly by conduction. Convection would greatly disrupt the linear temperature gradient and prevent the formation of a uniform liquid layer in the target. Convection will occur when the Rayleigh number of the helium gas column is larger than some critical value. The critical value for a column bounded by two infinite horizontal planes is 1700.³⁶ For a closed vertical cylinder, the critical value is 4300.³⁷
- (iii) An ICF target distorts the temperature gradient, because the thermal conductivity of the glass wall is much higher than that of the helium gas. The isotherms in the exchange gas curve around the target. The isotherms become more evenly spaced and more horizontal farther away from the target. When the helium gas column is 3 to 5 times the target radius, the isotherms are virtually horizontal. Therefore, the external linear temperature gradient is imposed on the helium envelope at a radius of 3 to 5 times the target radius.

- (iv) The final configuration is that of a uniform layer of liquid that is concentric inside the spherical ICF target. Therefore, the liquid layer is assumed to be uniform at any trial temperature gradient on the target and the bubble is assumed to be stationary.
- (v) The fluids are assumed to be incompressible, and the flows are assumed to be nondissipative and azimuthally symmetric.
- (vi) The multicomponent mixture inside the ICF target is assumed ideal.
- (vii) The temperature gradient does not appreciably change the thermodynamic and transport properties, namely, the density, viscosity, thermal conductivity and diffusion coefficients, which are defined at the average target temperature. The average target temperature is nearly the temperature found at the equator.
- (viii) It is assumed that the total local surface tension is the mole-fraction-weighted average of the pure-component surface tensions since the hydrogen mixture is essentially ideal.
- (ix) The velocity of the fluid is zero at the liquid-SGS interface, as the shell of the target is impermeable and is assumed to be stationary.
- (x) The vapor pressure at the vapor-liquid interface is assumed to be initially known at any trial iteration.
- (xi) Since the conductive heat flux in the vapor at the vapor-liquid interface is much smaller than the conductive heat flux in the liquid, the vapor-liquid interface is considered as a boundary in the energy equation. Therefore, the boundary condition on temperature is imposed at this interface.
- (xii) The mass fraction of one component in the liquid is assumed to be initially known, in addition to the pressure and temperature, for the ternary system.

The thermodynamic state of the fluid at the vapor-liquid is uniquely determined by the last three assumptions. The necessity of these assumptions is demonstrated in Section 2.3.5.2 by invoking the Gibb's phase rule.

2.2 Governing Equations

The liquid and vapor are considered to be incompressible, and the thermal conductivities, viscosities, and diffusion coefficients are considered to be constant in both phases. The effects of the thermal diffusion and viscous dissipation are considered negligible. Thus, the incompressible, nondissipative, constant property forms of the continuity, momentum, energy, and the mass diffusion-convection equations are considered in the liquid and vapor including the nonlinear convection terms. In the shell of the ICF target and/or the helium region, only the Laplacian form of the energy equation has to be considered.

The fundamental equations for incompressible flow of a Newtonian fluid with constant properties in spherical geometry are the continuity equation

$$\nabla \cdot \vec{v} = 0 \quad (2.1)$$

and the momentum equation

$$\vec{v} \cdot \nabla \vec{v} = \vec{g} - \frac{\nabla P}{\rho} + \nu \nabla^2 \vec{v} \quad (2.2)$$

where ρ , ν and $\vec{v}$ are, respectively, the density, kinematic viscosity, and the velocity of the fluids, and P is the pressure in the fluids.

It can be shown that the energy equation for the ternary system is

$$\rho \bar{c}_p \vec{V} \cdot \nabla T = k \nabla^2 T + \rho \sum_{i=1}^3 \sum_{j=1}^2 D_{ij} c_{pi} \nabla \omega_j \cdot \nabla T + \left(\sum_{i=1}^3 c_{pi} D_i^T \right) \frac{1}{T} \nabla T \cdot \nabla T \quad (2.3)$$

where c_{pi} 's are the specific heats of individual components and $\bar{c}_p$ is the mass-fraction-weighted average of the component specific heats. The energy equation for the binary and unary systems can be obtained as special cases of the above equation. The derivation of the energy equation can be found in Ref. 38 and is also shown in Appendix A.

The steady-state mass diffusion-convection equation in a ternary system for component i is

$$\rho \vec{V} \cdot \nabla \omega_i = \rho \sum_{j=1}^2 D_{ij} \nabla^2 \omega_j + D_i^T \left(\frac{1}{T} \nabla^2 T - \frac{1}{T^2} \nabla T \cdot \nabla T \right). \quad (2.4)$$

Here, the D_{ij} 's are the multicomponent diffusion coefficients. This reduces to the corresponding equation of the binary system if one considers only one equation and drops the second Laplacian term from the right-hand side. The derivation of the mass diffusion-convection equation can be found in Ref. 38 and is also shown in Appendix B.

These continuity and momentum equations are written in the primitive variables of velocity components, pressure and the fluid properties of mass density and kinematic viscosity. Although it is possible to obtain numerical solutions from these equations, the vorticity and stream function are used as the new variables of the flow field. The vector vorticity transport equation is given by

$$(\vec{v} \cdot \nabla) \vec{\zeta} = (\vec{\zeta} \cdot \nabla) \vec{v} + \nu \nabla^2 \vec{\zeta}. \quad (2.5)$$

The derivation of the vorticity transport equation is shown in Appendix C.

The vorticity is related to the velocity as

$$\vec{\zeta} = \nabla \times \vec{v}. \quad (2.6)$$

In spherical coordinates this gives

$$\zeta \hat{e}_\phi = \left(\frac{\partial v}{\partial r} - \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{v}{r} \right) \hat{e}_\phi \quad (2.7)$$

i.e., the vorticity is perpendicular to the plane of flow.

The modified vorticity Ω is used and is chosen such that ζ is definite at the center of the bubble. The modified vorticity is defined as

$$\Omega \hat{e}_\phi = r \left(\frac{\partial v}{\partial r} - \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{v}{r} \right) \hat{e}_\phi \quad (2.8)$$

Also used is the stream function Ψ which is related to the components of velocity as

$$u = \frac{1}{r^2 \sin \theta} \frac{\partial \Psi}{\partial \theta}, \quad v = -\frac{1}{r \sin \theta} \frac{\partial \Psi}{\partial r}. \quad (2.9)$$

The basic variables which are the radius r , temperature T , modified vorticity Ω , stream function Ψ , radial velocity u , tangential velocity v , mass

fraction of the component 1 in either phase ω_1 and mass fraction of the component 2 in either phase ω_2 are nondimensionalized as follows:

$$\eta = \frac{r}{a}, \quad \tilde{T} = \frac{(T - T_m)}{T_m}, \quad \tilde{u} = \frac{au}{\alpha}, \quad \tilde{v} = \frac{av}{\alpha},$$

$$\tilde{\Omega} = \frac{a\Omega}{\alpha}, \quad \tilde{\Psi} = \frac{\Psi}{\alpha a}, \quad (2.10)$$

$$\tilde{\omega}_1 = \frac{(\omega_1 - \omega_{1m})}{\omega_{1m}}, \quad \tilde{\omega}_2 = \frac{(\omega_2 - \omega_{2m})}{\omega_{2m}}$$

where the nondimensional quantities are indicated by the tilde; a is the radius at the vapor-liquid interface; α is the thermal diffusivity of either phase; T_m is the average temperature; ω_{1m} , and ω_{2m} are, respectively, the mass fraction of component 1 in either phase, and the mass fraction of component 2 in either phase for a given average target temperature.

Thus the governing equations in nondimensional form in the liquid and vapor regions are

$$\frac{\partial(\tilde{u}\tilde{\Omega})}{\partial\eta} + \frac{1}{\eta} \frac{\partial(\tilde{v}\tilde{\Omega})}{\partial\theta} = Pr \left(\frac{\partial^2 \tilde{\Omega}}{\partial\eta^2} + \frac{1}{\eta^2} \left(\frac{\partial^2 \tilde{\Omega}}{\partial\theta^2} + \frac{1}{\tan\theta} \frac{\partial\tilde{\Omega}}{\partial\theta} - \frac{\tilde{\Omega}}{\sin^2\theta} \right) \right), \quad (2.11)$$

$$\frac{\partial^2 \tilde{\Psi}}{\partial\eta^2} + \frac{1}{\eta^2} \left(\frac{\partial^2 \tilde{\Psi}}{\partial\theta^2} - \frac{1}{\tan\theta} \frac{\partial\tilde{\Psi}}{\partial\theta} \right) = -\tilde{\Omega} \sin\theta, \quad (2.12)$$

$$\begin{aligned} \bar{u} \frac{\partial \bar{T}}{\partial \eta} + \frac{\bar{v}}{\eta} \frac{\partial \bar{T}}{\partial \theta} = & \bar{\nabla}^2 \bar{T} + \frac{c_1 \omega_{1m}}{\alpha} \left(\frac{\partial \bar{\omega}_1}{\partial \eta} \frac{\partial \bar{T}}{\partial \eta} + \frac{1}{\eta^2} \frac{\partial \bar{\omega}_1}{\partial \theta} \frac{\partial \bar{T}}{\partial \theta} \right) \\ & + \frac{c_2 \omega_{2m}}{\alpha} \left(\frac{\partial \bar{\omega}_2}{\partial \eta} \frac{\partial \bar{T}}{\partial \eta} + \frac{1}{\eta^2} \frac{\partial \bar{\omega}_2}{\partial \theta} \frac{\partial \bar{T}}{\partial \theta} \right) + \frac{c_3}{\alpha} \left(\frac{\bar{\nabla} \bar{T} \cdot \bar{\nabla} \bar{T}}{\bar{T} + 1} \right), \end{aligned} \quad (2.13)$$

$$\begin{aligned} \frac{1}{\eta^2} \frac{\partial(\eta^2 \bar{u} \bar{\omega}_1)}{\partial \eta} + \frac{1}{\eta \sin \theta} \frac{\partial(\sin \theta \bar{v} \bar{\omega}_1)}{\partial \theta} = & \frac{1}{Le_1} \bar{\nabla}^2 \bar{\omega}_1 + \frac{1}{Le_2} \bar{\nabla}^2 \bar{\omega}_2 \\ & + TDN_1 \bar{\nabla} \cdot \left(\frac{1}{1 + \bar{T}} \bar{\nabla} \bar{T} \right) \end{aligned} \quad (2.14)$$

and

$$\begin{aligned} \frac{1}{\eta^2} \frac{\partial(\eta^2 \bar{u} \bar{\omega}_2)}{\partial \eta} + \frac{1}{\eta \sin \theta} \frac{\partial(\sin \theta \bar{v} \bar{\omega}_2)}{\partial \theta} = & \frac{1}{Le_3} \bar{\nabla}^2 \bar{\omega}_1 + \frac{1}{Le_4} \bar{\nabla}^2 \bar{\omega}_2 \\ & + TDN_2 \bar{\nabla} \cdot \left(\frac{1}{1 + \bar{T}} \bar{\nabla} \bar{T} \right). \end{aligned} \quad (2.15)$$

The above equations are respectively for the vorticity, stream function, temperature, mass fraction 1, and mass fraction 2, where $Pr = \nu/\alpha$ is the Prandtl number in either fluid. The derivation of the vorticity equation is detailed in Appendix C.

The following definitions have been used in the above equations

$$c_1 = \frac{(c_{p1} D_{11} + c_{p2} D_{21} + c_{p3} D_{31})}{\bar{c}_p}, \quad (2.16a)$$

$$c_2 = \frac{(c_{p1} D_{12} + c_{p2} D_{22} + c_{p3} D_{32})}{\bar{c}_p}, \quad (2.16b)$$

$$c_3 = \frac{(D_1^T c_{p1} + D_2^T c_{p2} + D_3^T c_{p3})}{\rho \bar{c}_p}, \quad (2.16c)$$

$$Le_1 = \frac{\alpha}{D_{11}}, \quad Le_2 = \frac{\alpha\omega_{1m}}{D_{12}\omega_{2m}}, \quad Le_3 = \frac{\alpha\omega_{2m}}{D_{21}\omega_{1m}}, \quad Le_4 = \frac{\alpha}{D_{22}}, \quad (2.17)$$

and

$$TDN_1 = \frac{D_1^T}{\alpha\rho\omega_{1m}}, \quad TDN_2 = \frac{D_2^T}{\alpha\rho\omega_{2m}}, \quad (2.18)$$

where Le_1 , Le_2 , Le_3 , and Le_4 can be referred to as Lewis Numbers and the c_{pi} 's are the specific heats of individual components. It should be noted that the conservative form of the governing equations is used in Eqs. (2.11), (2.14) and (2.15) for the convection terms.

The nondimensional gradient and Laplacian operators are defined as

$$\tilde{\nabla} = \hat{e}_\eta \frac{\partial}{\partial \eta} + \hat{e}_\theta \frac{1}{\eta} \frac{\partial}{\partial \theta}, \quad \tilde{\nabla}^2 = \frac{\partial^2}{\partial \eta^2} + \frac{2}{\eta} \frac{\partial}{\partial \eta} + \frac{1}{\eta^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{\eta^2 \tan \theta} \frac{\partial}{\partial \theta}. \quad (2.19)$$

The independent coordinates are η and θ only. For ease of notation, the tilde will be dropped on the nondimensional quantities.

2.3 Boundary Conditions

As the solutions of the field variables in the four-region nonisothermal situation in the presence of the vapor-liquid interface and body and pressure forces on the fluids are required, there are numerous boundary conditions. The most important ones are discussed in some detail, and the rest are indicated briefly.

2.3.1 Boundary conditions on temperature

2.3.1.1 Outside of the helium region ($r=d$)

An ICF target distorts the temperature gradient, because the thermal conductivity of the glass wall is much higher than that of the helium gas. The isotherms in the exchange gas curve around the target. The isotherms become more evenly spaced and more horizontal farther away from the target. Beyond a certain radius, the isotherms are virtually horizontal. Therefore, the external thermal gradient on the outer surface of the helium region is assumed to be linear in the vertical direction, i.e., $dT/dz|_{r=d}$ is constant at large radii. Hence, the temperature on the exterior surface of the helium can be written as

$$T(\theta) = T_m + \frac{dT}{dz} r \cos \theta. \quad (2.20)$$

2.3.1.2 SGS-helium interface ($r=c$)

The continuity of temperature and heat flux requires that

$$T_h = T_s, \quad \left(k \frac{\partial T}{\partial \eta} \right)_h = \left(k \frac{\partial T}{\partial \eta} \right)_s + q \quad (2.21a)$$

where q is the nondimensional radiative heat flux given by

$$q = \frac{-a\sigma(T_w^4 - T_s^4)}{T_m \left(\frac{P_s}{A_s \epsilon_s} + \frac{P_w}{A_w \epsilon_w} \right)}. \quad (2.21b)$$

The subscripts h, s and w refer to, respectively, the helium region, the spherical glass shell and the target chamber wall, σ is the Stefan-Boltzman constant, A is surface area, ϵ is emissivity and ρ is density.

2.3.1.3 Liquid-SGS interface ($r=b$)

Here again, the continuity of temperature and heat flux requires that

$$T_s = T_\ell, \quad \left(k \frac{\partial T}{\partial \eta} \right)_s = \left(k \frac{\partial T}{\partial \eta} \right)_\ell. \quad (2.22)$$

The subscripts s and ℓ refer to, respectively, the spherical glass shell and the liquid.

2.3.1.4 Vapor-liquid interface ($r=a$)

The continuity of the temperature and the heat flux at the vapor-liquid interface can be written as

$$T_\ell = T_v, \quad \left(k \frac{\partial T}{\partial \eta} \right)_\ell = \left(k \frac{\partial T}{\partial \eta} \right)_v + \frac{a}{T_m} \sum_{i=1}^3 (n_i h_{i\ell} - n_i h_{iv}) \quad (2.23)$$

where n_i and h_i are, respectively, the mass flux and enthalpy of the species i. The subscripts ℓ and v refer to, respectively, the liquid and the vapor. The last term represents the heat flux caused by evaporation and condensation.

2.3.1.5 At the center of the bubble ($r=0$)

There is a singularity at the center of the bubble due to the $1/r$ factor encountered in spherical geometry in the differential equations. By replacing the

energy equation in the spherical coordinates with its Cartesian equivalent, the singularity can be removed . The energy equation at the center is written as

$$u \frac{\partial T}{\partial z} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + c_1 \frac{\partial \omega_1}{\partial z} \frac{\partial T}{\partial z} + c_2 \frac{\partial \omega_2}{\partial z} \frac{\partial T}{\partial z} + \frac{1}{T} c_3 \frac{\partial T}{\partial z} \frac{\partial T}{\partial z}. \quad (2.24)$$

Only the convection term in the z-direction has been included since the energy flow is almost axial at the center. Additionally, the first derivatives normal to the z-direction are zero due to azimuthal symmetry.

2.3.2 Boundary conditions on vorticity

2.3.2.1 Liquid-SGS interface ($r=b$)

The effects of body and pressure forces on the liquid have to be explicitly imposed to develop the flow fields correctly. The Dirichlet boundary condition on vorticity at the liquid-SGS interface is implemented as follows:

$$\Omega_\ell(\eta = b/a, \theta) = \Omega_\ell(\eta = 1, \theta) + \int_1^{\frac{b}{a}} \left(\frac{\partial \Omega}{\partial \eta} \right)_\ell d\eta, \quad (2.25)$$

i.e., liquid vorticity values at the vapor-liquid interface are extrapolated to the liquid-SGS interface. The nondimensional form of the radial derivative of vorticity in liquid is given by

$$\frac{\partial \Omega}{\partial \eta} = \frac{a^2}{\mu \alpha} \frac{\partial P}{\partial \theta} - \frac{\rho a^3 \eta}{\mu \alpha} g_\theta + \frac{\rho \alpha \eta}{\mu} \left(u \frac{\partial v}{\partial \eta} + \frac{v}{\eta} \frac{\partial v}{\partial \theta} + \frac{uv}{\eta} \right) \quad (2.26)$$

where the first term on the right is due to pressure variation; the second term is due to gravity on the liquid and g_θ denotes the tangential component of gravity; the rest, which are due to the velocity components, make only small contributions. Appendix D outlines the derivation of this relation. A similar form for the normal definition of vorticity but without the convection terms can be found in Ref. 39. To calculate the angular derivatives of pressure, the pressure within the liquid has to be estimated. To that effect, the modified Young-Laplace relation for the balance of forces in the radial direction at the vapor-liquid interface is employed and the liquid side pressures are calculated from the vapor side pressures. The modified Young-Laplace relation⁴⁰ can be written in nondimensional form as

$$P_l(\eta = 1, \theta) = \left(P - \frac{2\mu\alpha}{a^2} \frac{\partial u}{\partial \eta} \right)_v + \left(\frac{2\mu\alpha}{a^2} \frac{\partial u}{\partial \eta} \right)_l - \frac{2\gamma}{a} - \rho_l \left(\frac{\alpha u}{a} \right)_l^2 \left(1 - \frac{\rho_l}{\rho_v} \right) \quad (2.27)$$

where the first term on the right is the total pressure from the vapor at any angular position at the vapor-liquid interface, the second term represents the normal viscous stress in the liquid, the third term is the normal stress due to the surface tension at the curved interface, and the last term is the stress due to momentum change of the mass flow across the interface. The pressure in the interior of the liquid is obtained by integration as follows:

$$P_l(\eta, \theta) = P_l(\eta = 1, \theta) + \int_1^\eta \frac{\partial P}{\partial \eta} d\eta \quad (2.28a)$$

in which

$$\begin{aligned} \frac{\partial P}{\partial \eta} = & \frac{\mu \alpha}{a^2} \left(\frac{\partial^2 u}{\partial \eta^2} + \frac{2}{\eta} \frac{\partial u}{\partial \eta} + \frac{1}{\eta^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{1}{\eta^2 \tan \theta} \frac{\partial u}{\partial \theta} - \frac{2u}{\eta^2} - \frac{2}{\eta^2} \frac{\partial v}{\partial \theta} - \frac{2}{\eta^2} \frac{v}{\tan \theta} \right) \\ & - \frac{\rho \alpha^2}{a^2} \left(u \frac{\partial u}{\partial \eta} + \frac{v}{\eta} \frac{\partial u}{\partial \theta} - \frac{u^2}{\eta} \right) - \rho g a \cos \theta \end{aligned} \quad (2.28b)$$

is the radial derivative of pressure that can be obtained from the radial component of the momentum equation; it accounts mainly for the pressure variation due to the radial component of liquid weight.

2.3.2.2 Vapor-liquid interface, ($r=a$), liquid side

The presence of the surface-tension gradient at the vapor-liquid interface manifests as a discontinuity in the shear stress across that interface. The shear stress condition can be written as

$$\tau_l + \frac{1}{a} \frac{\partial \gamma}{\partial \theta} = \tau_v. \quad (2.29)$$

The surface-tension gradient can be modeled as follows. Let us assume that the total local surface tension is the mole-fraction-weighted average of the pure-component surface tensions since the hydrogen mixture is essentially ideal. The pure-component surface tensions can be represented as a linear function of temperature as $\gamma_i = A_i - B_i T$ ($i = 1, 2, 3$), with A_i and B_i being characteristic positive constants⁴¹. Then, we can write the surface tension as $\gamma = x_1 \gamma_1 + x_2 \gamma_2 + x_3 \gamma_3$. Hence the surface-tension gradient can be written as

$$\frac{\partial \gamma}{\partial \theta} = \frac{\partial \gamma}{\partial T} \frac{\partial T}{\partial \theta} + \frac{\partial \gamma}{\partial x_1} \frac{\partial x_1}{\partial \theta} + \frac{\partial \gamma}{\partial x_2} \frac{\partial x_2}{\partial \theta} \quad (2.30)$$

where x_i is the liquid mole fraction of the i -th species and $x_1 + x_2 + x_3 = 1$. The factors $\frac{\partial x_1}{\partial \theta}$ and $\frac{\partial x_2}{\partial \theta}$ are written in terms of the mass fraction gradients as follows.

Liquid mole fractions x_i can be written in terms of liquid mass fractions ω_i as

$$x_i = \frac{\omega_i}{M_i} \left(\sum_{j=1}^3 \frac{\omega_j}{M_j} \right)^{-1} \quad i = 1, 2, 3 \quad (2.31)$$

where M_1 , M_2 , and M_3 are the pure component molecular weights, and $\sum_{j=1}^3 \frac{\omega_j}{M_j}$ is the inverse of local molecular weight of the liquid. One can then obtain $\frac{\partial \gamma}{\partial \theta}$ as

$$\frac{\partial \gamma}{\partial \theta} = \frac{\partial \gamma}{\partial T} \frac{\partial T}{\partial \theta} + \left(\frac{\partial \gamma}{\partial x_1} \frac{\partial x_1}{\partial \omega_1} + \frac{\partial \gamma}{\partial x_2} \frac{\partial x_2}{\partial \omega_1} \right) \frac{\partial \omega_1}{\partial \theta} + \left(\frac{\partial \gamma}{\partial x_1} \frac{\partial x_1}{\partial \omega_2} + \frac{\partial \gamma}{\partial x_2} \frac{\partial x_2}{\partial \omega_2} \right) \frac{\partial \omega_2}{\partial \theta}. \quad (2.32)$$

The resulting balance of shear stress can be written in terms of the vorticities of the fluids at the interface and the variation of the temperature and the mass-fractions along the angular direction as

$$\begin{aligned} \Omega_\ell = & -2 \left(\frac{\partial u}{\partial \theta} - v \right)_\ell + \frac{\mu_v \alpha_v}{\mu_\ell \alpha_\ell} \left(\Omega + 2 \left(\frac{\partial u}{\partial \theta} - v \right) \right)_v \\ & - \left(Ma_T \frac{\partial T}{\partial \theta} + Ma_{c1} \frac{\partial \omega_1}{\partial \theta} + Ma_{c2} \frac{\partial \omega_2}{\partial \theta} \right) \end{aligned} \quad (2.33)$$

where the subscripts ℓ and v respectively refer to the liquid and vapor phase, and Ma_T , Ma_{c1} , and Ma_{c2} can be referred to respectively as the thermal Marangoni number, the concentration Marangoni number due to component 1, and the concentration Marangoni number due to component 2. This terminology follows from the fact that the surface-tension-gradient-induced flows are also referred to

as Marangoni flows. The constants Ma_T , Ma_{c1} , and Ma_{c2} are written for the pure component, binary, and ternary systems as follows.

Pure-component system:

$$Ma_T = \frac{-aT_m B_1}{\mu_t \alpha_t} \quad (2.34a)$$

$$Ma_{c1} = 0 \quad (2.34b)$$

$$Ma_{c2} = 0. \quad (2.34c)$$

Binary system:

$$Ma_T = \frac{-aT_m}{\mu_t \alpha_t M} \left(B_1 \frac{\omega_1}{M_1} + B_2 \frac{1-\omega_1}{M_2} \right) \quad (2.35a)$$

$$Ma_{c1} = \frac{a\omega_{1m}}{\mu_t \alpha_t} \left((\gamma_1 - \gamma_2) \frac{\partial x_1}{\partial \omega_1} \right) \quad (2.35b)$$

$$Ma_{c2} = 0. \quad (2.35c)$$

Ternary system:

$$Ma_T = \frac{-aT_m}{\mu_t \alpha_t M} \left(B_1 \frac{\omega_1}{M_1} + B_2 \frac{\omega_2}{M_2} + B_3 \frac{(1-\omega_1-\omega_2)}{M_3} \right) \quad (2.36a)$$

$$Ma_{c1} = \frac{a\omega_{1m}}{\mu_t \alpha_t} \left((\gamma_1 - \gamma_3) \frac{\partial x_1}{\partial \omega_1} + (\gamma_2 - \gamma_3) \frac{\partial x_2}{\partial \omega_1} \right) \quad (2.36b)$$

$$Ma_{c2} = \frac{a\omega_{2m}}{\mu_t \alpha_t} \left((\gamma_1 - \gamma_3) \frac{\partial x_1}{\partial \omega_2} + (\gamma_2 - \gamma_3) \frac{\partial x_2}{\partial \omega_2} \right) \quad (2.36c)$$

where M is the mean molecular weight of the liquid; and ω_1 and ω_2 are the mass fractions in the liquid at the vapor-liquid interface.

2.3.2.3 Vapor-liquid interface, ($r=a$), vapor side

The definition of vorticity is used to evaluate the vapor vorticity at this interface

$$\Omega_v(\eta = 1, \theta) = \left(\frac{\partial v}{\partial \eta} - \frac{\partial u}{\partial \theta} + v \right)_v. \quad (2.37)$$

2.3.2.4 At the bubble center ($r=0$)

The modified vorticity is zero at this point.

2.3.3 Boundary conditions on stream function

2.3.3.1 Liquid-SGS interface ($r=b$)

The velocity of the fluid is zero at the liquid-SGS interface, as the shell of the target is impermeable and is assumed to be stationary. The stream function is therefore defined to be zero here. Additionally, the radial derivative of the stream function needs to be zero. Since this relation is redundant, it numerically verified rather than calculated.

2.3.3.2 Vapor-liquid interface, ($r=a$), liquid side

The stream function at this interface is found by integrating the radial velocities on the liquid side, using the relation between the radial velocity and the stream function as

$$\psi(\eta = 1, \theta) = \int_0^\theta u_r(\eta = 1, \theta) \sin \theta d\theta. \quad (2.38)$$

2.3.3.3 Vapor-liquid interface, ($r=a$), vapor side

The vapor stream function at the vapor-liquid interface is iterated for, along with the interior values, by using a modified form of the stream function equation. The known radial velocity is used in place of the tangential derivative of the stream function. The fictitious node introduced by the central-difference form of the second derivative of the stream function in the radial direction is eliminated by using the tangential velocity. The required set of equations is

$$\left. \frac{\partial \psi}{\partial \eta} \right|_{\eta=1} = -v_\theta(\eta = 1, \theta) \sin \theta, \quad (2.39a)$$

$$\frac{\partial^2 \psi}{\partial \eta^2} + \frac{1}{\eta^2} \frac{\partial^2 \psi}{\partial \theta^2} = -\Omega_v \sin \theta + u_v \cos \theta, \quad (2.39b)$$

This results in a stable iterative scheme for the vapor stream function at this interface. Details of this scheme can be found in Ref. 42.

2.3.4 Boundary conditions on velocities

2.3.4.1 Liquid-SGS interface ($r=b$)

The tangential liquid velocity at this interface is evaluated using the radial derivatives of stream function as shown in section 3.5.5.1.

2.3.4.2 Vapor-liquid interface ($r=a$)

The condition of continuity of energy flux at this interface can be used to obtain the radial liquid velocities as follows

$$\left(k \frac{\partial T}{\partial \eta}\right)_\ell = \left(k \frac{\partial T}{\partial \eta}\right)_v + \frac{a}{T_m} \sum_{i=1}^3 (n_{\ell i} h_{\ell i} - n_{v i} h_{v i}) \quad (2.40a)$$

where

$$\begin{aligned} (n_{\ell i} h_{\ell i} - n_{v i} h_{v i}) = & \left(\omega_i \rho u - \rho D_{i1} \frac{\partial \omega_1}{\partial r} - \rho D_{i2} \frac{\partial \omega_2}{\partial r} - D_i^T \frac{\partial T}{\partial r} \right)_\ell h_{\ell i} \\ & - \left(\omega_i \rho u - \rho D_{i1} \frac{\partial \omega_1}{\partial r} - \rho D_{i2} \frac{\partial \omega_2}{\partial r} - D_i^T \frac{\partial T}{\partial r} \right)_v h_{v i}. \end{aligned} \quad (2.40b)$$

The radial velocity on the vapor side in this expression can be written using the assumption of incompressibility of the fluids, in nondimensional form, as

$$u_v(\eta = 1, \theta) = \frac{\rho_\ell \alpha_\ell}{\rho_v \alpha_v} u_\ell(\eta = 1, \theta). \quad (2.41)$$

This allows one to take into account the effect of mass transfer due to evaporation and condensation.

The continuity of tangential velocities at this interface can be written, in nondimensional form as

$$v_v(\eta = 1, \theta) = \frac{\alpha_\ell}{\alpha_v} v_\ell(\eta = 1, \theta). \quad (2.42)$$

2.3.4.2 At the center of the bubble ($r=0$)

Because of the symmetry of the flow field about the vertical center line, the velocities at $\theta = 0$ and $\theta = \pi$ are radial. Using the estimate of the radial velocity at $\theta = 0$, the radial velocities can be written as

$$u_v(r = 0, \theta) = u_v(r = 0, \theta = 0) \cos \theta \quad (2.43)$$

and the tangential velocity at any direction can be written as

$$v_v(r = 0, \theta) = -u_v(r = 0, \theta = 0) \sin \theta. \quad (2.44)$$

The condition that the vapor vorticity at the center be zero is satisfied by these velocities.

2.3.5 Boundary conditions on mass fractions

2.3.5.1 Liquid-SGS interface ($r=b$)

The shell of the target is impermeable, therefore the concentration of the components in the binary and ternary systems can be determined by writing the flux relationship as

$$\left(D_{11} \omega_{1m} \frac{\partial \omega_1}{\partial \eta} + D_{12} \omega_{2m} \frac{\partial \omega_2}{\partial \eta} + \frac{1}{\rho} D_1^T \frac{1}{T} \frac{\partial T}{\partial \eta} \right) = 0 \quad i=1,2. \quad (2.45)$$

2.3.5.2 Vapor-liquid interface ($r=a$)

The profiles of the pressure, temperature, and the two mass fractions along the liquid-vapor interface have to be carefully considered, and to facilitate the computations the profiles must be specified in the beginning of the iterations.

The number of variables that are to be specified to uniquely determine the thermodynamic state of the system is given by the Gibb's⁴³ phase rule. Accordingly, the two-phase ($P=2$), multicomponent ($C=1$ or $C=2$ or $C=3$) system possesses the number of degrees of freedom F determined by $F = C - P + 2$. The number of degrees of freedom, which is the number of variables that have to be specified at the outset, is equal to one for the pure-component two-phase system, equal to two for the two-component two-phase system, and equal to three for the three-component two-phase system. The intensive properties that are assumed at the liquid-vapor interface are chosen to have cosine profiles along the interface.

The final temperature profile at the interface is obtained by iteration of the energy equation. In the binary system, the mass fraction of component 1 in the liquid and vapor is determined using Raoult's law once the saturation pressure is specified along the vapor-liquid interface, in addition to the final temperature profile. If the saturation pressures are not varied in the θ -direction but given the equilibrium values, the mass fraction variation is found to be very small. If the saturation pressure is varied parametrically, the mass fraction deviation from the mean can become quite large. In the ternary system, the mass fraction of component 2 in liquid and the mass fractions of the components 1 and 2 in vapor are determined using Raoult's law once the pressure, temperature, and the liquid mass fraction of component 1 along the interface are specified.

Assuming the liquid and vapor mixtures of hydrogen isotopes are nearly ideal, one can apply Raoult's law at the liquid-vapor interface as follows:

$$\omega_{1v} = \frac{\omega_{1\ell}}{\omega_{1mv}} (\omega_{1\ell} + 1) \frac{M_1 P_{s1}}{M_v P_{vt}} - 1, \quad \omega_{2v} = \frac{\omega_{2\ell}}{\omega_{2mv}} (\omega_{2\ell} + 1) \frac{M_2 P_{s2}}{M_v P_{vt}} - 1, \quad (2.46)$$

where P_v is the specified total vapor pressure at any point on the vapor-liquid interface; P_{s1} and P_{s2} are the saturation vapor pressures of components 1 and 2, respectively, and are known from the temperature profile specified along the vapor-liquid interface; and M_l and M_v are the mean molecular weights of the liquid and vapor mixture.

Also at the vapor-liquid interface, the radial mass fluxes of the individual components in the binary and ternary system should be continuous, and this condition can be written as

$$\begin{aligned} & \left(\rho \omega_m \alpha u (\omega_i + 1) - \rho \omega_m D_{i1} \frac{\partial \omega_1}{\partial \eta} - \rho \omega_m D_{i2} \frac{\partial \omega_2}{\partial \eta} - D_i^T T_m \frac{\partial T}{\partial \eta} \right)_l \\ & = \left(\rho \omega_m \alpha u (\omega_i + 1) - \rho \omega_m D_{i1} \frac{\partial \omega_1}{\partial \eta} - \rho \omega_m D_{i2} \frac{\partial \omega_2}{\partial \eta} - D_i^T T_m \frac{\partial T}{\partial \eta} \right)_v, \quad i=1,2. \end{aligned} \quad (2.47)$$

2.3.5.3 At the center of the vapor bubble ($r=0$)

Similar to the calculation of temperature at the center of the vapor bubble and to avoid the singularity in the diffusion-convection equation in the spherical coordinates, the corresponding Cartesian equivalent is used, and the convection term in the z -direction only is retained as the mass flux is predominantly axial at the center. The equation of component i is

$$\begin{aligned} u \frac{\partial \omega_i}{\partial z} &= D_{i1} \left(\frac{\partial^2 \omega_1}{\partial x^2} + \frac{\partial^2 \omega_1}{\partial y^2} + \frac{\partial^2 \omega_1}{\partial z^2} \right) + D_{i2} \left(\frac{\partial^2 \omega_2}{\partial x^2} + \frac{\partial^2 \omega_2}{\partial y^2} + \frac{\partial^2 \omega_2}{\partial z^2} \right) \\ &+ \frac{1}{\rho} D_i^T \left(\frac{1}{T} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) - \frac{1}{T^2} \left(\frac{\partial T}{\partial z} \right)^2 \right). \end{aligned} \quad (2.48)$$

2.3.6 Symmetry conditions

The symmetry conditions at $\theta = 0$, and $\theta = \pi$ are

$$\Omega_i = \psi_i = v_i = 0; \quad i = v, \ell \quad \text{Dirichlet boundary conditions} \quad (2.49a)$$

$$\frac{\partial T_i}{\partial \theta} = \frac{\partial \omega_{1i}}{\partial \theta} = \frac{\partial \omega_{2i}}{\partial \theta} = \frac{\partial u_i}{\partial \theta} = 0; \quad i = v, \ell. \quad \text{Neumann boundary conditions} \quad (2.49b)$$

2.4 Force Balance on the Vapor Bubble

For a given external temperature gradient, the bubble will be stationary at the center of the target when the total upward force cancels out the vapor weight. This is checked numerically by integrating the pressures and shear stresses on the vapor bubble. The total upward force F_z on the bubble is given by

$$F_z = 2\pi a^2 \int_0^\pi (-P_\pi \sin\theta \cos\theta - \tau_{r\theta} \sin^2\theta) d\theta \quad (2.50)$$

where the total pressure P_π and the shear stress $\tau_{r\theta}$ are defined as

$$P_\pi = \left(P - 2 \frac{\mu\alpha}{a^2} \frac{\partial u}{\partial \eta} \right) \Big|_{\eta=\pi}, \quad \tau_{r\theta} = \frac{\mu\alpha}{a^2} \left(\frac{\partial v}{\partial \eta} + \frac{\partial u}{\partial \theta} - v \right) \Big|_{\eta=\pi}. \quad (2.51)$$

The external temperature gradient is considered to be that required for the bubble to remain stationary at the center of the target if the total upward force F_z on the bubble is within a fraction of a percent of the vapor weight and if other checks for self-consistency are satisfied.

CHAPTER 3

NUMERICAL SOLUTION PROCEDURE

3.1 General Discussion

The numerical treatment of partial differential equations is, by itself, a vast subject. Partial differential equations are at the heart of many, if not most, computer analyses or simulations of continuous physical systems, such as fluids, electromagnetic fields and the human body. In most mathematics books, partial differential equations (PDEs) are classified into three categories, hyperbolic, parabolic and elliptic, on the basis of their characteristics, which are curves of information propagation.

From a computational point of view, the classification into these three canonical types is not very meaningful. If information on u (perhaps including time derivative information) is given at some initial time t_0 for all x , then the equations describe how $u(x,t)$ propagates itself forward in time, and the goal of the numerical code should be to track the time evolution with some desired accuracy. By contrast, if the goal is to find a single "static" function $u(x,y)$ which satisfies the equation within some (x,y) region of interest, and which has some desired behavior on the boundary of the region of interest, these problems are called boundary value problems. In general, it is not possible simply to "integrate in from the boundary" in the same sense that an initial value problem can be "integrated forward in time." Therefore the goal of a numerical code is somehow to converge on the correct solution everywhere at once.

Because all of the conditions on a boundary value problem must be satisfied "simultaneously," these problems usually result in, at least conceptually, to the solution of a large number of simultaneous algebraic equations. When

such equations are nonlinear, they are usually solved by linearization and iteration.

The system of governing equations for the problem at hand defines a boundary value problem. In the numerical iteration, the goal is to look for the situation in which the liquid layer is uniform in thickness. This means that the vapor bubble is required to be stationary when an appropriate external thermal gradient is imposed outside the helium region, and the aim of the computation is to determine such an external thermal gradient along with other parameters. A stationary bubble is formed when the resultant of the surface forces, due to pressure and shear and normal stresses on the bubble, points upward and cancels out the weight of the bubble. Such a condition is verified along the course of the numerical computations. The solution is obtained when several checks for self-consistency are found to be satisfactory.

As the numerical approach proceeds to search for the various parameters that will allow for a stationary bubble at the center of the target, it is necessary to check the consistency of the chosen parameters. A check for the agreement between the two different forms of the liquid vorticity at the liquid-SGS interface is required to obtain self-consistent results. This condition enables one to assess the acceptability of the assumed vapor pressure profile used to determine the liquid pressure profile at the vapor-liquid interface. The verification of the force balance on the bubble, the verification of the global mass balance, and the verification of the continuity of the local mass fluxes of the individual species at the liquid-vapor interface are also important checks.

3.2 Finite Difference Mesh

The mesh size at the interface of the vapor and liquid, at the interface of the liquid and SGS and at the interface of the SGS and the helium region, have to be nearly the same size to obtain accurate solutions. To accomplish this and avoid an excessive number of mesh points in regions in which variables do not vary rapidly, a radially varying mesh in the helium region and in the vapor is used. In the helium region this is done by radially incrementing the mesh size in geometric progression with the smallest mesh size at the SGS-helium interface. In the vapor region, the smallest mesh size is at the vapor-liquid interface, being of the order of the mesh size in the liquid and increasing in geometric progression toward the center of the bubble. The mesh structure and nomenclature are shown in Figure 3.1. Since the external linear temperature gradient is applied symmetrically in the vertical direction about the center line, it is sufficient to consider only one hemisphere. This is taken to be the right half of the concentric spherical system.

3.3 Numerical Algorithm

The diffusion terms of the vorticity, mass diffusion-convection and energy equations have been approximated by a central-difference scheme.⁴⁴ The same scheme was used for the stream function equation. Thus,

$$Q'_i = \frac{Q_r - Q_\ell}{2\Delta\eta}, \quad Q''_i = \frac{Q_r - 2Q_i + Q_\ell}{(\Delta\eta)^2}, \quad (3.1)$$

where Q is the generic quantity, $\Delta\eta$ is the nondimensional mesh size and the subscripts r , ℓ , and i indicate, respectively, the right, left and center nodes in the mesh. These discretization formulae are second-order accurate (see Appendix E).

Figure 3.1 Finite-difference mesh.

In the varying radial mesh in the vapor and helium regions, a different discretization procedure has to be adopted; the discretization formulae for the first and second derivatives in a varying mesh can be written as

$$Q'_i = \frac{Q_r - (1 - \beta^2)Q_i - \beta^2 Q_t}{(1 + \beta)\Delta r} \quad (3.2a)$$

and

$$Q''_i = \frac{2\beta\{Q_r - (1 + \beta)Q_i + \beta Q_t\}}{(1 + \beta)(\Delta r)^2}. \quad (3.2b)$$

The derivations of these formulae are shown in Appendix F. The factor β is the mesh expansion ratio and is defined as $\beta = \frac{\Delta r}{\Delta t}$. The discretization formulae are first-order accurate; but when the mesh expansion ratio β is close to unity, they are nearly second-order accurate.

A similar attempt to approximate the nonlinear convective terms failed. Unstable solutions were obtained even for fairly fine grids. This procedure would require very fine meshes to produce stable solutions.⁴⁵ There is a compromise between very fine grids to secure accurate and stable solutions and computer time available. Since the last represents a serious limitation, numerical schemes which ensure stability under reasonable grid sizes had to be devised. This is the case of upwind methods. These schemes emphasize the convection of a given property in the downstream direction. As a result they are considered to possess the transportive property,⁴⁴ in the sense that any perturbation in the flow is convected only in the downstream direction. These stable characteristics, however, are introduced at the expense of accuracy.

The convective terms appear in two different forms:

1. $\text{CONV} = \frac{\partial(u\Omega)}{\partial\eta} + \frac{1}{\eta} \frac{\partial(v\Omega)}{\partial\theta}$ in the vorticity equation, Eq. (2.11), and
 $\text{CONV} = \frac{1}{\eta^2} \frac{\partial(\eta^2 u \omega_i)}{\partial\eta} + \frac{1}{\eta \sin\theta} \frac{\partial(\sin\theta v \omega_i)}{\partial\theta}$ in the mass diffusion-convection equations, Eqs. (2.14) and (2.15). This form is called conservative in the literature.⁴⁶ It corresponds to a transformation of the kind

$$\tilde{\nabla} \cdot (\nabla \Omega) = \nabla \cdot (\tilde{\nabla} \Omega) \quad (3.3)$$

which is valid for an incompressible fluid. Even though equivalent, the distinct forms in Eq. (3.3) behave very differently under the same numerical procedure. It is a common belief that the conservative form (RHS of Eq. (3.3)) produces more accurate results for the same grid size.^{44,47-50} It has been reported, however, that under certain circumstances, they can lead to unstable solutions.⁵¹ In fact this was the case when trials were made with the conservative form for the energy equation. As a result, nonconservative forms were adopted. Appendix G contains a discussion of the general forms of the governing equations, conservative and nonconservative.

The vorticity (and mass diffusion-convection) convective terms were approximated by the so-called second upwind method.⁵² According to this procedure the velocities are linearly interpolated between mesh nodes. If η represents the coordinate in any given direction, whether r or θ , the convective term in this direction is approximated by

$$\frac{\partial}{\partial\eta}(u\Omega)_i \approx \frac{U_i \Omega_r - U_r \Omega_i}{\Delta\eta} \quad (3.4)$$

where

$$U_r = 0.5(u_i + u_{i+1}) \quad (3.5a)$$

$$U_l = 0.5(u_i + u_{i-1}) \quad (3.5b)$$

$$\Omega_r = \begin{cases} \Omega_i & \text{if } U_r > 0 \\ \Omega_{i+1} & \text{if } U_r < 0 \end{cases} \quad (3.5c)$$

$$\Omega_l = \begin{cases} \Omega_{i-1} & \text{if } U_l > 0 \\ \Omega_i & \text{if } U_l < 0 \end{cases} \quad (3.5d)$$

2. $\text{CONV} = u \frac{\partial T}{\partial \eta} + \frac{v}{\eta} \frac{\partial T}{\partial \theta}$ in the energy equation, Eq. (2.13). These

convective terms are approximated by the so-called first upwind method⁵²

$$u \frac{\partial T}{\partial \eta} \equiv u_i \frac{T_r - T_l}{\Delta \eta} \quad (3.6)$$

where

$$T_r = \begin{cases} T_i & \text{if } u_i > 0 \\ T_{i+1} & \text{if } u_i < 0 \end{cases} \quad (3.7a)$$

$$T_l = \begin{cases} T_{i-1} & \text{if } u_i > 0 \\ T_i & \text{if } u_i < 0 \end{cases} \quad (3.7b)$$

The main advantage of the "upwind" methods, used in this work, is to produce stable solutions for acceptable grid sizes. The main features of the upwind methods are:

- (1) The property is convected unchanged in the downstream direction.
- (2) The different assumptions regarding the velocities constitute the main concern of researchers in the fluid dynamics field. Two of the most popular models were used in this work and were referred to above, that is, the linear velocity distribution, which constitutes the second upwind method, and the constant velocity, which is characteristic of the first upwind scheme. Other schemes can be found in the literature.^{53,54} These schemes aim to confer more accuracy to the upwind methods, which in fact they do, making, however, the numerical algorithm more complex and, consequently, the computation phase more expensive.
- (3) Upwind methods are first-order approximations.

The iterative sequence of the numerical solutions of the equations is given briefly in the diagram in Figure 3.2. A more detailed flow diagram of the inner momentum loops for the liquid and the vapor is shown in Figure 3.3. At any iteration the energy equation converges quickly. In the multicomponent system, the mass diffusion-convection equations also converge quickly. The iterations for the vapor vorticity and stream function take a long time to converge, since the development of the vapor flow field for the given interface velocities takes substantial time. The liquid flow field can be computed in a relatively short time because there are fewer nodes in the liquid than in the vapor and because Dirichlet boundary conditions on the vorticity and stream function are used,

FLOW-CHART:

Figure 3.2 Simplified block diagram of the numerical computations.

Figure 3.3 Flow diagram for the separate inner momentum loops.

Eq. (2.49a). The separate inner momentum loops for the liquid and the vapor shown in Figure 3.3 greatly reduce the number of iterations needed for the whole flow field to converge, because the liquid flow field is governed by the surface-tension gradients and the interface mass transfer is quickly generated and changes very little after a few major iterations.

The efficiency of the computational algorithms, both in computational load and storage requirements, becomes the principal concern. The computer used for the numerical simulation is a Cray and is a vector machine. For these reasons, the iteration of the discretized equations is achieved by the Point Jacobi⁵⁵ technique. The computational load is reduced at the expense of additional storage. Other relaxation methods such as the Gauss-Seidel⁵⁵ line relaxation method may be more efficient on machines which do not vectorize.

3.4 Solution Technique - Point Jacobi Iteration

The governing equations define a boundary value problem, and hence the discretized equations are solved by a relaxation method. The details of this method can be found, for instance, in Ref. 55. In the iterative scheme, the node value is determined as the sum of the old value and the weighted average of the error function, which is a function of the values of the four surrounding nodes and of the center node itself. The computational algorithm is

$$\xi_{i,j} \leftarrow \xi_{i,j} + \frac{\omega_{\text{Jac}}}{D_5} (D_1 \xi_{i+1,j} + D_2 \xi_{i-1,j} + D_3 \xi_{i,j+1} + D_4 \xi_{i,j-1} - D_5 \xi_{i,j} + D_6) \quad (3.8)$$

where ξ is the generic quantity representing any variable of iteration. The coefficients D_1 to D_5 are those found in the discretized forms of the governing equations or the modified forms of them. The coefficient D_6 is due to the source

or sink terms. The quantity ω_{sor} , the relaxation factor, takes its values in the interval $0 \leq \omega_{\text{sor}} \leq 1$ for the point Jacobi iteration method.

The modified forms of the coefficients D_1 to D_6 are used in the energy equations at the SGS-helium interface, at the liquid-SGS interface and in the stream function equation for the vapor. Also, along the line of symmetry these coefficients are modified in the energy and mass diffusion-convection equations by using the symmetry conditions on the temperature and mass fractions. Thus, on the line of symmetry the temperature and mass fractions are obtained from iterations by modifying the coefficients D_1 to D_6 using the Neumann forms of the symmetry conditions. Eq. (2.49b).

The convergence of the solutions for each governing equation is based on the criterion

$$\text{DEVI} = |\xi_{i,j}^{k+1} - \xi_{i,j}^k| \quad (3.9)$$

where the deviation, DEVI, for any node in the solution domain is stipulated to be less than some specified value, depending on the nature of the values of the variable, and the superscript k refers to the k -th iteration.

3.5 Numerical Treatment of Boundary Conditions

3.5.1 Boundary conditions on temperature

3.5.1.1 SGS-helium interface ($r=c$)

The required boundary conditions are given by Eqs. (2.21a) and (2.21b). At this interface the discretized energy equation has two different sets of coefficients D_1 to D_6 , one each from the energy equation applied to the two adjoining regions. By using the technique of imaginary nodes, Ref. 56, and with

the interface boundary condition, a new set of coefficients $D_1 - D_6$ can be derived as

$$D_1 \leftarrow D_{1s} \frac{k_h \Delta\eta_s}{k_s \Delta\eta_h} \left(1 + \frac{D_{1h}}{D_{2h}} \right), \quad (3.10a)$$

$$D_2 \leftarrow D_{1s} + D_{2s}, \quad (3.10b)$$

$$D_3 \leftarrow D_{3s} + D_{1s} \frac{k_h \Delta\eta_s}{k_s \Delta\eta_h} \frac{D_{3h}}{D_{2h}}, \quad (3.10c)$$

$$D_4 \leftarrow D_{4s} + D_{1s} \frac{k_h \Delta\eta_s}{k_s \Delta\eta_h} \frac{D_{4h}}{D_{2h}}, \quad (3.10d)$$

$$D_5 \leftarrow D_{5s} + D_{1s} \frac{k_h \Delta\eta_s}{k_s \Delta\eta_h} \frac{D_{5h}}{D_{2h}}, \quad (3.10e)$$

and

$$D_6 \leftarrow D_{6s} + D_{1s} \frac{k_h \Delta\eta_s}{k_s \Delta\eta_h} \frac{D_{6h}}{D_{2h}} - 2 \frac{\Delta\eta_s}{k_s} \frac{a\sigma(T_w^4 - T_s^4)}{T_m \left(\frac{\rho_s}{A_s \epsilon_s} + \frac{\rho_w}{A_w \epsilon_w} \right)}. \quad (3.10f)$$

The left hand side represents the new values of the coefficients D_1 to D_6 , and the right-hand side is the function of the old values of the same coefficients from the adjoining regions as indicated by the subscripts h and s.

3.5.1.2 Liquid-SGS interface ($r=b$)

Again, the two difference sets of coefficients D_1 to D_6 of the energy equation at this interface can be reduced to one set using Eqs. (3.10a) to (3.10f) after replacing subscripts h and s by s and ℓ , respectively, and eliminating the last term on the right-hand side of Eq. (3.10f)

$$D_1 \leftarrow D_{1\ell} \frac{k_{sh}}{k_\ell} \frac{\Delta\eta_\ell}{\Delta\eta_s} \left(1 + \frac{D_{1s}}{D_{2s}} \right), \quad (3.11a)$$

$$D_2 \leftarrow D_{2\ell} + D_{2\ell}, \quad (3.11b)$$

$$D_3 \leftarrow D_{3\ell} + D_{1\ell} \frac{k_s}{k_\ell} \frac{\Delta\eta_\ell}{\Delta\eta_s} \frac{D_{3s}}{D_{2s}}, \quad (3.11c)$$

$$D_4 \leftarrow D_{4\ell} + D_{1\ell} \frac{k_s}{k_\ell} \frac{\Delta\eta_\ell}{\Delta\eta_s} \frac{D_{4s}}{D_{2s}}, \quad (3.11d)$$

$$D_5 \leftarrow D_{5\ell} + D_{1\ell} \frac{k_s}{k_\ell} \frac{\Delta\eta_\ell}{\Delta\eta_s} \frac{D_{5s}}{D_{2s}} \quad (3.11e)$$

and

$$D_6 \leftarrow D_{6\ell} + D_{1\ell} \frac{k_s}{k_\ell} \frac{\Delta\eta_\ell}{\Delta\eta_s} \frac{D_{6s}}{D_{2s}}. \quad (3.11f)$$

3.5.1.3 Vapor-liquid interface ($r=a$)

In the iteration procedure for solving the energy equation, the temperatures at the vapor-liquid interface are assumed to be known. In reality the latent heat transfer due to evaporation/condensation, in conjunction with the

far-field temperature gradient, determines the interface temperatures and the mass fractions of the individual species. Here the reverse process of letting the vapor-liquid interface temperature take preassigned values is employed to avoid the slow convergence of the energy equation since the interface temperature also depends on the interface energy flux.

3.5.2 Boundary conditions on vorticity

3.5.2.1 Liquid-SGS interface ($r=b$)

The liquid vorticity at the liquid-SGS interface is determined by numerically integrating Eq. (2.25).

3.5.2.2 Vapor-liquid interface ($r=a$)

The liquid vorticity at the vapor-liquid interface is computed using Eq. (2.33); the first-order derivatives are discretized using a second-order accurate forward-difference formulae.

The vapor vorticity at the vapor-liquid interface is given by Eq. (2.37). The required radial derivative of the tangential velocity at the liquid-vapor interface is evaluated by using second-order accurate backward-difference formulae.

3.5.3 Boundary conditions on stream function

3.5.3.1 Liquid-SGS interface ($r=b$)

The stream function at the liquid-SGS interface is zero.

3.5.3.2 Vapor-liquid interface ($r=a$)

Once the interfacial velocities are determined from Eqs. (2.40a) and (2.40b), the liquid stream function at the vapor-liquid interface is computed by numerically integrating Eq. (2.38).

The vapor stream function at the vapor-liquid interface is iterated for along with the stream function values in the interior of the vapor. The nondimensional discretized form of the equation for the vapor stream function at this interface is

$$D_2\psi_{i-1,j} + D_3\psi_{i,j+1} + D_4\psi_{i,j-1} - D_5\psi_{i,j} + D_6 = 0 \quad (3.12)$$

where

$$D_2 = 2, \quad (3.13a)$$

$$D_3 = \left(\frac{(\Delta\eta)^2}{\eta^2(\Delta\theta)^2} \right)_v, \quad (3.13b)$$

$$D_4 = \left(\frac{(\Delta\eta)^2}{\eta^2(\Delta\theta)^2} \right)_v, \quad (3.13c)$$

$$D_5 = \left(2 + 2 \frac{(\Delta\eta)^2}{\eta^2(\Delta\theta)^2} \right)_v \quad (3.13d)$$

and

$$D_6 = ((\Delta\eta)^2 \Omega \sin\theta - (\Delta\eta)^2 u \cos\theta - 2\eta\Delta\eta v \sin\theta). \quad (3.13e)$$

3.5.4 Boundary conditions on velocities

3.5.4.1 Liquid-SGS interface ($r=b$)

A special approach is adopted in the calculation of the liquid tangential velocities near the liquid-SGS interface. This contrivance is found necessary because the usual second-order central-difference forms for the liquid tangential velocities do not work well. The liquid velocities are obtained by using a cubic-polynomial fit to the generated stream function; this is necessary because the liquid flow is almost similar to boundary layer flow and there are sharp gradients in the radial direction in the field variables. By fitting a cubic polynomial of the stream function in the radial direction, it can be shown that

$$\left. \frac{\partial \psi}{\partial \eta} \right|_i = \frac{(-2\psi_{i-3} + 9\psi_{i-2} - 18\psi_{i-1} + 11\psi_i)}{6\Delta\eta}, \quad (3.14a)$$

$$\left. \frac{\partial \psi}{\partial \eta} \right|_{i-1} = \frac{(\psi_{i-3} - 6\psi_{i-2} + 3\psi_{i-1} + 2\psi_i)}{6\Delta\eta}, \quad (3.14b)$$

$$\left. \frac{\partial \psi}{\partial \eta} \right|_{i-2} = \frac{(-2\psi_{i-3} - 3\psi_{i-2} + 6\psi_{i-1} - \psi_i)}{6\Delta\eta} \quad (3.14c)$$

and

$$\left. \frac{\partial \psi}{\partial \eta} \right|_{i-3} = \frac{(-11\psi_{i-3} + 18\psi_{i-2} + 9\psi_{i-1} + 2\psi_i)}{6\Delta\eta} \quad (3.14d)$$

where i refers to the node at the liquid-SGS interface, and $i-1$, $i-2$, and $i-3$ refer to the three consecutively interior radial nodes. These expressions somewhat resemble those due to Briley.⁵⁷ These expressions can be found in Ref. 38 and

have been independently derived for the present work in Appendix H. The liquid tangential velocities at the corresponding nodes can thus be more accurately estimated from the definition of the stream function, the result being an accurate estimate of the mass flow along the liquid layer, which increases confidence in the numerical results of the global mass balance.

3.5.4.2 Vapor-liquid interface ($r=a$)

The liquid tangential velocity at the vapor-liquid interface is obtained from the liquid stream function field using the second-order accurate forward difference discretization for the radial derivative of the stream function and can be written as

$$v_t(\eta = 1, \theta) = -\frac{1}{\sin\theta} \left(\frac{-3\psi_{i,j} + 4\psi_{i+1,j} - \psi_{i+2,j}}{2\Delta\eta} \right)_i. \quad (3.15)$$

The local mass transfer at the vapor-liquid interface determines the local radial velocity in the liquid at this interface. The continuity of energy flux gives the condition for the liquid radial velocities as shown in Eqs. (2.40a) and (2.40b).

3.5.5 Boundary conditions on mass fractions

3.5.5.1 Liquid-SGS interface ($r=b$)

The mass fraction values at the liquid-SGS are found from the interior radial values by applying Eq. (2.45) which states that the mass fluxes are zero at this interface.

For the binary system, the discretized form of Eq. (2.45) gives

$$\omega_1(i,j) = \frac{4\omega_1(i-1,j) - \omega_1(i-2,j)}{3} \quad (3.16)$$

where i is the node in the liquid at the liquid-SGS interface, $i-1$ and $i-2$ are the two adjacent interior nodes.

For a ternary system, Eq. (2.45) gives the following two equations:

$$\left(D_{11}\omega_m \frac{\partial \omega_1}{\partial \eta} + D_{12}\omega_{2m} \frac{\partial \omega_2}{\partial \eta} + \frac{1}{\rho} D_i^T \frac{1}{T} \frac{\partial T}{\partial \eta} \right) = 0 \quad (3.17a)$$

and

$$\left(D_{21}\omega_m \frac{\partial \omega_1}{\partial \eta} + D_{22}\omega_{2m} \frac{\partial \omega_2}{\partial \eta} + \frac{1}{\rho} D_i^T \frac{1}{T} \frac{\partial T}{\partial \eta} \right) = 0. \quad (3.17b)$$

Writing the above equations in discretized form and rearranging terms gives

$$\begin{aligned} 3D_{11}\omega_m \omega_1(i,j) + 3D_{12}\omega_{2m} \omega_2(i,j) &= D_{11}\omega_m (4\omega_1(i-1,j) - \omega_1(i-2,j)) \\ &+ D_{12}\omega_{2m} (4\omega_2(i-1,j) - \omega_2(i-2,j)) \end{aligned} \quad (3.18a)$$

and

$$\begin{aligned} 3D_{21}\omega_m \omega_1(i,j) + 3D_{22}\omega_{2m} \omega_2(i,j) &= D_{21}\omega_m (4\omega_1(i-1,j) - \omega_1(i-2,j)) \\ &+ D_{22}\omega_{2m} (4\omega_2(i-1,j) - \omega_2(i-2,j)), \end{aligned} \quad (3.18b)$$

where i is the node in the liquid at the liquid-SGS interface, and $i-1$ and $i-2$ are the two adjacent interior nodes. This is a matrix equation of the form $[A][x] = [b]$ that

must be solved at each mesh point in the θ direction. These equations can also be solved by direct inversion. On a computer which vectorizes, the direct inversion method is much faster and computationally less expensive.

3.5.5.2 Vapor-liquid interface ($r=a$)

Raoult's law at the vapor-liquid interface can be written for a binary mixture, assuming the fluids to be ideal, as follows:

$$x_1 P_{s1} + x_2 P_{s2} = P_v \quad (3.19)$$

where x_1 and x_2 are the mole fractions of the components on the liquid side; P_{s1} and P_{s2} are the pure-component saturation vapor pressures; and P_v is the total vapor pressure. Noting that the mole fractions in the liquid sum to unity, Eq. (3.19) can be rewritten as

$$x_1 = \frac{P_v - P_{s2}}{P_{s1} - P_{s2}}. \quad (3.20)$$

Liquid mole fractions x_i can be written in terms of liquid mass fractions ω_i as

$$x_i = \frac{\omega_i}{M_i} \left(\sum_{j=1}^2 \frac{\omega_j}{M_j} \right)^{-1} \quad (3.21)$$

where M_1 and M_2 are the pure component molecular weights; and $\sum_{j=1}^2 \frac{\omega_j}{M_j}$ is the inverse of local molecular weight of the liquid. This gives

$$\omega_{1l}(i,j) = \frac{x_1}{\omega_{ml}} \frac{M_1}{\sum_{j=1}^2 \frac{\omega_j}{M_j}} - 1 \quad (3.22)$$

where i is the first radial node in the liquid at the vapor-liquid interface.

Once the mass fraction values on the liquid side are known, one can find the mass fraction values on the vapor side in the binary system as

$$\omega_{1v}(i,j) = \frac{\omega_{ml}}{\omega_{mv}} (\omega_{1l}(i,j) + 1) \frac{M_l P_{s1}}{M_v P_v} - 1 \quad (3.23)$$

where P_v is the specified total vapor pressure at any point on the vapor-liquid interface; P_{s1} is the saturation vapor pressure of component 1 and is known from the temperature profile specified along the vapor-liquid interface; and M_l and M_v are the mean molecular weights of the liquid and vapor mixture.

For the ternary system, Eq. (2.47) gives the following two equations:

$$\begin{aligned} & \left(\rho \omega_{1m} \alpha (\omega_1 + 1) - \rho \omega_{1m} D_{11} \frac{\partial \omega_1}{\partial \eta} - \rho \omega_{2m} D_{12} \frac{\partial \omega_2}{\partial \eta} - D_1^T T_m \frac{\partial T}{\partial \eta} \right)_l \\ & = \left(\rho \omega_{1m} \alpha (\omega_1 + 1) - \rho \omega_{1m} D_{11} \frac{\partial \omega_1}{\partial \eta} - \rho \omega_{2m} D_{12} \frac{\partial \omega_2}{\partial \eta} - D_1^T T_m \frac{\partial T}{\partial \eta} \right)_v \end{aligned} \quad (3.24a)$$

and

$$\begin{aligned} & \left(\rho \omega_{1m} \alpha (\omega_1 + 1) - \rho \omega_{1m} D_{21} \frac{\partial \omega_1}{\partial \eta} - \rho \omega_{2m} D_{22} \frac{\partial \omega_2}{\partial \eta} - D_2^T T_m \frac{\partial T}{\partial \eta} \right)_l \\ & = \left(\rho \omega_{1m} \alpha (\omega_1 + 1) - \rho \omega_{1m} D_{21} \frac{\partial \omega_1}{\partial \eta} - \rho \omega_{2m} D_{22} \frac{\partial \omega_2}{\partial \eta} - D_2^T T_m \frac{\partial T}{\partial \eta} \right)_v \end{aligned} \quad (3.24b)$$

Writing the above equations in discretized form, neglecting the thermal diffusion terms and rearranging gives

$$\begin{aligned}
& \left(\rho \omega_m \alpha u - \frac{3\rho \omega_m D_{11}}{2\Delta\eta} \right)_i \omega_u(i,j) - \left(\rho \omega_m \alpha u - \frac{3\rho \omega_m D_{11}}{2\Delta\eta} \right)_v (\text{fac2}) \omega_u(i,j) \\
& - \left(\frac{3\rho \omega_m D_{12}}{2\Delta\eta} \right)_i \omega_{2i}(i,j) + \left(\frac{3\rho \omega_m D_{12}}{2\Delta\eta} \right)_v (\text{fac4}) \omega_{2i}(i,j) \\
& = -(\rho \omega_m \alpha u)_i - \left(\frac{\rho \omega_m D_{11}}{2\Delta\eta} \right)_i (4\omega_u(i+1,j) - \omega_u(i+2,j)) \\
& \quad - \left(\frac{\rho \omega_m D_{12}}{2\Delta\eta} \right)_i (4\omega_{2i}(i+1,j) - \omega_{2i}(i+2,j)) \\
& \quad + (\rho \omega_m \alpha u)_v + \left(\frac{\rho \omega_m D_{11}}{2\Delta\eta} \right)_v (4\omega_{1v}(i-1,j) - \omega_{1v}(i-2,j)) \\
& \quad + \left(\frac{\rho \omega_m D_{12}}{2\Delta\eta} \right)_v (4\omega_{2v}(i-1,j) - \omega_{2v}(i-2,j)) \\
& \quad + \left(\rho \omega_m \alpha u - \frac{3\rho \omega_m D_{11}}{2\Delta\eta} \right)_v (\text{fac1}) - \left(\frac{3\rho \omega_m D_{12}}{2\Delta\eta} \right)_v (\text{fac3}) \quad (3.25a)
\end{aligned}$$

and

$$\begin{aligned}
& - \left(\frac{3\rho \omega_m D_{21}}{2\Delta\eta} \right)_i \omega_u(i,j) + \left(\frac{3\rho \omega_m D_{21}}{2\Delta\eta} \right)_v (\text{fac2}) \omega_u(i,j) \\
& + \left(\rho \omega_{2m} \alpha u - \frac{3\rho \omega_{2m} D_{22}}{2\Delta\eta} \right)_i \omega_{2i}(i,j) - \left(\rho \omega_{2m} \alpha u - \frac{3\rho \omega_{2m} D_{22}}{2\Delta\eta} \right)_v (\text{fac4}) \omega_{2i}(i,j) \\
& = -(\rho \omega_{2m} \alpha u)_i - \left(\frac{\rho \omega_m D_{21}}{2\Delta\eta} \right)_i (4\omega_u(i+1,j) - \omega_u(i+2,j)) \\
& \quad - \left(\frac{\rho \omega_{2m} D_{22}}{2\Delta\eta} \right)_i (4\omega_{2i}(i+1,j) - \omega_{2i}(i+2,j)) \\
& \quad + (\rho \omega_{2m} \alpha u)_v + \left(\frac{3\rho \omega_m D_{21}}{2\Delta\eta} \right)_v (4\omega_{1v}(i-1,j) - \omega_{1v}(i-2,j)) \\
& \quad + \left(\frac{\rho \omega_{2m} D_{22}}{2\Delta\eta} \right)_v (4\omega_{2v}(i-1,j) - \omega_{2v}(i-2,j)) \\
& \quad - \left(\frac{\rho \omega_m D_{21}}{2\Delta\eta} \right)_v (\text{fac1}) + \left(\rho \omega_{2m} \alpha u - \frac{3\rho \omega_{2m} D_{22}}{2\Delta\eta} \right)_v (\text{fac3}) \quad (3.25b)
\end{aligned}$$

where the following have been defined:

$$\text{fac1} = \frac{M_l P_{s1} \omega_{1m}}{M_v P_v \omega_{1mv}} - 1, \quad \text{fac2} = \frac{M_l P_{s1} \omega_{1m}}{M_v P_v \omega_{1mv}}, \quad (3.26a)$$

$$\text{fac3} = \frac{M_l P_{s2} \omega_{2m}}{M_v P_v \omega_{2mv}} - 1, \quad \text{fac4} = \frac{M_l P_{s2} \omega_{2m}}{M_v P_v \omega_{2mv}}. \quad (3.26b)$$

This is a matrix equation of the form $[A][x] = [b]$ that must be solved at each mesh point in the θ direction at the vapor-liquid interface. Again, these equations can be solved by direct inversion.

Once the mass fraction values on the liquid side are known, one can find the mass fraction values on the vapor side in the ternary system as

$$\omega_{1v}(i,j) = \frac{\omega_{1m}}{\omega_{1mv}} (\omega_{1l}(i,j) + 1) \frac{M_l P_{s1}}{M_v P_v} - 1, \quad \omega_{2v} = \frac{\omega_{2m}}{\omega_{2mv}} (\omega_{2l} + 1) \frac{M_l P_{s2}}{M_v P_v} - 1 \quad (3.27)$$

where P_v is the specified total vapor pressure at any point on the vapor-liquid interface; P_{s1} and P_{s2} are the saturation vapor pressures of components 1 and 2, respectively and are known from the temperature profile specified along the vapor-liquid interface; and M_l and M_v are the mean molecular weights of the liquid and vapor mixture.

3.5.6 Symmetry conditions

The fictitious nodes at the line of symmetry introduced by central-differencing the derivatives in the angular direction are eliminated by applying the Neuman condition on the temperature and the mass fractions, Eq. (2.49b). The

coefficients D_3 and D_4 are modified at the lines of symmetry, and the resulting equations are used to iterate for the temperature and the mass fractions at the line of symmetry.

3.6 Program Verification

The most common faults in the development of program software are programming errors. This can include both an error in programming the equations of motion or equations of state as well as errors in data table entries. Data tables, equations of motion, information equations, and the logical equations for control make up most software packages. Subtle errors in any of these can render a simulation result invalid over regions of the observables, state vectors, dependent and independent variables, and/or phase space. A simple sign reversal of the feedback in a complex multiloop system or high-order system of matrix/vector equations can lead to dynamics which are quite unlike the system being modeled.

A simple method for finding numerical errors used by Newton and many of the early numerical analysts is available for detecting errors in programs.⁵⁸ The method can be used to find errors in programming differential equations of motion, integration of differential equations, data tables, and logical equations associated with the flow of information in a system. A classical method for finding errors in data was to make a table of finite differences and look for discontinuities. This concept would be difficult to implement in a simulation as used in traditional numerical analysis, but a variation on the concept is to note that finite differences are the numerators in numerical differentiators; thus the first difference is approximately proportional to the first derivative of a function, the second difference is proportional to the second derivative, and so on. In

numerical form, the plot of a variable against its first difference is similar to a phase plane variable. For stable systems, the phase planes are bounded, thus a plot of the first difference of a variable against the variable itself is bounded for stable systems.

The method is to make phase-plane plots ("state vs. rate") for the primary parameters, state vectors or observables in a system. The phase plane plots are then carefully evaluated for zig-zag discontinuities. Phase planes of "state vs. rate" are useful for detecting large errors. In general, phase plane plots of higher-order derivatives can be made to detect smaller and smaller errors.

The observables for determination of the thermal gradient necessary to sustain a uniform liquid layer are temperature, vorticity and stream function. Phase plane plots of "state vs. rate" for these three observables have been done for analysis and detection of errors. The "state vs. rate" analysis was done for the binary H-D target with a 600- μm -diameter SGS, a 6.25- μm wall, 75 atm room-temperature fill pressure and an average temperature of 22 K. Figure 3.4 shows the phase plane plots for temperature along the liquid-SGS interface. It can be observed that there are no jump discontinuities. This gives us confidence in the solution obtained for the temperature equation. Figures 3.5 and 3.6 show "state vs. rate" plots for the vorticity along the liquid-SGS interface and stream function along the liquid-SGS interface, respectively. The smooth curves give us confidence in the solutions obtained for the vorticity and stream function equations. One of the branches in the "state vs. rate" plots is for the observables in the upper quarter of the target, while the other branch is for the observables in the lower quarter of the target.

Figure 3.4 "State vs. Rate" for temperature equation at liquid-SGS interface.

Figure 3.5 "State vs. Rate" for vorticity equation at liquid-SGS interface.

Figure 3.6 "State vs. Rate" for stream function equation at liquid-SGS interface.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Experimental Data

The cryogenic ICF target previously investigated,¹⁷ which is a thin-walled spherical microshell of a few hundred micrometers in diameter and contains the liquid fusion fuel and the vapor core, is centered between a pair of temperature plates, and the in-between space is filled with helium as the exchange gas. The temperatures of the top and bottom temperature plates can be adjusted separately, thus imposing a vertical temperature gradient on the target through the intervening helium region. The height of the gas column, which is the gap between the two temperature plates, is kept within critical Rayleigh number, which is about 4300 and is that of an equivalent cylinder, so that convection in the helium region is avoided. The configuration of the liquid layer inside the target can be visualized by Mach-Zehnder interferometry. The concentricity and the density of the interference fringes reveal whether the liquid layer is present and whether it is uniform. Details of the experimental procedures can be found in Ref. 59.

To obtain a uniform liquid layer, the temperature of the top and bottom temperature plates can be adjusted by controlling the flow of the liquid or gas helium coolant to the temperature plates. The external thermal gradient on the outside of the exchange gas is obtained as the ratio of the difference in temperature of the top and bottom temperature plates and the distance of separation.

4.2 Parameters of Targets under Study

Using the theoretical model developed in previous chapters, the linear thermal gradients that can bring about uniform liquid layers within cryogenic ICF targets can be computed. The theoretical model presented is utilized to find the far-field temperature gradients that form uniform liquid layers inside a deuterium (D_2) target, inside a hydrogen-deuterium (H-D) target and inside a deuterium-tritium (D-T) target. The D_2 target has a 200- μm diameter SGS, a 8.35 μm wall thickness and is filled with 133 atm of deuterium at room temperature. The H-D and the D-T targets have a 600- μm diameter SGS, a 6.25- μm wall thickness and are filled with 75 atm of equimolar mixture of hydrogen isotopes at room temperature. The H-D target is analyzed in two different ways. In one case the fluid inside the H-D target is assumed that the mixture remains binary, and in the other case it is assumed that the mixture is ternary when the target is cooled to cryogenic conditions. The D-T target is assumed to remain binary when the target is cooled to cryogenic conditions.

Some key issues of the behavior of the hydrogen mixtures under study and the estimation of the mole and mass fraction of the two phases are discussed next. The fill gas mixture in the H_2 - D_2 target, when cooled to cryogenic temperature, can remain binary, or because of the exchange reaction $H_2 + D_2 \rightleftharpoons 2HD$, can turn into a ternary mixture. Though the exchange reaction noted above is unlikely to take place without a catalyst, any minimum exposure to a catalyst is likely to turn the binary H-D into a ternary mixture. Since there is an uncertainty regarding the nature of the mixture inside the target, the cases of both the binary and ternary H-D mixtures formed from the same fill mixture are considered separately.

In the D-T target, the liquid-vapor mixtures are certainly ternary, due to the strong catalytic effect of the beta particle from the beta-decay of tritium which drives the exchange reaction $D_2 + T_2 \rightleftharpoons 2DT$ towards equilibrium. However, when allowing for the effect of the beta decay of the D-T mixture, the presence of the helium (He^3), which is the second product of the beta decay of tritium and whose effect is to make the D-T mixture at least quaternary has to be considered. Presuming that the ICF Target is freshly manufactured, the presence of helium in the D-T mixture can be neglected. In other situations the effect of the helium in D-T mixture should, in general, be considered. Because of the lack of research on the diffusion properties of a quaternary mixture, the presence of helium is been neglected. The vapor mole fractions of the ternary H-D and D-T mixtures at any mean target temperature are taken from Ref. 41. The values of the mole fractions and the mass fractions for the binary and ternary H-D mixtures and the binary D-T mixture can be found in tables in Appendix I.

The thickness of the liquid layer inside the D_2 , binary H-D and binary D-T targets can be found using simple thermodynamic arguments once the fill conditions are known. However, the liquid thickness inside the ternary H-D and D-T targets are somewhat ambiguous from the point of theoretical estimation. However, for the sake of simplicity it is assumed that the ICF target is filled with a equimolar binary hydrogen mixture (i.e., equimolar mixture containing H_2 and D_2 or D_2 and T_2) at certain pressure and temperature or equivalently at a certain molar density of the binary mixture, which upon cooling to cryogenic condition turns into a ternary mixture of equilibrium proportion tabulated in Ref. 41 and later condenses into liquid and vapor, preserving the molecular proportions of the individual species in the total mass. This kind of assumption is necessitated by the fact that Raoult's law at certain fill densities and cryogenic target

temperatures dictates the mean values of the mole fractions of the individual components which are quite different from the expected values of the mole fractions calculated from the kinetics of the exchange reactions discussed above. Thus there is an uncertainty regarding the mean mole fractions of the individual components if the exchange reaction is allowed to take place. Adopting the approach mentioned here we arrive at certain values of mean mole and mass fractions. Once the target size, liquid layer thickness and the mean mole and mass fractions are determined, the average properties of the liquid and the vapor phases can be determined.

The assumption that the external temperature gradients can be imposed on the outside of the helium region at about 3 to 5 times the target radius can be seen to be valid from the curves of Figures 4.1 - 4.9. The isotherms in the outer regions of the helium envelope are virtually horizontal as seen in Figures 4.1, 4.2, and 4.3 for the D_2 , H-D and D-T targets, respectively. In the outer regions of the helium envelope the vertical center-line temperature profiles as shown in Figures 4.4, 4.5 and 4.6 are nearly linear. Since the vertical center-line is taken at $\theta = 0$, the temperature can be seen to decrease in Figure 4.4 for the D_2 target, while the temperature increases for the H-D and D-T targets as seen in Figures 4.5 and 4.6. This is due to the fact that the temperature gradient across a D_2 target necessary to form a uniform liquid layer is negative while the temperature gradient across the H-D or D-T target necessary to form a uniform liquid layer is required to be positive. It should be noted that in Figures 4.4 - 4.6 the vertical axes for temperature are truncated.

In the outer regions of the helium envelope the vertical center-line energy fluxes as shown in Figures 4.7, 4.8 and 4.9 are nearly flat. When the thermal

Figure 4.1 Isotherms in helium exchange gas necessary to create a uniform liquid layer inside a D₂ target. The target has a 200- μm diameter SGS, a 8.35- μm wall, a 133 atm room-temperature fill pressure and an average temperature of 24 K. At this temperature, the liquid D₂ layer thickness is 4.28 μm .

Figure 4.2 Isotherms in helium exchange gas necessary to create a uniform liquid layer inside a binary H-D target. The target has a 600- μm diameter SGS, a 6.25- μm wall, a 75 atm room-temperature fill pressure and an average temperature of 22 K. At this temperature, the liquid H-D layer thickness is 6.85 μm .

Figure 4.3 Isotherms in helium exchange gas necessary to create a uniform liquid layer inside a binary D-T target. The target has a 600- μm diameter SGS, a 6.25- μm wall, a 75 atm room-temperature fill pressure and an average temperature of 22 K. At this temperature, the liquid D-T layer thickness is 6.93 μm .

Figure 4.4 Vertical center-line temperature profile in the 200-μm-diameter D₂ target at an average target temperature of 24 K. Temperature profile is plotted as a function of the nondimensional radial distance.

Figure 4.5 Vertical center-line temperature profile in the 600- μm -diameter binary H-D target at an average target temperature of 22 K. Temperature profile is plotted as a function of nondimensional radial distance.

Figure 4.6 Vertical center-line temperature profile in the 600- μm -diameter binary D-T target at an average target temperature of 22 K. Temperature profile is plotted as a function of nondimensional radial distance.

Figure 4.7 Vertical center-line energy flux in the 200- μm -diameter D₂ target at an average target temperature of 24 K. The energy flux is plotted as a function of nondimensional radial distance.

Figure 4.8 Vertical center-line energy flux in the 600- μm -diameter binary H-D target at an average target temperature of 22 K. The energy flux is plotted as a function of nondimensional radial distance.

Figure 4.9 Vertical center-line energy flux in the 600- μm -diameter binary D-T target at an average target temperature of 22K. The energy flux is plotted as a function of nondimensional radial distance.

gradients in the outer regions are linear, the energy flux will be constant; the near-flatness of the curves of the energy flux at the vertical center-line at large radii clearly indicates that the temperature gradients are almost linear in the outer regions of the helium envelope. Since the vertical center-line is taken at $\theta = 0$, the energy flux can be seen to be positive in Figure 4.7 for the D_2 target, while the energy flux is negative for the H-D and D-T targets as seen in Figures 4.8 and 4.9. The fact that the top of the D_2 target is cooler means that the heat flux in the radial direction at the top of the target is outward and removes the latent heat of phase transformation deposited where the vapor condenses. Since the top of the H-D and D-T targets are warmer, the heat flux in the radial direction at the top of the target is inward.

4.3 Numerical Mesh

The finite difference mesh has about 45 radial nodes in the vapor, about 13 to 17 radial nodes in the liquid, about 13 to 26 radial nodes in the shell and about 50 radial nodes in the helium region. The mesh has between 45 and 60 nodes in the angular direction. The mesh size in the angular direction is uniform; the radial mesh sizes in the vapor and helium regions are varied in geometric progression.

4.4 Parameters of Iteration

The relaxation parameters, ω_{sor} , and the convergence criterion, DEVI, for the 200- μm diameter D_2 target at an average target temperature of 24 K are shown in Table 4.1 Table 4.2 shows the relaxation parameters, ω_{sor} , and the convergence criterion, DEVI, for the 600- μm diameter binary H-D target at an

average target temperature of 22 K. Table 4.3 shows the relaxation parameters, ω_{sor} , and the convergence criterion, DEVI, for the 600- μm diameter ternary H-D target at an average target temperature of 22 K, while Table 4.4 shows the relaxation parameters, ω_{sor} , and the convergence criterion, DEVI, for the 600- μm diameter binary D-T target at an average target temperature of 22 K.

The relaxation parameters should be made as large as possible, but less than one, without causing the numerical scheme to diverge. It can be noted that the relaxation parameters for the energy equation for the helium region and for the SGS are larger than the relaxation parameters for the energy equation for the liquid and the vapor. The energy equation for the helium region and the SGS do not contain convection terms and the corresponding relaxation parameters can, in general, be larger than the relaxation parameters for the energy equation for the liquid and the vapor. It should be noted that for different target parameters, such as different target temperature, liquid layer thickness or target size, these relaxation parameters may change and are not known a priori.

		ω_{sor}	DEVI
energy equation	in helium	0.275	5(-8)
	in SGS	0.275	
	in liquid	0.125	
	in vapor	0.125	
vorticity equation	in liquid	0.675	1(-8)
	in vapor	0.775	1(-8)
stream function equation	in liquid	0.675	1(-9)
	in vapor	0.775	1(-8)

Table 4.1 Relaxation parameters and convergence criteria used for the D₂ target. The target has a 200- μm diameter SGS, a 8.35- μm wall, a 133 atm room-temperature fill pressure and an average temperature of 24 K.

		ω_{sor}	DEVI
energy equation	in helium	0.325	1(-8)
	in SGS	0.325	
	in liquid	0.250	
	in vapor	0.250	
vorticity equation	in liquid	0.425	1(-8)
	in vapor	0.425	1(-8)
stream function equation	in liquid	0.425	1(-9)
	in vapor	0.425	1(-8)
mass-diffusion-convection equation (component 1)	in liquid	0.425	1(-9)
	in vapor	0.425	1(-8)

Table 4.2 Relaxation parameters and convergence criteria used for the binary H-D target. The target has a 600- μm diameter SGS, a 6.25- μm wall, a 75 atm room-temperature fill pressure and an average temperature of 22 K.

		ω_{sor}	DEVI
energy equation	in helium	0.325	1(-8)
	in SGS	0.325	
	in liquid	0.250	
	in vapor	0.250	
vorticity equation	in liquid	0.425	1(-8)
	in vapor	0.425	1(-8)
stream function equation	in liquid	0.425	1(-9)
	in vapor	0.425	1(-8)
mass-diffusion-convection equation (component 1 and component 2)	in liquid	0.425	1(-9)
	in vapor	0.425	1(-8)

Table 4.3 Relaxation parameters and convergence criteria used for the ternary H-D target. The target has a 600- μm diameter SGS, a 6.25- μm wall, a 75 atm room-temperature fill pressure and an average temperature of 22 K.

		ω_{cor}	DEVI
energy equation	in helium	0.325	1(-8)
	in SGS	0.325	
	in liquid	0.250	
	in vapor	0.250	
vorticity equation	in liquid	0.425	1(-8)
	in vapor	0.425	1(-8)
stream function equation	in liquid	0.425	1(-9)
	in vapor	0.425	1(-8)
mass diffusion-convection equation (component 1)	in liquid	0.425	1(-9)
	in vapor	0.425	1(-8)

Table 4.4 Relaxation parameters and convergence criteria used for the binary D-T target. The target has a 600- μm diameter SGS, a 6.25- μm wall, a 75 atm room-temperature fill pressure and an average temperature of 22 K.

4.5 Results for D₂ Target

Using hydrogen data compiled by P.C. Souers,⁴¹ the vertical temperature gradient across the target that produces a uniform liquid layer was calculated. Figure 4.10 shows the experimental temperature gradient, taken from Ref. 59, across the target necessary to form a uniform liquid layer and theoretical values of the temperature gradient, predicted from Model II in Ref. 35, across the target necessary to form a uniform liquid layer. Figure 4.10 also shows the predicted values of the temperature gradient across the target from the current model. One notes that the theoretical data obtained from the present model are in concurrence with the experimental data and earlier theoretical values. The predictions of the present model are in better agreement with the experimental

Figure 4.10 Thermal gradient across the target necessary to create a uniform liquid layer in the 200- μ m diameter D₂ target. The thermal gradient is plotted as a function of average target temperature. The experimental values were taken from Ref. 59. The solid line is the theoretical prediction from Model II, Ref. 35.

data than those of the earlier model. A plot of the far-field linear temperature gradients predicted by the present model that are required for uniform liquid layers versus the average target temperature is shown in Figure 4.11. The shape of the theoretical curve for the far-field temperature gradient from the present model is similar to the experimental and theoretical curves found in Figure 4.10.

A uniform liquid layer can be created in a single-component system by making the top of the target colder than the bottom. This negative temperature gradient produces a surface-tension gradient which draws liquid upward. This upward motion of fuel is aided by liquid evaporating from the bottom and condensing at the top of the target. As it turns out, this latter effect is much more dominant than the motion of fuel induced by the surface-tension gradient. As the target becomes colder, more hydrogen condenses and the weight of the liquid increases. To counteract the increased downward fluid flows from the liquid weight gain, a larger temperature gradient is required to provide more mass transfer and a larger surface-tension gradient. This explains why the magnitude of the temperature gradient necessary for a uniform liquid layer increases as the average temperature of a D_2 target decreases from 32 K to 24 K.

The reason a smaller temperature gradient is needed when a D_2 target is cooled below 24 K, however, is less readily apparent. When a target is cooled, the increase in liquid thickness levels off. This is because the target is a closed system, and when the temperature approaches the fuel's triple point, virtually all of the fuel has already been liquefied; therefore, there is little change in liquid thickness near the triple point as shown in Figure 4.12. Also, surface tension steadily increases when temperature is being lowered, but there is a sharp

Figure 4.11 Thermal gradient outside the helium region required to form a uniform liquid layer in the 200- μ m diameter D₂ target. The thermal gradient is plotted as a function of average target temperature.

Figure 4.12 Thickness of a uniform liquid layer within a D₂ target. The thickness is plotted as a function of average target temperature.

increase in surface tension versus liquid volume when a target's liquid thickness limit is approached, which can be seen in Figure 4.13(a). A similar condition exists for liquid viscosity, shown in Figure 4.13(b). It is believed that this sudden increase in surface tension and viscosity as compared to the negligible increase in liquid thickness is responsible for the smaller temperature gradient requirement near the fuel's triple point.

The fact that the top of the D_2 target is cooler means that the heat flux in the radial direction at the top of the target is outward and removes the latent heat of phase transformation deposited where the vapor condenses. The heat of evaporation at the bottom of the target is furnished by the inward flowing radial heat flux. The magnitude of the temperature gradient at the vapor-liquid interface is small, approximately -0.162 K/cm, as shown in Figure 4.14. The temperature difference across the vapor-liquid interface is smaller than the temperature difference across the target, which is a few μm away, because of the large heats of transformation brought about by interface mass transfer. The temperature-induced surface-tension gradients are small because of the very small variation of temperature along the vapor-liquid interface. The flow field inside the D_2 target is illustrated in Figures 4.15(a), (b) and (c) which clearly show the unidirectional flow of vapor because of the small temperature-induced surface-tension gradients. It should be noted that the horizontal axis (nondimensional radius) and the vertical axis (velocity) in Figures 4.15(b) and (c) are not the same. The vertical axis (velocity) in Figure 4.15(b) is expanded to show the details of the velocity profile in the vapor. The horizontal axis (nondimensional radius) in Figure 4.15(c) is also expanded to show details of the velocity profile in the liquid.

(a)

(b)

Figure 4.13 (a) D₂ surface tension plotted against the thickness of a uniform liquid layer. (b) Viscosity of liquid D₂ plotted against the thickness of a uniform liquid layer.

Figure 4.14 Temperature across vapor-liquid interface, and across the target, necessary to create a uniform liquid layer in a 200- μm diameter D_2 target at an average target temperature of 24 K.

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(a)

Figure 4.15 (a) Flow field inside the 200- μm diameter D_2 target at an average target temperature of 24 K. (b) Velocity profile along horizontal center-line in vapor. (c) Velocity profile along horizontal center-line in liquid.

4.6 Results for Hydrogen-Deuterium Target

It has been shown³⁵ that the two major forces that are responsible for bringing about a uniform liquid layer inside an ICF target are the liquid-vapor interfacial tension gradient and the saturated vapor pressure difference. For a single-component, two-phase system, the liquid-vapor interfacial tension and the saturated vapor pressure are functions of temperature only. However, according to the phase rule,⁴³ all of the thermodynamic quantities including these two will no longer be a single function of temperature for a multicomponent, multiphase system. For instance, for a binary system having two phases, the quantities will be a function of temperature and the mixture ratio of the two components in the system.

A change in the mixture ratio in the liquid layer will have an effect on the total liquid-vapor interfacial tension. The interfacial tensions of pure hydrogen and pure deuterium are both decreasing functions of temperature. However, at a given temperature the interfacial tension of deuterium is, in general, higher than that of hydrogen. Because of the phase rule, the overall liquid-vapor interfacial tension is now a function of not only the temperature but also the mixture ratio. Hence, if the enrichment of deuterium near the bottom of the target is high enough, the total interfacial tension near the bottom will become higher even when the bottom of the target is kept warmer than the top. If this is so, the total interfacial tension gradient will point downward and work together with gravity in moving the liquid downward. The configuration of the liquid layer, therefore, depends on the competition between the mass flow rate brought by the evaporation and condensation and that brought by the interfacial tension gradient plus the gravity. If the enrichment of deuterium near the bottom is low, the total interfacial tension gradient will point upward.

When the top of the helium envelope is cooler than the bottom, the external linear thermal gradient that achieves a uniform liquid layer is denoted as negative, since temperature decreases in the assumed positive z -direction. A uniform liquid layer inside the cryogenic multicomponent target is obtained when the top of the target is kept warmer than its bottom, i.e., the external linear thermal gradient is required to be positive.

The experimental data⁵⁹ and the theoretical values of these external linear thermal gradients are shown in Figure 4.16 for the 600- μm diameter target with 6.25- μm wall thickness, filled with 75 atm of 50%-50% mixture of H_2 and D_2 at room temperature. One can note that the numerical results for the H-D target agree well with the experimental data. A preliminary analysis of the required far-field thermal gradients that will give rise to uniform liquid H-D layers inside the same ICF target with the H-D mixture treated as a ternary mixture of H_2 , D_2 , and HD is also shown in Figure 4.16. There is very little difference between the results obtained from the binary and ternary mixture treatments of the H-D liquid. It is therefore concluded that results obtained assuming a binary mixture can be reliably used, removing much of the complexity and computational expense involved with assuming a ternary mixture.

In the multicomponent system of the H-D fluid inside the ICF target, the surface-tension gradients play a vital role in forming the uniform liquid layers. The surface tension, being a thermodynamic quantity, is a function of the local temperature and concentration. The surface tension decreases with temperature but increases with the concentration of the less volatile component, namely, D_2 , in the case of a H-D mixture. The variation of surface tension because of the concentration of the less volatile component is larger in magnitude than the

Figure 4.16 Thermal gradients outside the helium region required to form uniform liquid layers in the 600- μm diameter H-D target. The thermal gradient is plotted as a function of average target temperature.

variation of surface tension with temperature for multicomponent liquid layers inside the ICF target. The imposed positive external temperature gradient induces surface-tension gradients at the vapor-liquid interface such that the sum of the temperature-induced and concentration-induced surface-tension gradients at the vapor-liquid interface are negative, i.e., the surface tension is larger at the top than at the bottom of the vapor-liquid interface. The upward increasing surface tensions draw the liquid in the direction opposite to that of gravity, resulting in a recirculatory flow in the liquid and vapor. The required surface-tension gradients are dominated by component separation, because the more volatile component, hydrogen, tends to accumulate on the cold side since its vapor pressure is higher than that of deuterium.

The angular variation of the surface-tension gradients in the binary H-D mixture is illustrated in Figure 4.17. The temperature-induced and concentration-induced surface-tension gradients and the total surface-tension gradients are plotted individually. The surface-tension gradient values are in nondimensional form, and the dimensional values in dyn/cm can be obtained by multiplying the axis values by $a / (\mu_t \alpha_t)$ with the values of the three individual constants taken in cgs units.

The flow field in the binary system of the H-D target at the mean target temperature of 22 K is shown in Figures 4.18(a), (b) and (c). The velocity profile at the mid-plane of the target is also shown at the bottom. Circular flow patterns prevail for both the vapor and liquid phases. This shows that the fluid flows are dominated by the liquid-vapor interfacial tension gradient. It should be noted that the horizontal axis (nondimensional radius) and the vertical axis (velocity) in Figures 4.18(b) and (c) are not the same. The vertical axis (velocity) in

Figure 4.17 Normalized surface tension gradients at the vapor-liquid interface of the 600- μm -diameter binary H-D target at an average target temperature of 22 K. The surface tension gradient is plotted as a function of angular position.

(a)

Figure 4.18 (a) Flow field inside the 600- μm diameter binary H-D target at an average target temperature of 22 K. (b) Velocity profile along horizontal center-line in vapor. (c) Velocity profile along horizontal center-line in liquid.

Figure 4.18(b) is expanded to show the details of the velocity profile in the vapor. The horizontal axis (nondimensional radius) in Figure 4.18(c) is also expanded to show details of the velocity profile in the liquid.

The mass fraction variation of H_2 is illustrated in Figure 4.19. This plot shows that the liquid layer near the top of the target is enriched with deuterium and thus the direction of the overall interfacial tension gradient points upward and acts against gravity to bring about a uniform liquid layer. One notes that the deviation of the liquid and vapor mass fractions from the mean values is small.

4.7 Results for Deuterium-Tritium Target

Within the limitations posed by the uncertainties in the thermophysical properties of the hydrogen isotopes and by the neglect of the effect of beta-decay of tritium, an analysis of the required far-field thermal gradient that will give rise to uniform liquid D-T layers inside a spherical shell ICF target has been carried out with the D-T mixture treated as a binary mixture of D_2 and T_2 , and the results are shown in Figure 4.20 for a 600- μm diameter target with 6.25- μm wall thickness, filled with 75 atm of 50%-50% mixture of D_2 and T_2 at room temperature. These results indicate that the thermal gradients needed to support uniform liquid D-T layers inside a spherical ICF target are comparable to those for H-D layers. A preliminary analysis indicates that the effect of beta-decay heating of tritium will be a minor effect for targets containing liquid fuel layers thinner than 500 μm ; however, detailed theoretical analysis and experimental data will be needed for conclusive verification.

Figure 4.19 Mass fraction contours of H_2 in the-600- μm diameter binary H-D target at an average target temperature of 22 K.

Figure 4.20 Thermal gradients outside the helium region required to form uniform liquid layers in the 600- μm diameter binary D-T target. The thermal gradient is plotted as a function of average target temperature.

CHAPTER 5

SUMMARY AND CONCLUDING REMARKS

A numerical model has been developed to describe the thermally induced behavior of a liquid layer of hydrogen isotopes inside a spherical Inertial Confinement Fusion (ICF) target and to calculate the far-field temperature gradient which will sustain a uniform liquid layer. This method is much faster than the trial-and-error method previously employed.³⁸ The effects of the surface-tension gradients and the interfacial mass transfer in the formation of the uniform liquid layers of pure-component and multicomponent fuel mixtures have been studied. The present work is summarized and concluded as follows.

- (1) Using the theoretical model, the values of the externally applied thermal gradients that give rise to uniform liquid layers of hydrogen inside a cryogenic spherical-shell ICF target are calculated, and the results compared with the existing experimental data. The results from this model are in good agreement with the experimentally measured far-field temperature gradients for the formation of uniform layers inside targets filled, respectively, with pure-component D_2 and with a H-D mixture. Calculations have also been done for targets filled with a D-T mixture.
- (2) Behavior of liquid hydrogen isotopes inside a spherical-shell target has been analyzed. The behavior of a single-component liquid hydrogen (D_2) inside an ICF target, when subjected to a temperature gradient, is different from that of a multicomponent liquid hydrogen (H-D or D-T) due to the effects of component separation.
- (3a) A uniform liquid layer can be created in a single-component system by making the top of the target colder than the bottom. This negative

temperature gradient produces a surface-tension gradient which draws liquid upward. This upward motion of fuel is aided by liquid evaporating from the bottom and condensing at the top of the target. As it turns out, this latter effect is much more dominant than the motion of fuel induced by the surface-tension gradient.

- (3b) In the multicomponent system of the H-D fluid inside the ICF target, the surface-tension gradients play a vital role in forming the uniform liquid layers. A uniform liquid layer inside the cryogenic multicomponent target is obtained when the top of the target is kept warmer than its bottom, i.e., the external linear thermal gradient is required to be positive.
- (4) The method of flow field generation using the vorticity derivatives in the liquid region has been successful since the gravity and pressure terms are the dominant factors that generate the vorticity field and also since the convection terms in the vorticity derivative of the liquid are small.

There are two major disadvantages associated with the present code. They can be summarized as follows:

- (1) Calculation of the pure-component ICF target requires eight (8) separate relaxation parameters; four for the temperature equations in the four regions; two for the vorticity equations in the liquid and vapor regions; and two for the stream function equations in the liquid and vapor regions. Calculation of the multicomponent ICF target requires ten (10) relaxation parameters for the binary mixture and twelve (12) for the ternary mixture; the additional relaxation parameters arise from the calculation of the mass diffusion-convection equations in the liquid and vapor regions. The optimum values for the different relaxation parameters are not known a

priori. Since the governing equations are coupled and nonlinear, changing one relaxation parameter affects the convergence of other equations.

- (2) The thermal gradients that give rise to uniform liquid layers thicker than 20 μm are difficult to compute because of the cosine approximations made in the selection of the trial set of parameters at the vapor-liquid interface which are valid only for small Reynolds number flows. Above a liquid layer thickness of 20 μm , the necessary liquid and vapor momentum fields exhibit high Reynolds numbers and higher-order variations in the field variables so that the simple cosine approximations to the trial set of parameters at the vapor-liquid interface will no longer be sufficient.

Some areas of research which deserve further investigation have been disclosed throughout this thesis , namely:

- (1) The origin of the instabilities for conservative energy equation.
- (2) The use of higher-order upwind methods,⁶⁰ which produce lower-order truncation errors and stable solutions.

APPENDIX A

DERIVATION OF ENERGY EQUATION

The derivation of the energy equation can be found in Ref. 38 and is included here for ease of reference.

The steady-state energy equation can be derived as the divergence of the energy flux equated to zero. The energy flux $\tilde{e}$ is defined as

$$\tilde{e} = -k\nabla T + \sum_{i=1}^3 \tilde{n}_i h_i. \quad (A.1)$$

By substituting the definition of mass flux $\tilde{n}_i$, for the ternary system, the energy flux can be written as

$$\tilde{e} = -k\nabla T + \sum_{i=1}^3 h_i \left(\omega_i \rho \tilde{v} - \rho \sum_{k=1}^2 D_{ik} \nabla \omega_k - D_i^T \nabla \ln T \right). \quad (A.2)$$

As the divergence of the energy flux is zero in steady state, using Eq. (A.1) one can show that

$$\nabla \cdot \tilde{e} = 0 = -k\nabla^2 T + \sum_{i=1}^3 h_i (\nabla \cdot n_i) + \sum_{i=1}^3 n_i \cdot \nabla h_i. \quad (A.3)$$

The second term in the above equation can be eliminated because the divergence of mass flux is also zero in steady state. Then, with the help of the definition of mass flux and noting that

$$\nabla h_i = c_{pi} \nabla T, \quad (A.4)$$

it can be shown that the divergence of the energy flux equated to zero reduces to

$$0 = -k\nabla^2 T + \left(\sum_{i=1}^3 (\omega_i c_{pi}) \right) \rho \tilde{v} \cdot \nabla T - \rho \sum_{i=1}^3 c_{pi} \sum_{k=1}^2 D_{ik} \nabla \omega_k \cdot \nabla T - \sum_{i=1}^3 c_{pi} D_i^T (\nabla \ln T) \cdot \nabla T. \quad (A.5)$$

Then, by defining the average specific heat as the mass-fraction-weighted average of the component specific heats, it can be shown that the energy equation for the ternary system is

$$\rho \bar{c}_p \tilde{v} \cdot \nabla T = k \nabla^2 T + \rho \sum_{i=1}^3 \sum_{k=1}^2 D_{ik} c_{pi} \nabla \omega_k \cdot \nabla T + \left(\sum_{i=1}^3 c_{pi} D_i^T \right) \frac{1}{T} \nabla T \cdot \nabla T. \quad (A.6)$$

The energy equation for the binary and the unary systems can be obtained as special cases of the above equation.

APPENDIX B

DERIVATION OF MASS DIFFUSION-CONVECTION EQUATION

The derivation of the mass diffusion-convection equation can be found in Ref. 38 and is included here for ease of reference.

The steady-state mass diffusion-convection equation can be shown to be the divergence of the mass flux set to zero. By assuming the Onsager form for the diffusion flux, the mass flux in a ternary system can be written as

$$\vec{n}_i = \omega_i \rho \vec{v} - \rho \sum_{k=1}^2 D_{ik} \nabla \omega_k - D_i^T \nabla \ln T \quad (\text{B.1})$$

where the first term is the convection flux, the second term is the diffusion flux, and the third term is the flux due to thermal diffusion.

In steady state

$$\nabla \cdot \vec{n}_i = 0. \quad (\text{B.2})$$

By taking the divergence of the mass flux Eq. (B.1) one can show that

$$\nabla \cdot (\omega_i \rho \vec{v}) = \rho \sum_{k=1}^2 \nabla \cdot (D_{ik} \nabla \omega_k) + \nabla \cdot (D_i^T \nabla \ln T). \quad (\text{B.3})$$

By using the equation of continuity and the assumption of incompressibility one can simplify the convection terms and show that

$$\rho \vec{v} \cdot \nabla \omega_i = \rho \sum_{k=1}^2 D_{ik} \nabla^2 \omega_k + D_i^T \nabla \cdot \left(\frac{1}{T} \nabla T \right). \quad (\text{B.4})$$

Then it follows that

$$\rho \vec{v} \cdot \nabla \omega_i = \rho \sum_{k=1}^2 D_{ik} \nabla^2 \omega_k + D_i^T \left(\frac{1}{T} \nabla^2 T - \frac{1}{T^2} \nabla T \cdot \nabla T \right). \quad (\text{B.5})$$

This equation of the ternary system reduces to the corresponding equation of the binary system if one considers only one equation and drops the first Laplacian term from the right-hand side.

APPENDIX C

DERIVATION OF THE VORTICITY EQUATION

The Navier-Stokes equation for a fluid of constant density and viscosity is

$$(\vec{v} \cdot \nabla) \vec{v} = -\nabla \frac{P}{\rho} + \nu \nabla^2 \vec{v} + \vec{g}. \quad (C.1)$$

Replacing the nonlinear term by its equivalent form given by the vector identities, this vector equation becomes

$$\nabla \left(\frac{1}{2} \vec{v} \cdot \vec{v} \right) - \vec{v} \times (\nabla \times \vec{v}) = -\nabla \frac{P}{\rho} + \nu \nabla^2 \vec{v} + \vec{g}. \quad (C.2)$$

The vorticity equation is obtained by taking the curl of the above equation and noting that the curl of the gradient of any scalar is zero. Hence

$$\nabla \times (\vec{v} \times \vec{\zeta}) = \nu \nabla^2 \vec{\zeta}. \quad (C.3)$$

Using vector identities, the left-hand side may be expanded to give

$$\nabla \times (\vec{v} \times \vec{\zeta}) = \vec{v} (\vec{\nabla} \cdot \vec{\zeta}) - (\vec{v} \cdot \nabla) \vec{\zeta} + (\vec{\zeta} \cdot \nabla) \vec{v}. \quad (C.4)$$

However, $\vec{\nabla} \cdot \vec{\zeta} = 0$, since the divergence of the curl of any vector is zero and $\vec{\nabla} \cdot \vec{v} = 0$ from the continuity equation. Therefore, the vorticity transport equation becomes

$$(\vec{v} \cdot \nabla) \vec{\zeta} = (\vec{\zeta} \cdot \nabla) \vec{v} + \nu \nabla^2 \vec{\zeta}. \quad (C.5)$$

The LHS of Eq. (C.5) can be expanded to give

$$(\vec{v} \cdot \nabla) \vec{\zeta} = \left[(u \hat{e}_r + v \hat{e}_\theta) \cdot \left(\frac{\partial}{\partial r} \hat{e}_r + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{e}_\theta \right) \right] [\zeta \hat{e}_\phi]. \quad (\text{C.6})$$

Carrying out the indicated operations yields

$$(\vec{v} \cdot \nabla) \vec{\zeta} = \left(u \frac{\partial \zeta}{\partial r} + v \frac{1}{r} \frac{\partial \zeta}{\partial \theta} \right) \hat{e}_\phi, \quad (\text{C.7})$$

or

$$(\vec{v} \cdot \nabla) \vec{\zeta} = \left[\frac{\partial(u\zeta)}{\partial r} + \frac{1}{r} \frac{\partial(v\zeta)}{\partial \theta} - \zeta \left(\frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} \right) \right] \hat{e}_\phi. \quad (\text{C.8})$$

The first term on the RHS of Eq. (C.5) can be expanded to give

$$(\vec{\zeta} \cdot \nabla) \vec{v} = \left[(\zeta \hat{e}_\phi) \cdot \left(\frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \hat{e}_\phi \right) \right] [u \hat{e}_r + v \hat{e}_\theta]. \quad (\text{C.9})$$

Again, carrying out the indicated operations gives

$$(\vec{\zeta} \cdot \nabla) \vec{v} = \frac{u \zeta}{r \sin \theta} \frac{\partial \hat{e}_r}{\partial \phi} + \frac{v \zeta}{r \sin \theta} \frac{\partial \hat{e}_\theta}{\partial \phi} \quad (\text{C.10})$$

or

$$(\vec{\zeta} \cdot \nabla) \vec{v} = \frac{\zeta}{r} \left(u + \frac{v}{\tan \theta} \right) \hat{e}_\phi. \quad (\text{C.11})$$

From the continuity equation,

$$\frac{1}{r^2} \frac{\partial(r^2 u)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(\sin \theta v)}{\partial \theta} = 0, \quad (\text{C.12})$$

which can be rewritten as

$$\frac{u}{r} + \frac{v}{r \tan \theta} = - \left(\frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right). \quad (\text{C.13})$$

Combining Eqs. (C.11) and (C.13) gives

$$(\vec{\zeta} \cdot \nabla) \vec{v} = -\zeta \left(\frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right) \hat{e}_\phi. \quad (\text{C.14})$$

The second term on the RHS of Eq. (C.5) can be expanded as

$$v \nabla^2 \vec{\zeta} = \frac{v}{r} \left[\frac{\partial}{\partial \theta} \left(\frac{1}{r^2 \sin \theta} \left(\frac{\partial(r \sin \theta \zeta)}{\partial \theta} \right) \right) + \frac{\partial}{\partial r} \left(\frac{1}{\sin \theta} \left(\frac{\partial(r \sin \theta \zeta)}{\partial r} \right) \right) \right] \hat{e}_\phi, \quad (\text{C.15})$$

or

$$v \nabla^2 \vec{\zeta} = v \left(\frac{\partial^2 \zeta}{\partial r^2} + \frac{2}{r} \frac{\partial \zeta}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \zeta}{\partial \theta^2} + \frac{1}{r^2 \tan \theta} \frac{\partial \zeta}{\partial \theta} - \frac{\zeta}{r^2 \sin^2 \theta} \right) \hat{e}_\phi. \quad (\text{C.16})$$

Combining Eqs. (C.8), (C.14) and (C.16) gives

$$\begin{aligned} \left[\frac{\partial u \zeta}{\partial r} + \frac{1}{r} \frac{\partial v \zeta}{\partial \theta} - \zeta \left(\frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} \right) \right] \hat{e}_\phi &= -\zeta \left(\frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{u}{r} \right) \hat{e}_\phi \\ &+ v \left(\frac{\partial^2 \zeta}{\partial r^2} + \frac{2}{r} \frac{\partial \zeta}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \zeta}{\partial \theta^2} + \frac{1}{r^2 \tan \theta} \frac{\partial \zeta}{\partial \theta} - \frac{\zeta}{r^2 \sin^2 \theta} \right) \hat{e}_\phi. \end{aligned} \quad (\text{C.17})$$

The vorticity equation can then be written as

$$\frac{\partial(u\zeta)}{\partial r} + \frac{1}{r} \frac{\partial(v\zeta)}{\partial \theta} = \nu \left(\frac{\partial^2 \zeta}{\partial r^2} + \frac{2}{r} \frac{\partial \zeta}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \zeta}{\partial \theta^2} + \frac{1}{r^2 \tan \theta} \frac{\partial \zeta}{\partial \theta} - \frac{\zeta}{r^2 \sin^2 \theta} \right) - \frac{u\zeta}{r}. \quad (\text{C.18})$$

By using the modified vorticity, defined as $\Omega = r\zeta$, this becomes

$$\frac{\partial(u\Omega)}{\partial r} + \frac{1}{r} \frac{\partial(v\Omega)}{\partial \theta} = \nu \left(\frac{\partial^2 \Omega}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 \Omega}{\partial \theta^2} + \frac{1}{r^2 \tan \theta} \frac{\partial \Omega}{\partial \theta} - \frac{\Omega}{r^2 \sin^2 \theta} \right). \quad (\text{C.19})$$

APPENDIX D

DERIVATION OF RADIAL DERIVATIVE CONDITION ON VORTICITY

The radial derivative of the vorticity incorporates the effect of body and pressure forces in the flow field. This relationship is derived from the angular momentum equation.

In the spherical coordinate system the momentum equation in the angular direction is given, considering that the flow field has azimuthal symmetry, as

$$u \frac{\partial v}{\partial r} + \frac{v}{r} \frac{\partial v}{\partial \theta} + \frac{uv}{r} = -\frac{1}{\rho r} \frac{\partial P}{\partial \theta} + g_\theta + v \left(\nabla^2 v + \frac{2}{r^2} \frac{\partial u}{\partial \theta} - \frac{v}{r^2 \sin^2 \theta} \right). \quad (D.1)$$

The modified definition of vorticity can be written as

$$\Omega = r \left(\frac{\partial v}{\partial r} - \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{v}{r} \right). \quad (D.2)$$

Differentiation of the above definition of vorticity gives

$$\frac{1}{r} \frac{\partial \Omega}{\partial r} = \left(\frac{\partial^2 v}{\partial r^2} + \frac{2}{r} \frac{\partial v}{\partial r} - \frac{1}{r} \frac{\partial^2 u}{\partial r \partial \theta} \right). \quad (D.3)$$

The third term on the RHS of Eq. (D.1) can be eliminated by taking the angular derivative of the continuity equation

$$\frac{1}{r} \frac{\partial (\nabla \cdot \vec{v})}{\partial \theta} = 0. \quad (D.4)$$

This gives

$$-\frac{1}{r} \frac{\partial^2 u}{\partial \theta \partial r} = \frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 v}{\partial \theta^2} + \frac{1}{r^2 \tan \theta} \frac{\partial v}{\partial \theta} - \frac{v}{r^2 \sin^2 \theta}. \quad (D.5)$$

Combining Eqs. (D.3) and Eq. (D.5) gives

$$\frac{1}{r} \frac{\partial \Omega}{\partial r} = \left(\frac{\partial^2 v}{\partial r^2} + \frac{2}{r} \frac{\partial v}{\partial r} + \frac{1}{r^2} \frac{\partial^2 v}{\partial \theta^2} + \frac{1}{r^2 \tan \theta} \frac{\partial v}{\partial \theta} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} - \frac{v}{r^2 \sin^2 \theta} \right). \quad (D.6)$$

Noting that

$$\nabla^2 v = \frac{\partial^2 v}{\partial r^2} + \frac{2}{r} \frac{\partial v}{\partial r} + \frac{1}{r^2} \frac{\partial^2 v}{\partial \theta^2} + \frac{1}{r^2 \tan \theta} \frac{\partial v}{\partial \theta}. \quad (D.7)$$

we can combine Eqs. (D.6) and Eq. (D.7) to give

$$u \frac{\partial v}{\partial r} + \frac{v}{r} \frac{\partial v}{\partial \theta} + \frac{uv}{r} = -\frac{1}{\rho r} \frac{\partial P}{\partial \theta} + g_\theta + v \left(\frac{1}{r} \frac{\partial \Omega}{\partial r} \right). \quad (D.8)$$

Rearranging terms yields

$$\frac{\partial \Omega}{\partial r} = \frac{1}{\mu} \frac{\partial P}{\partial \theta} - \frac{\rho r g_\theta}{\mu} + \frac{\rho r}{\mu} \left(u \frac{\partial v}{\partial r} + \frac{v}{r} \frac{\partial v}{\partial \theta} + \frac{uv}{r} \right). \quad (D.9)$$

In nondimensional form this becomes

$$\frac{\partial \Omega}{\partial \eta} = \frac{a^2}{\mu \alpha} \frac{\partial P}{\partial \theta} - \frac{\rho a^3 \eta g_\theta}{\mu \alpha} + \frac{\alpha}{\mu} \rho \eta \left(u \frac{\partial v}{\partial \eta} + \frac{v}{\eta} \frac{\partial v}{\partial \theta} + \frac{uv}{\eta} \right). \quad (D.10)$$

APPENDIX E

FINITE DIFFERENCE APPROXIMATION OF DERIVATIVES

The first step in obtaining a numerical solution by a digital computer is the transformation of the partial differential equation into a form such that the differentiation can be performed by numerical calculations. The derivative of a function at a given point can be represented by finite-difference approximation using a Taylor series expansion of the function about that point. Let $f(x)$ be a function that can be expanded in a Taylor series. Then, a Taylor series expansion of the functions $f(x+\Delta x)$ and $f(x-\Delta x)$ about x as illustrated in Fig. E.1 is given as

$$f(x + \Delta x) = f(x) + (\Delta x)f'(x) + \frac{(\Delta x)^2}{2!}f''(x) + \frac{(\Delta x)^3}{3!}f'''(x) + \dots \quad (E.1)$$

$$f(x - \Delta x) = f(x) - (\Delta x)f'(x) + \frac{(\Delta x)^2}{2!}f''(x) - \frac{(\Delta x)^3}{3!}f'''(x) + \dots \quad (E.2)$$

where primes denote derivatives with respect to x .

To obtain expressions for the finite-difference form of the first-order derivative $f'(x)$, Eqs. (E.1) and (E.2) are solved for $f'(x)$ as

$$f'(x) = \frac{f(x + \Delta x) - f(x)}{(\Delta x)} - \frac{(\Delta x)}{2}f''(x) - \frac{(\Delta x)^2}{6}f'''(x) \dots \quad (E.3)$$

$$f'(x) = \frac{f(x) - f(x - \Delta x)}{(\Delta x)} + \frac{(\Delta x)}{2}f''(x) - \frac{(\Delta x)^2}{6}f'''(x) \dots \quad (E.4)$$

Figure E.1 Nomenclature for a Taylor series representation.

Adding Eqs. (E.3) and (E.4) gives

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2(\Delta x)} - \frac{(\Delta x)^2}{6} f'''(x) \dots \quad (\text{E.5})$$

From Eqs. (E.3) to (E.4) the following approximations can be written, respectively, for the first derivative of a function $f(x)$ about the point x .

$$f'(x) = \frac{f(x + \Delta x) - f(x)}{(\Delta x)} + O(\Delta x) \quad \text{forward difference} \quad (\text{E.6})$$

$$f'(x) = \frac{f(x) - f(x - \Delta x)}{(\Delta x)} + O(\Delta x) \quad \text{backward difference} \quad (\text{E.7})$$

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2(\Delta x)} + O[(\Delta x)^2] \quad \text{central difference} \quad (\text{E.8})$$

Here the notation $O(\Delta x)$ is used to show that the error involved is of the order of Δx , or first-order accurate: similarly $O[(\Delta x)^2]$ is for the error of the order of $(\Delta x)^2$, or second-order accurate.

Finite-difference representations of the second-order derivative $f''(x)$ about the point x can be shown to be

$$f''(x) = \frac{f(x) - 2f(x + \Delta x) + f(x + 2\Delta x)}{(\Delta x)^2} + O(\Delta x) \quad \text{forward difference} \quad (\text{E.9})$$

$$f''(x) = \frac{f(x - 2\Delta x) - 2f(x - \Delta x) + f(x)}{(\Delta x)^2} + O(\Delta x) \quad \text{backward difference} \quad (\text{E.10})$$

$$f''(x) = \frac{f(x - \Delta x) - 2f(x) + f(x + \Delta x)}{(\Delta x)^2} + O[(\Delta x)^2] \quad \text{central difference} \quad (\text{E.11})$$

The central-difference representation is second-order accurate whereas the forward and backward differences are first-order accurate.

APPENDIX F

DERIVATION OF FIRST DERIVATIVE AND SECOND DERIVATIVE FOR UNEQUAL MESH SPACING

The numerical solution of differential equations consists essentially in obtaining the numerical values of the unknown at some nodal points, spaced along the axis for ordinary differential equations, and the plane for two-dimensional partial differential equations. To obtain the nodal values of the unknown, Q , the derivatives of Q appearing in the differential equation are approximated by a Taylor expansion. For equal mesh spacing, these expansions can be found in any numerical methods book. For the unequal spacing used, the numerical formula for both the first derivative and the second derivative will be derived.

The Taylor series of $y(x+\Delta x)$ about x is given by

$$\begin{aligned} y(x + \Delta x) &= y(x) + (\Delta x)y'(x) + \frac{(\Delta x)^2}{2!}y''(x) + \frac{(\Delta x)^3}{3!}y'''(x) + \dots \\ &= \sum_{n=0}^{\infty} \frac{(\Delta x)^n}{n!}y^n(x) \end{aligned} \quad (F.1)$$

where $y^n(x)$ stands for $\frac{d^n y}{dx^n}$, $y^0(x) = y(x)$, and $0! = 1$.

Applying Eq. (F.1) with the symbols of Figure F.1, the Taylor series expansion at $Q(i + \Delta r)$ and at $Q(i - \Delta \ell)$ is

$$Q_r = Q_i + (\Delta r)Q'_i + \frac{(\Delta r)^2}{2!}Q''_i + \frac{(\Delta r)^3}{3!}Q'''_i + \dots \quad (F.2)$$

and

$$Q_r = Q_i - (\Delta \ell) Q'_i + \frac{(\Delta \ell)^2}{2!} Q''_i - \frac{(\Delta \ell)^3}{3!} Q'''_i + \dots \quad (F.3)$$

Figure F.1 Unequal spacing of mesh points.

Multiplying Eq. (F.2) by $(\Delta \ell)^2$ and Eq. (F.3) by $(\Delta r)^2$ and subtracting the two equations gives

$$(\Delta \ell)^2 Q_r - (\Delta r)^2 Q_l = \{(\Delta \ell)^2 - (\Delta r)^2\} Q_i + \{(\Delta \ell)^2 (\Delta r) + (\Delta r)^2 (\Delta \ell)\} Q'_i + \dots \quad (F.4)$$

Letting $\beta = \frac{\Delta r}{\Delta \ell}$ and rearranging terms gives, for the first derivative

$$Q'_i = \frac{Q_r - (1 - \beta^2) Q_i - \beta^2 Q_l}{(1 + \beta) \Delta r} \quad (F.5)$$

Multiplying Eq. (F.2) by $(\Delta \ell)$ and Eq. (F.3) by (Δr) and adding the two equations gives

$$(\Delta \ell)Q_r + (\Delta r)Q_\ell = \{(\Delta \ell) + (\Delta r)\}Q_i + \left\{ \frac{(\Delta \ell)(\Delta r)^2 + (\Delta r)(\Delta \ell)^2}{2} \right\}Q_i'' + \dots \quad (\text{F.6})$$

Again, letting $\beta = \frac{\Delta r}{\Delta \ell}$ and rearranging terms gives, for the second derivative

$$Q_i'' = \frac{2\beta\{Q_r - (1+\beta)Q_i + \beta Q_\ell\}}{(1+\beta)(\Delta r)^2}. \quad (\text{F.7})$$

If the nodal points are equally spaced, $\beta = 1$, then these formulae reduce to the usual central-difference scheme.

APPENDIX G

GENERAL FORM OF A CONSERVATION LAW

The laws of fluid dynamics are well established and can be formulated in many equivalent ways. For instance, they can be deduced from the observation that the behavior of a physical system is completely determined by conservation laws. This corresponds to the statement that during the evolution of a fluid a certain number of properties, such as mass, generalized momentum and energy, are "conserved." Not only are the basic properties of mass, momentum and energy conserved during the whole process at all times but these three conditions completely determine the behavior of the system. The only additional information concerns the specification of the nature of the fluid (for example, incompressible fluid, perfect gas, viscous fluid, etc.).

The concept of conservation, as mentioned above, means that the variation of a conserved (intensive) flow quantity within a given volume is due to the net effect of some internal sources and of the amount of the quantity which is crossing the boundary surface. This amount is called the flux, and its expression results from the mechanical and thermodynamical properties of the fluid. The sources attached to a given flow quantity are assumed to be known from basic studies. The fluxes and sources are, in general, dependent on the space-time co-ordinates as well as on the fluid motion.

The fluxes are generated from two contributions: one due to the convective transport of the fluid and another due to the molecular motion, which is always present even when the fluid is at rest. The effect of the molecular motion expresses the tendency of a fluid towards equilibrium and uniformity, since differences in the intensity of the quantity being considered create a

transfer in space so as to reduce the nonhomogeneity. This contribution to the total flux is proportional to the gradient of the corresponding quantity, since it has to vanish for a homogeneous distribution and therefore acts as a diffusive effect.

Let us consider a scalar quantity per unit volume U , acting in an arbitrary volume Ω , fixed in space, bounded by a closed surface S . The local intensity of U varies through the effect of fluxes, which express the contributions from the surrounding points to the local value and through sources Q . The flux vector $\vec{F}$ contains two components, a diffusive contribution $\vec{F}_D$ and a convective part $\vec{F}_C$. The general form of a conservation law is expressed in stating that the variation per unit time of the quantity U within the volume Ω ;

$$\frac{\partial}{\partial t} \int_{\Omega} U d\Omega \quad (G.1)$$

should be equal to the net contribution from the incoming fluxes through the surface S , with the surface element vector $d\vec{S}$ pointing outward

$$-\oint_S \vec{F} \cdot d\vec{S} \quad (G.2)$$

plus contributions from the sources of the quantity U .

These sources can be divided into volume and surface sources, Q_v and $\vec{Q}_s$, and the total contribution is

$$\int_{\Omega} Q_v d\Omega + \oint_S \vec{Q}_s \cdot d\vec{S} \quad (G.3)$$

Hence the general form of the conservation equation for the quantity U is

$$\frac{\partial}{\partial t} \int_{\Omega} U d\Omega + \oint_S \vec{F} \cdot d\vec{S} = \int_{\Omega} Q_v d\Omega + \oint_S \vec{Q}_s \cdot d\vec{S} \quad (G.4)$$

or, with Gauss's theorem, for continuous fluxes and surface sources:

$$\int_{\Omega} \frac{\partial U}{\partial t} d\Omega + \int_{\Omega} \vec{\nabla} \cdot \vec{F} d\Omega = \int_{\Omega} Q_v d\Omega + \int_{\Omega} \vec{\nabla} \cdot \vec{Q}_s d\Omega. \quad (G.5)$$

This last form leads to the differential form of the conservation law, since Eq. (G.5) is written for an arbitrary volume Ω :

$$\frac{\partial U}{\partial t} + \vec{\nabla} \cdot \vec{F} = Q_v + \vec{\nabla} \cdot \vec{Q}_s \quad (G.6)$$

An essential aspect of the conservation law lies in the observation that the internal variations of U , in the absence of volume sources, depend only on the flux contribution through the surface S and not the flux values inside the volume Ω . Separating the flux vector into its two components $\vec{F}_c$ and $\vec{F}_D$, a more precise form of the equation can be obtained. The convective part of the flux vector $\vec{F}_c$, attached to the quantity U in a flow of velocity $\vec{v}$, is the amount of U transported with the motion, and is given by

$$\vec{F}_c = \vec{v}U. \quad (G.7)$$

The diffusive flux is defined as the contribution present in fluids at rest, due to the molecular, thermal agitation. It can be expressed by the generalized, gradient law of Fick:

$$\vec{F}_D = -\kappa \rho \vec{\nabla} u \quad (\text{G.8})$$

where u is the quantity U per unit mass, i.e. $U = \rho u$, ρ is the specific mass of the fluid and κ a diffusivity constant. Eq (G6) then becomes

$$\frac{\partial(\rho u)}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v} u) = \vec{\nabla} \cdot (\kappa \rho \vec{\nabla} u) + Q_v + \vec{\nabla} \cdot \vec{Q}_s \quad (\text{G.9})$$

This equation is the general form of a transport equation for the quantity $U = \rho u$ and is in conservative form. Observe that the diffusivity constant κ has units of m^2/s for any quantity U .

The law of mass conservation is a general statement of kinematic nature, that is, independent of the nature of the fluid or of the forces acting on it. It expresses the empirical fact that, in a fluid system, mass cannot disappear from the system nor be created. The quantity U is, in this case, the specific mass. No diffusive flux exists for the mass transport, which means that mass can be transported only through convection. Chemical reactions will not be considered, hence no sources will have to be introduced. The general conservation equation then becomes

$$\frac{\partial}{\partial t} \int_{\Omega} \rho d\Omega + \oint_{\Sigma} \rho \vec{v} \cdot d\vec{S} = 0 \quad (\text{G.10})$$

and in differential form

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0. \quad (\text{G.11})$$

The differential form of the general conservation equation can be written in another way. If Eq. (G.11) multiplied by u is subtracted from the left-hand side of Eq. (G.7) we obtain

$$\rho \frac{\partial u}{\partial t} + \rho \vec{v} \cdot \vec{\nabla} u = \vec{\nabla} \cdot (\kappa \rho \vec{\nabla} u) + Q_v + \vec{\nabla} \cdot \vec{Q}_s. \quad (G.12)$$

The difference between Eq. (G.7) and Eq. (G.12) lies in the conservative form of the equations. Equation (G.12) is not in conservation form and a straightforward discretization will generally not conserve the property u in the numerical simulation. It is important to note that this conservation property is linked to the convective term.

APPENDIX H

DERIVATION OF VELOCITIES FROM A CUBIC FIT ON STREAM FUNCTION

The derivation of the velocities from a cubic fit on the stream function can be found in Ref. 38 and is included here for ease of reference.

In the following the expressions for the first and second derivatives of a cubic polynomial fit on a function on four equally spaced points are derived. The results are utilized in calculating the required velocities and vorticities from the stream function field near the liquid-SGS interface.

A third-order polynomial expansion of the generic variable Q can be written as

$$Q = a_1\eta^3 + a_2\eta^2 + a_3\eta + a_4. \quad (H.1)$$

where η is taken to be the radial position. To determine the four constants we need the values of the function at four points. If the radial position at the liquid-SGS interface is designated as i and $\Delta\eta$ as the radial distance between any two adjacent nodes in the liquid, the following equations can be obtained by substituting the relative radial positions and the corresponding function values:

$$Q_i = a_1\Delta\eta^3 + a_2\Delta\eta^2 + a_3\Delta\eta + a_4, \quad (H.2)$$

$$Q_{i-1} = a_4, \quad (H.3)$$

$$Q_{i-2} = -a_1\Delta\eta^3 + a_2\Delta\eta^2 - a_3\Delta\eta + a_4 \quad (H.4)$$

and

$$Q_{i-3} = -8a_1\Delta\eta^3 + 4a_2\Delta\eta^2 - 2a_3\Delta\eta + a_4. \quad (\text{H.5})$$

Here we have assumed that the last radial position ($\eta=0$) is one node interior to the liquid-SGS interface.

By solving the above system of four simultaneous equations, the expressions for the constants a_1 , a_2 , a_3 , and a_4 can be shown to be

$$a_1 = \frac{(-Q_{i-3} + 3Q_{i-2} - 3Q_{i-1} + Q_i)}{(6\Delta\eta^3)}, \quad (\text{H.6})$$

$$a_2 = \frac{(3Q_{i-2} - 6Q_{i-1} + 3Q_i)}{(6\Delta\eta^2)}, \quad (\text{H.7})$$

$$a_3 = \frac{(Q_{i-3} - 6Q_{i-2} + 3Q_{i-1} + 2Q_i)}{(6\Delta\eta)} \quad (\text{H.8})$$

and

$$a_4 = Q_{i-1}. \quad (\text{H.9})$$

Then the first derivatives at the four radial positions are

$$\left. \frac{dQ}{d\eta} \right|_i = 3a_1\Delta\eta^2 + 2a_2\Delta\eta + a_3 = \frac{(-2Q_{i-3} + 9Q_{i-2} - 18Q_{i-1} + 11Q_i)}{6\Delta\eta}, \quad (\text{H.10})$$

$$\left. \frac{dQ}{d\eta} \right|_{i-1} = a_3 = \frac{(Q_{i-3} - 6Q_{i-2} + 3Q_{i-1} + 2Q_i)}{6\Delta\eta}, \quad (\text{H.11})$$

$$\left. \frac{dQ}{d\eta} \right|_{i-2} = 3a_1\Delta\eta^2 - 2a_2\Delta\eta + a_3 = \frac{(-2Q_{i-3} - 3Q_{i-2} + 6Q_{i-1} - Q_i)}{6\Delta\eta} \quad (H.12)$$

and

$$\left. \frac{dQ}{d\eta} \right|_{i-3} = 12a_1\Delta\eta^2 - 4a_2\Delta\eta + a_3 = \frac{(-11Q_{i-3} + 18Q_{i-2} - 9Q_{i-1} + 2Q_i)}{6\Delta\eta}. \quad (H.13)$$

At the radial position i , the liquid-SGS interface, the second derivative can be shown to be

$$\left. \frac{d^2Q}{d\eta^2} \right|_i = 6a_1\Delta\eta + 2a_2 = \frac{(-Q_{i-3} + 4Q_{i-2} - 5Q_{i-1} + 2Q_i)}{\Delta\eta^2}. \quad (H.14)$$

In a similar fashion, using cubic fit one can show that the second derivative at the liquid-vapor interface is

$$\left. \frac{d^2Q}{d\eta^2} \right|_i = \frac{(-Q_{i+3} + 4Q_{i+2} - 5Q_{i+1} + 2Q_i)}{\Delta\eta^2} \quad (H.15)$$

where node i is on the liquid-vapor interface itself.

The formulae for the first derivatives are used to calculate the tangential velocities from the stream function field using the first radial derivatives of the stream function at the nodes near the liquid-SGS interface. The second derivatives are utilized to check the vorticities using the stream function equation at the liquid-vapor and liquid-SGS interfaces.

APPENDIX I

DATA TABLES

For the sake of simplicity it is assumed that the ICF target is filled with a equimolar binary hydrogen mixture (i.e., equimolar mixture containing H₂ and D₂ or D₂ and T₂) at certain pressure and temperature or equivalently at a certain molar density of the binary mixture, which upon cooling to cryogenic condition turns into a ternary mixture of equilibrium proportion tabulated in Ref. 41, and shown in the tables below.

Mean Temperature (K)	Mole Fraction				Mass Fraction			
	In Liquid		In Vaopr		In Liquid		In Vapor	
	H ₂	D ₂	H ₂	D ₂	H ₂	D ₂	H ₂	D ₂
20	0.465	0.535	0.727	0.273	0.303	0.697	0.571	0.429
22	0.447	0.553	0.679	0.321	0.288	0.712	0.514	0.486
24	0.400	0.600	0.605	0.395	0.250	0.750	0.434	0.566
26	0.341	0.659	0.519	0.481	0.206	0.794	0.351	0.649
28	0.276	0.724	0.422	0.578	0.160	0.840	0.268	0.732

Table I.1 Mean composition of the liquid and vapor of the binary H-D mixture inside the ICF target.

Mean Temperature (K)	Mole Fraction				Mass Fraction			
	In Liquid		In Vaopr		In Liquid		In Vapor	
	H ₂	D ₂	H ₂	D ₂	H ₂	D ₂	H ₂	D ₂
20	0.389	0.449	0.620	0.233	0.254	0.587	0.475	0.357
22	0.363	0.448	0.558	0.264	0.235	0.581	0.413	0.389
24	0.316	0.471	0.478	0.309	0.200	0.597	0.338	0.437
26	0.266	0.504	0.399	0.362	0.164	0.622	0.269	0.489
28	0.213	0.549	0.318	0.427	0.128	0.658	0.204	0.549

Table I.2 Mean composition of the liquid and vapor of the ternary H-D mixture inside the ICF target.

Mean Temperature (K)	Mole Fraction				Mass Fraction			
	In Liquid		In Vapor		In Liquid		In Vapor	
	H ₂	D ₂	H ₂	D ₂	H ₂	D ₂	H ₂	D ₂
20	0.482	0.518	0.624	0.376	0.384	0.616	0.526	0.474
22	0.491	0.509	0.609	0.391	0.392	0.608	0.510	0.490
24	0.479	0.521	0.580	0.420	0.380	0.620	0.480	0.520
26	0.471	0.529	0.558	0.442	0.372	0.628	0.457	0.543
28	0.451	0.549	0.527	0.472	0.354	0.646	0.427	0.573

Table I.3 Mean composition of the liquid and vapor of the binary D-T mixture inside the ICF target.

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