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A ONE-DIMENSIONAL MODEL FOR COAXIAL FLOWING

STREAMS WITH CONDENSATION

Steve Andes

March 1976

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STREAMS WITH CONDENSATION

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ABSTRACT

An analytical model is developed to identify the basic phenomena present in the high temperature flow (2700°K) of two gaseous coaxial streams. The one-dimensional model potentially has application for design of hardware and test conditions for conducting a laser isotope separation feasibility experiment. The processes of interest are those of coupled flow dynamics, liquid condensation of metal vapors, and gaseous diffusion. The stream tubes may initially consist of pure or combinations of an inert carrier—nitrogen, or metal vapor—uranium. A computer code, LISP (Laser Isotope Separation Program), follows from the model. Output from the LISP code is presented in three test cases in Figures 5 through 15. They involved stream differences in velocity up to 90,000 mm/sec and in temperatures of 1100°K . The rate controlling process for the cases cited was found to be diffusion. However, condensation was present. Further use of the LISP code should continue to give a better understanding into the coupled processes of diffusion, condensation, and flow dynamics.

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NOMENCLATURE

A	Stream flow area
a	Inner stream radius
c	Gas concentration
C_p	Gas specific heat capacity at constant pressure
D	Binary diffusion coefficient
$\dot{E}$	Gas energy flux
G	Gas mass flux
g	Mass fraction of condensate
ΔG^*	Free energy of formation of a critical sized nucleus
h	Gas specific enthalpy
J	Droplet nucleation rate
J^i, J^0	Diffusive mass flux defined by equations (15) and (16)
K	Boltzmann constant
K_1	Constant defined in Equation (8)
L	Uranium vapor latent heat of vaporization
M	Gas Mach number
m	Gas mass
N_A	Avogadro's number of molecules
P	Gas pressure
Q_1, Q_2, Q_3	Defined by equations (78) through (80)
R	Universal gas constant
Re	Reynolds number
r	Stream radius
S	Vapor degree of saturation
T	Gas temperature

t	Time
u	Gas velocity
V	Gas volume
α	Constant defined in equation (7)
β	Ratio defined by equations (62), (63), and (66)
α_c, α_i	Energy accommodation coefficient for condensate and inert gases, respectively.
γ	Gas specific heat ratio
λ	Ratio defined in equation (45)
μ	Gas molecular weight
ξ	Fraction of arriving molecules which penetrate the drop surface
ρ	Gas density
σ	Liquid uranium surface tension
χ	Gas mass fraction

Subscripts

c	Condensate
$conv$	Convection
cr	Critical
D	Drop, diffusion
g	Gas
i	Inert
L	Liquid
T	Total
V	Vapor

- x Axial
- x_1 Position
- ∞ Flat film conditions

Superscripts

- i Inside stream
 - 0 outside stream
 - *
- Critical condition

INTRODUCTION

The present study was undertaken to analytically model an experimental method which is being considered as a means of laser isotope separation. The method, which is shown in Figure 1, involves flowing uranium vapor or a uranium/inert gas mixture at an elevated temperature through an inner tube. The gas leaves the tube and comes into contact with a flowing colder inert gas. As these two streams diffuse the static pressure of the uranium vapor goes below that of its vapor pressure and spontaneous condensation occurs. Since condensation depletes the available gaseous uranium (only gas phase vapor can be used for isotope separation), it is desirable to keep condensation to a minimum

Figure 1. Isotope separation model.

The purposes of the experiment are to first arrive at a kinetically optimum, nonreacting mixture of uranium and inert gas. Second, the uranium vapor must be in sufficient quantity that subsequent excitation by a laser is both feasible and economical (minimum depletion by condensation or diffusion once the laser is used). To achieve these purposes determination of the spatial

state properties of the two streams and the concentrations of inert, vapor and condensed species is necessary. This requires that the basic processes of mass transfer, condensation, and flow dynamics be properly coupled together. This paper will show how these processes can be mathematically coupled. The results of the parameter studies are presented to support the proposed experimental program. Finally, the necessary information to run the code will be given.

ANALYTICAL MODEL

There have been a number of papers in the last few years which have considered condensation effects of metal vapor in supersonic nozzles⁽¹⁻⁴⁾ All of these are one dimensional models and use classical nucleation theory for prediction of condensation. The proposed model also is a one-dimensional compressible flow technique with the inclusion of the classical approach to condensation. This approach is taken as opposed to the statistical mechanical view because of its excellent agreement with experiments of condensing metallic vapors. The present model differs from those cited in that the condensation conditions are created due to the mass transfer of a colder inert gas, and not through adiabatic expansion of the gases in a nozzle. This present approach requires a different formulation of the conservation equations. The assumptions involved in the model are presented under three classifications: mass transfer, flow dynamics, and condensation.

MASS TRANSFER —

1. Mass diffuses according to Fick's law.
2. The binary diffusion coefficient is constant.

3. Mass that is transferred mixes uniformly within the individual stream control volume.

FLOW DYNAMICS —

1. Flow is one-dimensional, inviscid, and compressible.
2. Gases behave as perfect gases.
3. Condensed vapor has same velocity as the gas.
4. Flow is nonsteady due to mass transfer between the two stream tubes.
5. Flow is laminar ($Re_D \approx 40 - 150$).

CONDENSATION —

1. Condensation calculations are based on classical nucleation theory.
2. Drops appear due to homogeneous nucleation.
3. Drops that reach critical size are the ones that can grow.
4. Drop radius is much less than the mean free path.
5. The Oswatitsch assumption that the drop pressure, P_D , is equal to the flat film saturation pressure at the drop temperature, $P_\infty(T_D)$, is not valid, i.e.,

$$P_D \neq P_\infty(T_D).$$

This is because the uranium surface tension is large and $P_D \gg P_\infty(T_D)$ especially for drops having radii in the region $(5 - 200) \times 10^{-7}$ mm.

MASS DIFFUSION EQUATION

If one considers only significant mass diffusion in the radial direction for coaxial streams and diffusion equation takes the form

$$\frac{\partial c}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r D \frac{\partial c}{\partial r} \right). \quad (1)$$

With the assumptions of a constant diffusion coefficient, D , and considering an outer infinite boundary Cranks⁽⁵⁾ centerline axial solution ($r = 0$) can be extended to the following form

$$c^i(0,t) = c^0 + (c^i - c^0)(1 - e^{-a^2/4Dt}). \quad (2)$$

Imposing the following initial conditions

$$c_v^i = c_v(0,0)$$

$$c_v^0 = 0$$

$$c_i^i = 0$$

$$c_i^0 = c_i(0,0)$$

on Eq. (2) gives the time dependent concentration on centerline of the inner coaxial stream. This can be expressed by

$$c_v^i(0,t) = c_v(0,0) \left(1 - e^{-a^2/4Dt} \right) \quad (3)$$

and

$$c_i^i(0,t) = c_i(0,0) e^{-a^2/4Dt} \quad (4)$$

If $C_i^i \neq 0$, which is the situation where a carrier gas plus pure uranium vapor is not being flowed in the inner stream tube, the initial bulk gas properties of the inside stream can be adjusted to achieve $C_i^i = 0$ so that use of Eqs. (3) and (4) can be made. This is done simply by combining properties of the inside gases weighted by the proper proportions in which they exit. You now have a "new gas" flowing in the inner stream tube whose properties are reflective of the vapor and inert constituents. This "new gas" now is not inert and so $C_i^i = 0$ and Eqs. (3) and (4) become applicable once again. Caution must be used, however, in that the "new gas" properties must now be used in all subsequent calculations.

The two previous time dependent equations will be used to determine the quantities of vapor and inert being transferred in both inner and outer streams.

CONSERVATION EQUATIONS

The following set of equations will be derived for the inner stream since it is the one in which condensation is considered. The set of equations for the outside stream are obtained by using a zero mass fraction condensate condition in the inner stream equations.

MASS — The total amount of mass per unit volume contained in the inner stream can be expressed by

$$\rho^i - \sum_{j=1}^n \rho_j^i = 0. \quad (n = \text{number of species}) \quad (5)$$

Expanding gives

$$\rho^i = \rho_v + \rho_i. \quad (6)$$

The density present can be determined by using Eqs. (3) and (4) one obtains the following:

$$\rho^i(0,t) = C_v(0,0)\left(1 - e^{-\alpha/t}\right)\mu_v + C_i(0,0)e^{-\alpha/t}\mu_i \quad (7)$$

and

$$\alpha = a^2/4D.$$

Using this equation and taking the necessary derivatives of Eqs. (3) and (4) one obtains the following:

$$\frac{d\rho^i}{dt} = -\mu_v K_1 e^{-\alpha/t} C_v(0,0) + \mu_i K_1 e^{-\alpha/t} C_i(0,0) \quad (8)$$

where

$$K_1 = \frac{a^2}{4Dt^2}.$$

Specifying origin of inert and vapor as superscripts i,0

$$\frac{d\rho^i}{dt} = -K_1 e^{-\alpha/t} C_v^i(0,0)\mu_v + K_1 e^{-\alpha/t} C_i^0(0,0)\mu_i \quad (9)$$

This shows that the time rate of change of total density is only a function of the diffusion process. This is because condensation takes place at the same rate that vapor is consumed thereby causing no net change in total density. The total density, ρ^i , is expressed by

$$\frac{d\rho^i}{dt} = K_1 e^{-\alpha/t} \left[C_i^0(0,0)\mu_i - C_v^i(0,0)\mu_v \right] \quad (10)$$

The gas density, ρ_g , is found by setting

$$\rho_g = \rho_v + \rho_i - \rho_c.$$

Taking the time derivative of this equation where $\rho_c = g\rho^i$

$$\frac{d\rho_g}{dt} = (1 - g) \left[\frac{d\rho_v}{dt} + \frac{d\rho_i}{dt} \right] - \rho^i \frac{dg}{dt}. \quad (11)$$

This gives the time variation of the gas density of the inner stream and is a function of the diffusive processes as well as the rate of change of condensed vapor.

CONTINUITY — Taking a control volume, Figure 2, and summing all the mass fluxes crossing the boundaries due to convection and diffusion gives

$$G_x^i \delta y - G_x^i \delta y - \frac{dG_x^i}{dx} \delta x \delta y - G_D^i \delta x + G_D^0 \delta x, \quad (12)$$

assuming a unit width surface. Rearranging gives

$$\frac{dG_x^i}{dx} \delta x \delta y = -G_D^i \delta x + G_D^0 \delta x. \quad (13)$$

Figure 2. Continuity equation control volume

We can set this equal to a total density change to include the nonsteady flow condition in the form,

$$\frac{dG_x^i}{dx} \delta x \delta y = -G_D^i \delta x + G_D^0 \delta x = \frac{d\rho^i}{dt} \delta x \delta y. \quad (14)$$

Defining also from Fick's law the diffusive mass fluxes to be

$$G_D^i = J^i = -\rho^i D \nabla x_v, \quad (15)$$

and

$$G_D^0 = J^0 = -\rho^0 D \nabla X_i \quad (16)$$

Rearranging Eq. (14) results in an expression for determining the nonsteady convective mass flux, now assuming a concentric cylindrical flow,

$$dG_x^i = J^0 - J^i \frac{2}{a} dx \quad (17)$$

MOMENTUM — From the control volume shown in Figure 3 a momentum balance is performed. This summation includes the diffusive as well as the convective momentum in the axial direction. The assumption is made here that the diffusive (radial) momentum is small compared to the convective (axial) momentum. The diffusive terms, however, carry with themselves an axial velocity component and therefore are not small, and are considered in the above

Figure 3. Momentum balance control volume.

balance. Summing the forces and respective momentum gives for a unit width

$$-\frac{d}{dx} (P \delta y)_x^i \delta x = \frac{d}{dx} (uG)_x^i \delta y \delta x + (u_x G_D^i) \delta x - (u_x G_D^0) \delta x. \quad (18)$$

Performing the differentiation and substituting $a = \delta y$, results in

$$-\frac{d}{dx} (Pa)_x^i = \frac{d}{dx} (uG)_x^i a + (u_x G_D^i) - (u_x G_D^0). \quad (19)$$

Expanding and substituting from Fick's law gives

$$-dP_x^i = u^i \left[\frac{J^0}{a} - \frac{J^i}{a} \right] dx + (G du)_x^i + (u^i J^i - u^0 J^0) \frac{dx}{a}. \quad (20)$$

Using the perfect gas equation of state

$$P = \frac{\rho(1-g)RT}{\mu_g} = \frac{\rho_g RT}{\mu_g}, \quad (21)$$

and the continuity equation

$$G = \frac{\rho_g u}{(1-g)} = \rho u, \quad (22)$$

the momentum equation becomes

$$- \frac{dP}{P} \frac{(RT)}{\mu} = \frac{u^i}{1-g} du + \frac{J^0}{\rho_g a} \left[u^i - u^0 \right] dx. \quad (23)$$

Substituting the definition of Mach number

$$u^2 = M^2 \frac{\gamma RT}{\mu} \quad (24)$$

gives

$$- \frac{dP}{P} \left(\frac{RT}{\mu} \right) = \frac{M^2}{1-g} \left(\frac{\gamma RT}{\mu} \right) \frac{du}{u} + \frac{M^2 \gamma RT}{\mu} \frac{J^0}{\rho_g a} \left[1 - \frac{u^0}{u^i} \right] dt \quad (25)$$

Now dividing through by $\gamma RT/\mu$, results in

$$- \frac{dP}{P} \left(\frac{1}{\gamma} \right) = \frac{M^2}{1-g} \frac{du}{u} + \frac{M^2 J^0}{\rho_g a} \left[1 - \frac{u^0}{u^i} \right] dt \quad (26)$$

Solving for du/u the momentum equation becomes, for concentric stream flow

$$\frac{du}{u} = - \frac{(1-g)}{\gamma M^2} \frac{dP}{P} - \frac{2(1-g)J^0}{\rho_g a} \left[1 - \frac{u^0}{u^i} \right] dt \quad (27)$$

ENERGY — The energy equation is obtained by summing the terms shown in Figure 4 that cross the control volume. The assumption is made that no condensed vapor crosses the boundary. Additionally, once vapor leaves it does not diffuse in and, conversely, the inert doesn't leave the control

volume once it enters. The terms are defined as follows per unit area:

Figure 4. Energy flux control volume.

$$\dot{E}_{\text{conv},x} = \left(\begin{array}{c} \text{convective energy} \\ \text{flux at } x \end{array} \right) = G_x^i \delta y \left(h + \frac{u_x^2}{2} \right)^i \quad (28)$$

$$\dot{E}_{\text{conv},x+\delta x} = \left(\begin{array}{c} \text{convective energy} \\ \text{flux at } x + \delta x \end{array} \right) = \left\{ G_x^i \left(h + \frac{u_x^2}{2} \right)^i + \frac{d}{dx} \left[G_x \left(h + \frac{u_x^2}{2} \right)^i \right] \delta x \right\} \delta y \quad (29)$$

$$\dot{E}_D^0 = \left(\begin{array}{c} \text{diffusive energy flux enter-} \\ \text{ing from outside stream} \end{array} \right) = J^0 \left(h_i x_i + \frac{u_x^2}{2} \right)^0 \delta x \quad (30)$$

$$\dot{E}_D^i = \left(\begin{array}{c} \text{diffusive energy flux leav-} \\ \text{ing from inner stream} \end{array} \right) = J^i \left(h_v x_v + \frac{u_x^2}{2} \right)^i \delta x \quad (31)$$

Summing the terms and making the necessary cancellation gives

$$- \frac{d}{dx} \left[G_x \left(h + \frac{u_x^2}{2} \right)^i \right] \delta x \delta y - J^i \left(h_v x_v + \frac{u_x^2}{2} \right)^i \delta x + J^0 \left(h_i x_i + \frac{u_x^2}{2} \right)^0 \delta x = 0. \quad (32)$$

Rearranging and setting $a = \delta y$

$$d \left[G_x \left(h + \frac{u_x^2}{2} \right)^i \right] = -J^i \left(h_v x_v + \frac{u_x^2}{2} \right)^i \frac{dx}{a} + J^0 \left(h_i x_i + \frac{u_x^2}{2} \right)^0 \frac{dx}{a} \quad (33)$$

Expanding the left hand terms and noting that all variables are considered to refer to inside parameters unless superscripted otherwise

$$G_X dh + G_X u du + \left(h + \frac{u^2}{2}\right) dG_X = -J^i \left(h_V X_V + \frac{u_X^2}{2}\right) \frac{dx}{a} + J^0 \left(h_i X_i + \frac{u_X^2}{2}\right) \frac{dx}{a} \quad (34)$$

Expanding the third term from the left in Appendix A results in

$$\left(h + \frac{u^2}{2}\right) dG_X = \left[J^0 h_i^i X_i^i - J^i h_V^i X_V^i + J^0 \frac{u_X^2}{2} - J^i \frac{u_X^2}{2} \right] \frac{dx}{a} \quad (35)$$

Dividing Eq. (34) by G_X and substituting Eq. (35), and making the necessary cancellations, the energy equation becomes,

$$dh + u du = J^0 \frac{(1-g)}{\alpha \rho_g} \left[X_i^0 h_i^0 - X_i^i h_i^i \right] dt - \frac{(1-g)}{2\alpha \rho_g} J^0 u^2 \left[1 - \left(\frac{u^0}{u}\right)^2 \right] dt \quad (36)$$

The change in enthalpy may be handled by beginning with its definition;

$$h^i = \sum_{j=1}^n x_j h_j, \quad (n = \text{No. of species}). \quad (37)$$

Expanding,

$$d \left[X_V h_V + X_i h_i + X_C h_C \right] \quad (38)$$

and using the definition of h_C to be

$$h_C = h_V^i - L - C_{pL}(T - T_D) \quad (39)$$

gives, assuming $C_{pL}(T - T_D)$ is small compared to the latent heat of vaporization, L , Eq. (38) becomes

$$d \left[(X_V + g) h_V + X_i h_i - gL \right]. \quad (40)$$

Defining

$$C_{pT} = (X_V + g) C_{pV} + X_i C_{p_i} \quad (41)$$

equation (40) becomes

$$C_{pT} dT - g dL - L dg. \quad (42)$$

Substituting into Eq. (36) one obtains

$$C_{p_T} dT = g dL + L dg - u du + \frac{(1-g)}{\alpha \rho_g} J^0 \left[x_i^{0,0} h_i^0 - x_i^i h_i^i \right] dt - \frac{(1-g)}{2\alpha \rho_g} J^0 u^2 \left[1 - \left(\frac{u^0}{u} \right)^2 \right] dt \quad (43)$$

Substituting the results of the momentum equation (Eq. (27)) and the mach number relationship we have

$$C_{p_T} dT = g dL + L dg - \frac{M^2 \gamma R T}{\mu} \left[- \frac{(1-g)}{\gamma M^2} \frac{dp}{p} - \frac{(1-g)}{\rho_g a} J^0 \left[1 - \frac{u^0}{u} \right] dt \right] + \frac{(1-g)}{\alpha \rho_g} J^0 \left[x_i^{0,0} h_i^0 - x_i^i h_i^i \right] dt - \frac{(1-g)}{2\alpha \rho_g \mu} M^2 \gamma R T \left[1 - \left(\frac{u^0}{u} \right)^2 \right] dt. \quad (44)$$

Multiplying by $(\gamma - 1) \frac{u}{\gamma R T}$ which is equal to $1/C_p$, and dividing by $\eta(C_{p_T}/C_p)$, which is defined as the "temperature dependent"/"isentropic" specific heat ratio, gives for concentric streams

$$\frac{dT}{T} = \frac{g}{C_{p_T}} dL + \lambda dg + \eta \frac{(\gamma - 1)}{\gamma} (1 - g) \frac{dp}{p} + \eta M^2 \frac{(\gamma - 1)}{\rho_g a} 2(1 - g) J^0 \left[1 - \frac{u^0}{u} \right] dt + \frac{2(1-g)}{\alpha \rho_g} J^0 \left[\frac{x_i^{0,0} h_i^0 - x_i^i h_i^i}{C_{p_T}} \right] - \eta \frac{(1-g)}{\alpha \rho_g} J^0 M^2 (\gamma - 1) \left[1 - \left(\frac{u^0}{u} \right)^2 \right] dt. \quad (45)$$

The function γ is defined as

$$\lambda = \frac{L}{C_{p_T} T}.$$

Equation (45) gives a first order differential equation for determining the static temperature. The unknown is the differential change in pressure dp/P which will be dealt with now.

COMBINING CONTINUITY AND MOMENTUM

The continuity equation is defined as

$$G_x = \frac{\dot{m}_x}{A} = \frac{\rho_g u_x}{(1-g)} \quad (46)$$

Differentiating Eq. (46) and dividing through by G_x

$$\frac{d\rho_g}{\rho_g} + \frac{du}{u} + \frac{dg}{1-g} = \frac{(1-g)}{\rho_g u} dG \quad (47)$$

Substituting Eq. (17) and the momentum equation (Eq. (27)) results in

$$\begin{aligned} \frac{d\rho_g}{\rho_g} - \frac{(1-g)}{\gamma M^2} \frac{dP}{P} - \frac{(1-g)}{\rho_g a} J^0 \left[1 - \frac{u^0}{u^i} \right] dt + \frac{dg}{1-g} \\ = \frac{(1-g)}{\rho_g u} \frac{J^0}{a} dx - \frac{(1-g)}{\rho_g u} \frac{J^i}{a} dx \end{aligned} \quad (48)$$

Knowing that the density is a function not only of pressure and temperature, but is also a function of molecular weight it can be denoted by

$$\rho_g = f(P, T, \mu). \quad (49)$$

Using the chain rule one obtains

$$d\rho_g = \left(\frac{\partial \rho_g}{\partial P} \right)_{T, \mu} dP + \left(\frac{\partial \rho_g}{\partial T} \right)_{P, \mu} dT + \left(\frac{\partial \rho_g}{\partial \mu} \right)_{T, P} d\mu. \quad (50)$$

Using the perfect gas relationship of Eq. (21) and Eq. (17) the partials become

$$\left(\frac{\partial \rho_g}{\partial P} \right)_{T, \mu} = \frac{\rho_g}{P}, \quad (51)$$

$$\left(\frac{\partial \rho_g}{\partial T} \right)_{P, \mu} = - \frac{\rho_g}{T}, \quad (52)$$

$$\left(\frac{\partial \rho_g}{\partial \mu} \right)_{P, T} = \frac{\rho_g}{\mu}. \quad (53)$$

Substituting Eqs. (51) - (53) into Eq. (50) and dividing through by the

density ρ_g

$$\frac{d\rho_g}{\rho_g} = \frac{dP}{P} - \frac{dT}{T} + \frac{d\mu}{\mu}. \quad (54)$$

Substituting the result into Eq. (48) and combining terms gives,

$$\frac{dP}{P} \left[\frac{\gamma M^2 - (1 - g)}{\gamma M^2} \right] = - \frac{dg}{1 - g} + \frac{dT}{T} + \frac{(1 - g)}{\rho_g a} J^0 \left[1 - \frac{u^0}{u^i} \right] dt - \frac{d\mu}{\mu}. \quad (55)$$

Now substituting the energy equation for dT/T and combining terms results in

$$\begin{aligned} \frac{dP}{P} \left[\frac{\gamma M^2 - (1 - g) - \eta M^2 (1 - g)}{\gamma M^2} \right] &= \frac{g}{C_{pT}} dL + \left[\lambda + \frac{1}{1 - g} \right] dg \\ &+ \frac{2(1 - g)J^0}{\rho_g a} \left[(\gamma - 1)\eta M^2 + 1 \right] \left[1 - \frac{u^0}{u^i} \right] dt + \frac{2(1 - g)J^0}{a\rho_g} \left[\frac{x_i^0 h_i^0 - x_i^i h_i^i}{C_{pT}} \right] dt \\ &- \frac{d\mu}{\mu} + \frac{2(1 - g)}{a} J^0 - J^i dt - \eta(1 - g) \frac{J^0 M^2}{a\rho_g} (\gamma - 1) \left[1 - \left(\frac{u^0}{u^i} \right)^2 \right] dt. \quad (56) \end{aligned}$$

A solution of this last equation will give the static pressure at the axial position along the stream. Simultaneous solution of Eqs. (27), (45), (54), and (56) will adequately describe the state variables of the inner stream. Left unsolved, however, is the condensation parameter g and the rate at which condensation occurs, dg/dt . These two parameters will now be dealt with.

CLASSICAL NUCLEATION THEORY

DROP NUCLEATION EQUATIONS — Numerous derivations of the classical nucleation rate, J , have been conducted⁽⁶⁻⁷⁾. It takes the basic form

$$J = \left(\frac{P_v}{KT} \right)^2 \frac{1}{\rho_L} \left[\frac{2\mu_v \sigma}{\pi N_A} \right]^{1/2} \exp \left(- \frac{\Delta G^*}{KT} \right) \quad (57)$$

where ΔG^* is defined as the free energy of formation of a critical sized nucleus, r^* . Hill (8) has adequately shown that ΔG^* is the sum of three terms which gives a maximum when

$$\Delta G^* = \frac{4}{3} \pi (r^*)^2 \sigma. \quad (58)$$

Hence the critical sized nucleus is given by

$$r^* = \frac{2\sigma}{\rho_L RT \ln(P/P_\infty)}, \quad (59)$$

and is the radius at which spontaneous homogeneous condensation will occur.

The degree of saturation is defined by the relationship

$$S = \ln(P/P_\infty) \quad (60)$$

where P_∞ is the flat film saturation pressure. When

$S < 1$ the flow is unsaturated

$S = 1$ the flow is saturated

$S > 1$ the flow is supersaturated

Growth will occur when $S \geq 1$ but not until a critical supersaturation ratio is reached. This critical ratio is defined as the condition when nuclei capable of further growth form at a rate of one per unit volume per unit time. That is,

$$S = S_{cr} \quad \text{when} \quad J = 1 \text{ nuclei mm}^{-3}\text{-sec}^{-1}.$$

DROP GROWTH EQUATIONS — The use of kinetic theory can be employed to calculate the rate at which mass and energy impinge upon the drop surface since the drop radius is much less than the mean free path. Hill (8) has shown that the rate at which drops grow is the difference between the condensation and evaporation rates multiplied times ξ which is defined as that fraction of arriving molecules which penetrate the surface. The growth rate equation is therefore

$$\frac{dr}{dt} = \frac{\xi}{\rho_L} (\beta - \beta_D), \quad (61)$$

where

$$\beta = P_v / (2\pi RT)^{1/2} \quad (62)$$

and

$$\beta_D = P_D / (2\pi RT_D)^{1/2}. \quad (63)$$

The drop pressure is given by the Helmholtz equation

$$P_D = P_\infty(T_D) \exp \frac{2\sigma}{\rho_L RT_D r_D} \quad (64)$$

where r_D is the drop radius and $P_\infty(T_D)$ is the flat film saturation pressure evaluated at the drop temperature, T_D . Hill further states that the rate of energy flux to the drop must be balanced by the rate of increase of its internal energy. Mathematically this becomes

$$\begin{aligned} & \text{Internal Energy} \\ & \frac{4}{3} \pi r^3 \rho_L C_{pL} \frac{dT_D}{dt} + 4\pi r^2 \left(\frac{dr}{dt} \right) \rho_L \left[\frac{\gamma}{\gamma - 1} RT - L \right] = \\ & \text{(external energy addition)} \quad \text{(energy due to growth)} \\ & 4\pi r^2 \left\{ \begin{array}{l} \text{Arriving Vapor} \\ \left[\begin{array}{l} \xi \beta \quad + \quad (1 - \xi) \beta \end{array} \right] KRT \\ \text{(condensing)} \quad \text{(reflected)} \end{array} \right. - \begin{array}{l} \text{Leaving Vapor} \\ (1 - \xi) \beta_K R \left[T + \alpha_i (T_D - T) \right] \\ \text{(reflected)} \end{array} \\ & \quad - \begin{array}{l} \text{Leaving Vapor} \\ \xi \beta_D KRT_D \\ \text{(evaporating)} \end{array} - \left. \begin{array}{l} \text{Noncondensable Vapor} \\ \beta_c \alpha_c K_c R_c T_D - T \end{array} \right\} \end{aligned} \quad (65)$$

In Eq. (65) β_c is defined as

$$\beta_c = \rho_{v_i} / (2\pi RT)^{1/2}, \quad (66)$$

and the two accommodation coefficients α_i and α_c are defined as the fraction of energy transported to the drop by the arriving molecules. Since little data is known about liquid-gas accommodation coefficients I have chosen to use a high value (1 - 0.8) as suggested by Hill⁽⁸⁾.

Dividing Eq. (65) by $(4\pi r^2)RT$ and cancelling like terms gives

$$\begin{aligned} \frac{rCp_L}{3RT} \rho_L \left(\frac{dT_D}{dt} \right) = & \xi \beta K \left(1 - \frac{\beta_D T_D}{\beta T} \right) - (1 - \xi) \beta K \alpha_i \left(\frac{T_D}{T} - 1 \right) \\ & - \beta_c \alpha_c K \left(\frac{R_c}{R} \right) \left(\frac{T_D}{T} - 1 \right) - \frac{\rho_L}{RT} \left(\frac{dr}{dt} \right) \left[\frac{\gamma}{\gamma - 1} RT - L \right] \end{aligned} \quad (67)$$

Since the change in internal energy of the drop due to external temperature change is small compared to the rate at which the condensing liquid gives its latent heat to the drop the term

$$\frac{rCp_L}{3RT} \rho_L \left(\frac{dT_D}{dt} \right) \approx 0 \quad (68)$$

and Eq. (67) becomes

$$\begin{aligned} \xi \beta K \left(1 - \frac{\beta_D T_D}{\beta T} \right) - (1 - \xi) \beta K \alpha_i \left(\frac{T_D}{T} - 1 \right) - \beta_c \alpha_c K \left(\frac{R_c}{R} \right) \left(\frac{T_D}{T} - 1 \right) \\ - \frac{\rho_L}{RT} \left(\frac{dr}{dt} \right) \left[\frac{\gamma}{\gamma - 1} RT - L \right] \approx 0. \end{aligned} \quad (69)$$

Substituting Eq. (61) and $\lambda = (\gamma - 1)L/\gamma RT$ and dividing through by β gives

$$\begin{aligned} \xi K \left(1 - \frac{\beta_D T_D}{\beta T} \right) - (1 - \xi) K \alpha_i \left(\frac{T_D}{T} - 1 \right) - \frac{\beta_c}{\beta} \alpha_c K \left(\frac{R_c}{R} \right) \left(\frac{T_D}{T} - 1 \right) \\ + \xi \left(1 - \frac{\beta_D}{\beta} \right) \frac{\gamma}{\gamma - 1} (\lambda - 1) \approx 0. \end{aligned} \quad (70)$$

From kinetic theory⁽⁹⁾, considering only the translational energy of a molecule, the number of degrees of freedom, z , gives the value of the constant K ;

$$K = 3/2$$

$$(z = 3 \text{ for monatomic gas})$$

and

$$K = 5/2$$

(z = 5 for diatomic gas)

Dividing Eq. (70) by $K = 5/2$ and solving for T_D gives

$$T_D = T \left\{ \frac{\xi \left(1 - \frac{\beta_D T_D}{\beta T} \right) + \xi \left(\frac{2}{5} \right) \left(\frac{\gamma}{\gamma - 1} \right) \left(1 - \frac{\beta_D}{\beta} \right) (\lambda - 1)}{(1 - \xi) \alpha_i + \left(\frac{3}{5} \right) \left(\frac{R_c}{R} \right) \alpha_c \left(\frac{\beta_c}{\beta} \right)} + 1 \right\}. \quad (71)$$

Equation (71) is an implicit algebraic equation. To solve this equation one must guess the value of T_D and calculate the liquid density of uranium⁽¹⁰⁾ based on the relationship

$$\rho_L = -1.0328 \times 10^{-3} T_D(^{\circ}\text{K}) + 18.717 \quad (72)$$

Then it is necessary to calculate the equilibrium vapor pressure⁽¹¹⁾ at that temperature from

$$P_{\infty}(T_D) = \left[10^{5.88 - 25230/T_D(^{\circ}\text{K})} \right] 1.013 \times 10^5 \text{ (pascal)}. \quad (73)$$

with these values P_D can be evaluated from Eq. (64) knowing the average drop radius size r_D . The average drop radius size can be estimated from the set of ordinary differential equations to be derived in a subsequent section. Once known, however, iterative solution of Eq. (71) is possible until convergence is achieved. A Newton Raphson iteration technique was found to be adequate with convergence achieved in 5 - 7 iterations.

DROP GROWTH RATE EQUATIONS

The previous section gave the tools to calculate the conditions for drop growth. This section deals with determining the rate at which they grow. Hill⁽⁸⁾ has shown that starting with a droplet of size r_0 , which is slightly greater than r^* , to assure growth, the radius of the drop as it goes from x to x_1 , is given by

$$r_{x_1} = r_0 + \int_x^{x_1} \frac{1}{u} \frac{dr}{dt} dx. \quad (74)$$

The surface area by the time it reaches x is

$$4\pi \left[r_{x_1} \right]^2. \quad (75)$$

Further Hill finds that the total number of nuclei formed per second in the volume $A(x) dx$ is just $J(x) A(x) dx$. The rate of condensing liquid then as the drop travels the distance dx becomes

$$\dot{m}_c = \rho_L 4\pi \left[r_{x_1} \right]^2 J(x) A(x) dx \frac{dr}{dt} \frac{dx}{u}. \quad (76)$$

Taking into account also droplets which now spontaneously appear at x_1 (those that have reached the critical sized radius) the normalized condensation rate, dg/dx become

$$\frac{dg}{dx} = \frac{4\pi\rho_L}{\dot{m}} \left[\int_0^x \left(r_{x_1} \right)^2 J(x) A(x) \frac{1}{u} \left(\frac{dr}{dt} \right) dx + \frac{r_0^3}{3} J(x_1) A(x_1) \right]. \quad (77)$$

Equation (77) can be broken down into four first-order ordinary differential equations. They are:

$$\frac{dQ_3}{dx} = 8\pi JA \quad (78)$$

$$\frac{dQ_2}{dx} = \left[Q_3 \frac{1}{u} \left(\frac{dr}{dt} \right) + 8\pi J A r_0 \right] \quad (79)$$

$$\frac{dQ_1}{dx} = \left[Q_2 \frac{1}{u} \left(\frac{dr}{dt} \right) + 4\pi J A r_0^2 \right] \quad (80)$$

$$\frac{dg}{dx} = \frac{\rho_L}{\dot{m}} \left[Q_1 \frac{1}{u} \left(\frac{dr}{dt} \right) + \frac{4\pi}{3} J A r_0^3 \right]. \quad (81)$$

The condensate mass fraction, g , is found by simply integrating Eqs. (78)-(81)

The average drop size radius, r_D , to be used in Eq. (64) to find the drop temperature is calculated by setting

$$r_D = \left(2Q_1/Q_3\right)^{1/2}. \quad (82)$$

This gives a surface averaged radius for the drop temperature calculations.

LISP COMPUTER CODE

The Laser Isotope Separation Program (LISP) code consists of the system of equations derived previously and are solved numerically with the CDC system simulation program CSSL3⁽¹²⁾. It was chosen because of the versatility and many options available in the CSSL language, and the ability to also link programs written in Fortran IV. The LISP code is arranged in the following sections:

- INPUTS — Consists of the constants used in the program.
- INITIAL — Portion of program that calculates initial values for the numerical integrators.
- DYNAMIC — Control region for program termination.
- DERIVATIVE — Consists of the differential and algebraic equations necessary to solve the particular problem.
- OUTPUT — Output statement to print those variables desired at each calculational interval.
- TERMINAL — CSSL dummy statement — no real function.

Each of these sections will now be discussed in greater detail.

INPUTS — This section defines those parameters which remain constant and are denoted by a "CONSTANT" statement. The variables and their definitions are given in the order in which they appear in LISP.

<u>Code Input Constants</u>	<u>Definition</u>
RU	Universal gas constant — $\frac{\text{gm} - \text{mm}^2}{\text{gm}_{\text{mole}} - ^\circ\text{K} - \text{sec}^2}$
MOLI	Outer stream molecular weight — gm/gm _{mole}
GAMMI	Inert gas (nitrogen) specific heat ratio — dimensionless
ROUT	Outer stream radius — mm
PIE	Constant π , 3.14159
MOLV	Inner stream molecular weight — gm/gm _{mole}
GAMMV	Condensable vapor (uranium) specific heat ratio — dimensionless
NA	Avagadro's number — molecules/gm _{mole}
KB	Boltzmann constant — gm-mm ² /sec ² -°K
CONVF1	Conversion factor
FUG1	Constant used to calculate uranium liquid density in equation (72)
FUG2	Constant used to calculate uranium liquid density in equation (72)
CC3	Conversion factor
FF2	Conversion factor to convert cal/gm-°K to mm ² /sec ² -°K
DLDX	The differential change in the vapor latent heat of vaporization — mm/sec ²
DADX	The differential change in the flow area — mm

Code Input Constants

Definition

POI	Outside stream initial static pressure — Pascal
TOI	Outside stream initial static temperature — °K
VELOI	Outside stream initial velocity — mm/sec
CPLC	Specific heat of liquid uranium — $\text{mm}^2/\text{sec}^2\text{-}^\circ\text{K}$
Z	Exponential function "e" — 2.71828 ...
PIT	Inside stream initial static pressure — Pascal
TII	Inside stream initial static temperature — °K
VELII	Inside stream initial velocity — mm/sec
D	Binary diffusion coefficient — mm^2/sec
EPS	Drop surface penetration coefficient defined in equation (61) — dimensionless
ALPHA	Thermal accommodation coefficient — dimensionless
SIGMA	Uranium surface tension — gm/sec^2
L	Uranium latent heat of vaporization — mm^2/sec^2
FF	Factor multiplied times the critical drop radius to assure growth — dimensionless
A	Inside stream radius — mm
ION	Initial contamination level present in flow field — molecules
RADIUS	Initial drop radius — mm
MAXSTP	Maximum value of the independent variable — mm

<u>Code Input Constants</u>	<u>Description</u>
VAPMOL	Uranium molecular weight — gm/gm _{mole}
INEMOL	Inert (nitrogen) molecular weight — gm/gm _{mole}
AA0,BB0,CC0,DD0, EE0,FF0,GG0,HH0	Coefficients of least square fit to calculate temperature dependency of uranium specific heat (1405 °K — 5000 °K)
AA1,BB1,CC1,DD1, EE1,FF1,GG1,HH1, JJ1	Coefficients of least square fit to calculate temperature dependency of nitrogen specific heat (100 °K - 3000 °K)

INITIAL — The initial portion of the program uses the input constants to calculate initial values for the numerical integrators. This section is broken up into two sections. One for calculating those initial properties required in the outer stream and the other for those properties in the inner stream. The two sections are designated by "COMMENT" cards.

DYNAMIC — This section contains only the termination statement, TERMT(). Program execution stops when this function is satisfied.

DERIVATIVE — This section contains the algebraic and differential equations necessary to solve the flow dynamics, mass transfer, and condensation processes. The section is divided into the following "COMMENT" fields:

- INTEGRATION CONTROL
- MASS, CONCENTRATION AND MASS FRACTION RELATIONSHIPS
- CALCULATION OF OUTER STREAM PROPERTIES
- CALCULATION OF INNER STREAM PROPERTIES

- CONDENSATION CALCULATION
- ITERATION FOR DROP TEMPERATURE
- LEAST SQUARE VAPOR SPECIFIC HEAT — URANIUM
- LEAST SQUARE INERT SPECIFIC HEAT — NITROGEN

Within each of the fields are the related equations and parameters necessary to calculate the processes indicated.

OUTPUT — The current output variables are printed as a function of the independent variables, T, and include, but are not limited to, the following:

<u>Output Variable</u>	<u>Definition</u>
T	Current axial position — mm
PI	Inner stream static pressure — Pascal
TI	Inner stream static temperature — °K
UI	Inner stream flow velocity — mm/sec
CI	Inner stream concentration — $\text{gm}_{\text{mole}}/\text{mm}^3$
RHOI	Inner stream flow density — gm/mm^3
MUI	Inner stream molecular weight — $\text{gm}/\text{gm}_{\text{mole}}$
TIMEI	Inner stream time — seconds
CIV	Inner stream vapor concentration — $\text{gm}_{\text{mole}}/\text{mm}^3$
CII	Inner stream inert concentration — $\text{gm}_{\text{mole}}/\text{mm}^3$
PO	Outer stream static pressure — Pascal

<u>Output Variable</u>	<u>Definition</u>
T0	Outer stream static temperature — °K
U0	Outer stream flow velocity — mm/sec
CO	Outer stream concentration — $\text{gm}_{\text{mole}}/\text{mm}^3$
RH00	Outer stream flow density — gm/mm^3
MU0	Outer stream molecular weight — $\text{gm}/\text{gm}_{\text{mole}}$
TIME0	Outer stream time — seconds
COV	Outer stream vapor concentration — $\text{gm}_{\text{mole}}/\text{mm}^3$
COI	Outer stream inert concentration — $\text{gm}_{\text{mole}}/\text{mm}^3$
S	Degree of saturation defined in equation (60)
G	Mass of condensate per total inside stream mass — gm_C/gm_T
J	Nucleation rate defined in equation (57) — $\text{nuclei}/\text{mm}^3\text{-sec}$
RCRIT	Critical drop radius defined in equation (59) — mm
D1RDX	Droplet growth rate defined in equation (61) — mm/mm
PD	Drop pressure calculated from equation (64) — Pascal
TD	Drop temperature calculated from iterative solution of equation (71) — °K

Output Variable

Definition

FRCTCV

Mass of condensate per gram of vapor of the
inner stream — gm_c/gm_v

A sample listing of the LISP program is included as well as a copy of the numerical and graphical output. The graphical output was performed using a post processor, CSSLPLT, available only at LLL. However, line printer plots are available within the CSSL package.

LISP CODE RESULTS

Three example problems will be illustrated with LISP. The following initial conditions exist in the outer and inner stream tubes.

Case I — Initial Velocity and Temperature Gradient

Outer: Nitrogen gas (mol. wt = 28.016)

Temperature = 1600°K

Pressure = 35 pascal

Velocity = 1.0×10^4 mm/sec

Radius = 50 mm

Inner: Uranium gas (mol. wt = 238.03)

Temperature = 2700°K

Pressure = 35 pascal

Velocity = 1.0×10^5 mm/sec

Radius = 10 mm

The mutual diffusion coefficient for N_2 and U gas at these conditions is $D = 1.0 \times 10^6$ mm²/sec.

Case II — Initial Temperature Gradient

The same above conditions exist except the initial velocities are now both set equal to 1.0×10^5 mm/sec.

Case III — No Initial Gradients

The same conditions as Case I except both initial velocities are set equal to 1.0×10^5 mm/sec and both static stream temperatures are equal to 2700°K.

The results from the three cases are graphically illustrated in Figures 5 - 15. Generally they show rapid mass and thermal equilibrium occurring within the radius of the stream tube. This is, of course, due to the extremely large diffusion coefficient which exist at these low pressures. The time involved is approximately .05 ms. The fraction of vapor that is condensing is small. The diffusion process at this pressure depletes the available vapor much more rapidly than does the condensation process.

Comparing the first two cases shows that the initial velocity gradient case enhances the mixing process. This is especially clear comparing Figures 6 - 11 with thermal equilibrium being reached in about a third of the distance for Case I compared to Case II.

Case III shows very little occurring since both streams are initially at thermal and velocity equilibrium. The difference in molecular weight does cause density changes in the two stream tubes, however, as can be seen by Figure 15. The velocity variation takes essentially the same profile as exhibited by Case II in Figure 13. Otherwise no appreciable state changes took place from the initial conditions through the 5 mm distance.

Figure 5. Case I steam pressure variation.

Figure 6. Case I stream temperature variation.

Figure 7. Case I stream density variation.

Figure 8. Case I stream velocity variation.

Figure 9. Case I vapor depletion rate.

Figure 10. Case II steam pressure variation.

Figure 11. Case II stream temperature variation.

Figure 12. Case II stream density variation.

Figure 13. Case II stream velocity variation.

Figure 14, Case II vapor depletion rate.

Figure 15. Case III stream density variation.

CONCLUSIONS AND RECOMMENDATIONS

A number of observations can be drawn about the LISP computer code from the three test cases reported previously.

1. The LISP code seems to adequately handle the processes of diffusion and condensation.
2. State variables converge to acceptable steady state values with the probable exception of the velocity. The significance of the velocity error on the total problem is small but for completeness it should be eliminated in the future.
3. The problem set over which the program was exercised is a diffusion dominated process. Future work should include higher pressures to exercise code capability in regions where condensation and diffusive effects are more in balance.
4. The rate at which the processes in the program take place is extremely sensitive to the magnitude of the diffusion coefficient. Therefore it is of utmost importance that one determine this variable with extreme accuracy.
5. The drop temperature, Figures 6 and 11, did not significantly differ from the ambient gas temperature except for a brief period of time during initial gas drop growth. For these conditions the Oswatitsch assumption can be invoked.

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PROGRAM ISOTOPE
COMMENT ISOTOPE SEPARATION FOR CENTERLINE SOLUTION
REAL INEMOL
CONSTANT RU=8.3143E+9, MOLI=28.016, GAMMI=1.4, ROUT=50.
CONSTANT PIE=3.14159, MOLV=238.03, GAMMV=1.667, NA=6.022E+23
CONSTANT KB=1.3805E-14, CONVF1=1.0133E+5, FUG=-1.0328E-3, FUG1=18.717
CONSTANT CC3=1.0E3, FF2=4.184E+9, DLDX=0., DADX=0.
CONSTANT POI=35.000, TOI=2700., VELOI=1.E5, CPLC=4.79068E+10, Z=2.71828
CONSTANT PII=35.000, TII=2700., VELII=1.E5, D=1.0E6, EPS=.9, ALPHA=1.
CONSTANT SIGMA=1550., L=2.0285E+13, FF=1.3, A=10., ION=0., RADIUS=1.4E-7
CONSTANT MAXSTP=1.0, COVI=0., MOVI=0., CIII=0., MIII=0.
CONSTANT AAO=1.19902E1, BBO=-2.00007E-2, CCO=2.24651E-5, ...
DDO=-1.12867E-8, EEO=3.09632E-12, FFO=-4.78648E-16, ...
GGO=3.91308E-20, HHO=-1.31567E-24
CONSTANT AAI=3.4502, BBI=9.82068E-4, CCI=-6.1695E-6, ...
DDI=1.64418E-8, EEI=-1.95103E-11, FFI=1.23579E-14, ...
GGI=-4.3617E-18, HHI=8.10689E-22, JJI=-6.19244E-26
CONSTANT VAPMOL=238.03, INEMOL=28.016
INITIAL
COMMENT CALCULATE INITIAL PROPERTIES OF THE OUTER STREAM
COII = POI/(RU* TOI)
RHOOI = COII * MOLI
AO = 1.* PIE * ((ROUT*ROUT)-(A*A))
AT = PIE*ROUT*ROUT
MASSOI = RHOOI * AO * 1.
MOII = MASSOI
COMMENT CALCULATE INITIAL PROPERTIES OF THE INNER STREAM
PSATI = 10.*(5.88-25230./TII)*CONVF1
BIVIT = PSATI/PII
BIIIT = (PII-PSATI) / PII
XXIVIT = BIVIT*VAPMOL/MOLV
XXIIIT = BIIIT*INEMOL / MOLV
CIVI = PII/(RU* TII)
RHOII = CIVI * MOLV
MACHII = VELII / SQRT(GAMMV*RU*TII/MOLV)
AI = PIE * A * A
MDOTII = VELII * RHOII * 1.
MASSII = RHOII * AI * 1.
MIVI = MASSII
VAPINT = MIVI
INEINT = MOII
MASII = MASSII
MASOI = MASSOI
END
DYNAMIC
TERMT (T.GE. 5.)
DERIVATIVE CALC
COMMENT MASS, CONCENTRATION AND MASS FRACTION RELATIONSHIPS
CINTERVAL CCCI=.1
MINTERVAL HMINT= 1.E-9
MERROR UI= 1.E-7, UO= 1.E-7
INTEGER MB
PROCEDURAL(COE1=TIMEI,A,D)
COE1 = 0.0
IF (TIMEI.GT.0.0) COE1=A*A/(4.*D*TIMEI*TIMEI)
END
PROCEDURAL(COE2=TIMEI,A,D)
COE2 = 1.0

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IF (TIME1.GT.0.0) COE2=A*A/(4.*D*TIME1)
!!      END
      EXPOS = 1.-(1./EXP(COE2))
      PROCEDURAL(COE7=TIME1,EXPOS)
      COE7 = 1.
      IF (TIME1.GT.0.0) COE7 = EXPOS
      END
      HMIVD = COE7 * MIVI
      HMOV = VAPINT-HMIVD
      EXP00 = 1.-(1./EXP(COE2))
      PROCEDURAL(COE8=TIME1,EXP00)
      COE8 = 1.
      IF (TIME1.GT.0.0) COE8=EXP00
      END
      HMOI = COE8*MOII
      HMII = INEINT -HMOI
      HMOLTI = (HMII/MOLI) + (HMIVD/MOLV)
      HMOLTO = (HMOI/MOLI) + (HMOV/MOLV)
      HBMIIV = HMIVD/HMOLTI/MOLV
      HBMOV = HMOV/HMOLTO/MOLV
      HBMIII = HMII/HMOLTI/MOLI
      HBMOI = HMOI/HMOLTO/MOLI
      MTOTAL = MO + MI
      THERMO = (MOV*CPGOV+MOI*CPGOI)*TO / FF2
      ENEGYO = THERMO+(MO*UO*UO/(2.*FF2))
      THERMI = (MIV*CPGIV+MII*CPGII)*TI/FF2
      ENEGYI = THERMI+(MI*UI*UI/(2.*FF2))
      ENEGYT = ENEGYI + ENEGYO
      DEBUG 2 , 1.0
      TERM = COE1/ Z**COE2
      EXPREO = 1.-(1./EXP(COE2))
      EXPRES = 1.-(1./EXP(COE2))
      PROCEDURAL(COE4=TIME1,EXPRES)
      COE4 = 1.
      IF (TIME1.GT. 0.0) COE4= EXPREO
      END
      PROCEDURAL(COE3=TIME1,EXPRES)
      COE3 = 1.
      IF (TIME1.GT. 0.0) COE3 = EXPRES
      END
      MIV = MIVDIF - G*MI
      PROCEDURAL(MIVDIF=MIVI,COE3,HBMIIV,HBMOV)
      IF (HBMIIV.LE.HBMOV) GO TO NEXT
      MIVDIF = COE3 * MIVI
      NEXT..CONTINUE
      END
      DIMIV = DERIVT(MASII,MIV,T,SMIV)
      MOV = VAPINT - MIVDIF
      DIMOV = DERIVT(0.0,MOV,T,SMO)
      MII = INEINT - MOI
      DIMII = DERIVT(0.0,MII,T,STO)
      PROCEDURAL(MOI=MOII,COE4,HBMIII,HBMOI)
      IF (HBMOI.LE.HBMIII) GO TO NEXT1
      MOI = MOII * COE4
      NEXT1..CONTINUE
      END
      DIMOI = DERIVT(MASOI,MOI,T,SMOI)
      MO = MOV + MOI
      MDOTO = DERIVT(MASSOI,MO,T,STMO)
      MI = (MIVDIF+MOII-MOI) / (1.-G)
      MDOTI = DERIVT(MASSII,MI,T,STMI)

```

```

XXOV = MOV / MO
XXOI = MOI / MO
XXII = MII / MI
XXIV = MIV / MI
ARRAY PIIITS(15),POIOVS(15)
ARRAY SMIV(15),SMOI(15),STMO(15),STMI(15),SXXII(15)
ARRAY SXXIV(15),SXXOI(15),SMO(15),SXXOV(15),STO(15)
COMMENT CALCULATING OUTER STREAM PROPERTIES
VDIFO = 1. - UI / UO
MODT = RHOO*AO*UO
ZMSQO = ZBO*MCHSQO
UIUOSQ = 1. - UISQ/UOSQ
CPO = (XXOV*XXIVIT)*CPGOV+(XXOI+XXIIIT*XXOV)*CPGOI
DIA = AO / (2.*A)
GMMO = GAMO - 1.
RHODT = RHOO*((DIP0/PO)-(D1TO/TO)+MUODT/MUO)
RHOO = INTEG(RHODT,RHOOI)
DDOV = -RHOOI*(COE3-1.)*AI/AO
DIOVDT = DERIVT(0.0,DDOV,TIMEI,DDOVSS)
JOV = DDOVDT
DDII = -RHOOI * (COE4-1.)
DDIIDT = DERIVT(0.0,DDII,TIMEI,DDIISS)
RHOOOV = XXOV * RHOO
COV = RHOOOV / MOLV
RHOOOI = XXOI * RHOO
COI = RHOOOI / MOLI
CPOUT = JOV / (GOUT*DIA)
CPOUTM = CPOUT *VDIFO
GMSQO = GAMO * MCHSQO
EHOUT = CPO * TO
DIFFCO = (CPGIV*TI- CPGOV*TO)/EHOUT
PROCEDURAL(JO=RHOO,D.DXXI,TIMEI)
JO = -RHOO*D*(-DXXI)
IF(TIMEI.EQ.0.0) JO = 0.0
END
ARRAY MUOSS(15)
MUODT = DERIVT(MOLI,MUO,T,MUOSS)
POUT1 = -(PO*GMSQO)/(GMSQO*(1.-ZBO)+ZMSQO-1.)
POUT2 = CPOUTM * (GMMO*ZMSQO+1.)
POUT3 = CPOUT * DIFFCO
POUT4 = CPOUT*UIUOSQ*GMMO*ZMSQO/ 2.
POUT5 = MUODT / MUO-(JOV-JII)/(GOUT*DIA)
DIP0 = POUT1*(POUT2+POUT3 - POUT4-POUT5 )
PO = INTEG(DIP0,POI)
CUO1 = DIP0/(PO* GAMO * MACHO * MACHO )
CUO2 =CPOUTM
DIUO = -UO * ( CUO1 + CUO2)
UO = INTEG(DIUO,VELOI)
TOUT1 = GMMO*DIP0*ZBO / (PO*GAMO)
TOUT2 =CPOUTM * GMMO * ZMSQO
TOUT3 = POUT3
TOUT4 = POUT4
D1TO = TO*(TOUT1 + TOUT2 + TOUT3 - TOUT4)
TO = INTEG(D1TO,TOI)
UOSQ = UO *UO
ZBO = GAMO*RU / (MUO*GMMO*CPD)
GOUT = RHOO*UO
CO = RHOO / MUO
MOLIO = MOI/MOLI
MOLVO = MOV/MOLV

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MOLEO = MOLIO + MOLVO
BIO = MOLIO/MOLEO
BVO = MOLVO/MOLEO
POI = PO*BIO
POV = PO * BVO
MUO = BIO*MOLI+ BVO*MOLV
PROCEDURAL(JI=RHOI,D,DXXV,TIMEI)
JI = -RHOI * D * (-DXXV)
IF (TIMEI.EQ.0.0) JI = 0.0
END
GAMO = GAMMV * XXOV + GAMMI * XXOI
MACHO = UO / SQRT(GAMO * RU * TO / MUO)
MCHSQO = MACHO*MACHO
DTD XO = 1. / UO
TIMEO = INTEG(DTD XO,0.)
ARRAY SDXXV(15),SDXXI(15)
DIFXXV = XXOV-XXIV
DIFXXI = XXII-XXOI
DXXV = DERIVT(1.,DIFXXV,T,SDXXV)
DXXI = DERIVT(1.,DIFXXI,T,SDXXI)
COMMENT CALCULATION OF INNER STREAM PROPERTIES
CPI = (XXIV*XXIVIT)*CPGIV+(XXII+XXIIIT*XXIV)*CPGII
DTDX = 1. / UI
TIMEI = INTEG(DTD X,0.)
LAMBDA = L / (CPI * TI)
MCHSQI = MACHI * MACHI
ARRAY DDI VSS(15),DDOISS(15),DDI ISS(15)
DDIV = -RHOII*(COE3-1.)
DDIVDT = DERIVT(0.0,DDIV,TIMEI,DDIVSS)
JIV = DDIVDT
DDOI = -RHOII*(COE4-1.)*AO/AI
DDOIDT = DERIVT(0.0,DDOI,TIMEI,DDOISS)
JOI = DDOIDT
ARRAY MUISS(15)
MUIDT = DERIVT(MOLV,MUI,T,MUISS)
RHOIDT=RHOI*((DIPI/PI)-(DITI/TI))+MUIDT/MUI
RHOI = INTEG(RHOIDT,RHOII)
CI = RHOI / MUI
CIV = RHOIIV / MOLV
RHOIIV= XXIV* RHOI
RHOIII = XXII * RHOI
CII = RHOIII / MOLI
ZBI = GAMI*RU / (MUI*GMMI*CPI)
ZE = 1.- G
GMMI = GAMI - 1.
CPCOF = 2 *JOI / (GIN*A)
CPCOFF= CPCOF * VDIFI
DIFFCP= (CPGOI * TO - CPGII * TI) / (CPI * TI)
UISQ = UI * UI
MDOTIT= RHOI*UI*AI
MIDT = MDOTIT/ ZE
VDIFI = 1. - UO / UI
ZMSQI = ZBI*MCHSQI
UQUISQ = 1. - (UOSQ/UISQ)
CP1 = ((2./ZE)+(LAMBDA)) * DIG
CP2 = CPCOFF*(GMMI*ZMSQI+ 1.)
CP3 = CPCOF * DIFFCP
CP4 = ZMSQI*GMMI*CPCOF*UQUISQ/ 2.
CP5 = -(GAMI*MCHSQI)/(GAMI*MCHSQI-ZE-ZMSQI*ZE*GMMI)
CP6 = MUIDT / MUI-(2.*(JOI-JIV)/(GIN*A))

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D1PI = CP5*(CP1 + CP2 + CP3 - CP4-CP6 ) * PI
PI = INTEG(D1PI,PII)
CT1 = GMMI * ZE * D1PI*ZBI / (PI * GAMI )
CT3 = LAMBDA * DIG
CT4 = ZMSQI * GMMI * CPCOFF
CT5 = CP3
CT6 = CP4
DITI = TI * ( CT1 + CT3 + CT4 + CT5 - CT6 )
TI = INTEG(DITI,TII)
CU1 = ZE * D1PI / (GAMI * MCHSQI * PI )
CU2 = CPCOFF
DIUI = -UI * ( CU1 + CU2 )
UI = INTEG(DIUI,VELII)
MOLII = MII/MOLI
MOLIV = MIV/MOLV
MOLEI = MOLII + MOLIV
BII = MOLII/MOLEI
BIV = MOLIV / MOLEI
PIII = PI * (BII+BIIIT)
PVI = PI * BIVIT
MUI = BII*MOLI + BIV*MOLV
GIN = RHOI*UI
GAMI = GAMMV * XXIV + GAMMI * XXII
MACHI = UI / SQRT( GAMI * RU * TI / MUI )
COMMENT CONDENSATION CALCULATIONS
COND = G * MI
FRCTCV = COND/MIV/XXIVIT
ROSO = RO * RO
D1Q3H = 8. * PIE * J * AI
D1Q3 = FCNSW(JDIF,0.0,D1Q3H,D1Q3H)
Q3 = INTEG(D1Q3,0.0)
D1Q2 = Q3 * DIRDX + D1Q3 * RO
Q2 = LIMINT(D1Q2,0.0,0.0,1.E20)
D1Q1 = Q2 * DIRDX + (D1Q3 * ROSQ/2.)
Q1 = LIMINT(D1Q1,0.0,0.0,1.E20)
ROCU = ROSQ * RO
PROCEDURAL(DIG=Q1,DIRDX ,D1Q3,ROCU,RHOLI,MDOTIT,JDIF)
DIG=0.0
IF(JDIF.GE.0.0.AND.ROCU.GE.0.0) ....
DIG = (Q1*DIRDX+(D1Q3*ROCU/6.))*RHOLI /MDOTIT
END
G = LIMINT(DIG,0.0,0.0,1.0)
RO = FF * RCRIT
SCHK = S-1.
S = PVI/PINF
SINFT = FCNSW(SCHK,S,1.00001,S)
PINF = 10.**(5.88-25230./TI) * CONVF1
RHOLI = (FUG*TI+FUG1)/ CC3
RHOLIQ = (FUG*TD+FUG1)/ CC3
DIRDX = EPS *(BE-BD)/(UI*RHOLI)
JDIF = J - 1.
COMB = FCNSW(JDIF,0.0,1.,1.)
R = INTEG(DIRDX,RADIUS)
RCRIT = 2.*SIGMA *MOLV/(RHOLI*RU*TI*ALOG(SINFT))
RCSQ = RCRIT * RCRIT
PROCEDURAL(J=SIGMA.MOLV,PI,TI,RHOLI ,SINFT)
J=0.0
CJ1 = 5.394533E15*SQRT(SIGMA*VAPMOL)*(PVI/TI)**2 /RHOLI
CJ2 = 1.755843E-5*(SIGMA/TI)**3 *(VAPMOL/(RHOLI *ALOG(SINFT)))*2
IF(CJ2.LT.300.) J= CJ1/2**CJ2

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END
PD = PINF * Z** (2.*SIGMA*MUI/(RHOLQ*RU*TD*RBAR))
PROCEDURAL (RBAR=Q1,Q3,RADIUS)
RBAR = RADIUS
Q11 = SQRT(Q1*Q1)
IF(Q3.GT.0.0) RBAR=SQRT(2.*Q11/Q3)
END
IN = 2.*RU * PIE
BC = PIII /SQRT(IN*TI/INEMOL)
BE = PVI / SQRT(IN*TI / VAPMOL )
BD = PD / SQRT(IN*TD / VAPMOL )
COMMENT ITERATION FOR DROP TEMPERATURE
PROCEDURAL (TD=RBAR,SIGMA,TI,RU,VAPMOL,INEMOL,LAMBDA,COMB,GAMMV,EPS,...
ALPHA,MUI,PVI,PIII)
ARRAY GG(2),F(2),SUB(2)
INTEGER INC,N
TD = TI
IF (LUMB.EQ.0) GO TO SEVENN
TD1 = TI
TD2 = TI + 100.
INC = 0
TWONE..INC = INC + 1
N = 0
TD = TD1
GG(1) = TD
NN = 1
GO TO EIGHT
NINE..TD=TD2
GG(2) = TD
NN = 2
GO TO EIGHTT
TRTEN..GG(2) = TD
EIGHTT..CONTINUE
EIGHT..N = N + 1
RHOLQ = (-0.001032*TD + 18.717)/1000.
EXP0 = 5.88 - (25230./TD)
PINFTD = (10.**EXP0)*101325.
EXP01 = 2.*SIGMA*VAPMOL/(RHOLQ*RU*TD*RBAR)
PD = PINFTD*(2.7183**EXP01)
INNER = 6.2831853*RU
BETA = PVI/SQRT (INNER*TI/VAPMOL)
BETAD = PD/SQRT (INNER*TD/VAPMOL)
BETAC = PIII/SQRT (INNER*TI/INEMOL)
RATIO = BETAD/BETA
TERM1 = EPS*(1.-(RATIO*TD)/TI)
TERM2 = EPS*(1.-RATIO)*2.*GAMMV*(LAMBDA-1.)/(3.*(GAMMV-1.))
TERM3 = ALPHA*((1.-EPS)+.6*BETAC*VAPMOL/(BETA*INEMOL))
F(NN) = TI*(((TERM1 +TERM2)/TERM3)+1.)
SUB(NN) =F(NN)- TD
IF(N.LE.1) GO TO NINE
GPRIME = (F(2)-F(1))/(GG(2)-GG(1))
IF(N.EQ.2) GO TO ELEVEN
TEST1 = ABS(SUB(1))
TEST2 = ABS(SUB(2))
IF(TEST1.LE.TEST2) GO TO ELVEN
GG(1) = GG(2)
F(1) = F(2)
ELVEN..CONTINUE
ELEVEN..TD = GG(1)-(F(1)/GPRIME)
CONV = ABS( TD - GG(1) )

```

```

      IF(CONV.LE. .005) GO TO SEVEN
      IF(N.LE. 20) GO TO TRTEN
SEVEN..CONTINUE
SEVEN..CONTINUE
END
T20 = T0*T0
T30 = T20 * T0
T40 = T30 * T0
T50 = T40 * T0
T60 = T50 * T0
T70 = T60 * T0
T80 = T70 * T0
T21 = T1*T1
T31 = T21 * T1
T41 = T31 * T1
T51 = T41 * T1
T61 = T51 * T1
T71 = T61 * T1
T81 = T71 * T1
COMMENT LEAST SQUARE VAPOR SPECIFIC HEAT - URANIUM
LAST1 = AAO+ BBO*T0 + CCO*T20 + DDO*T30 + EEO*T40
LAST2 = FFO*T50 + GGO*T60 + HHO*T70
CPGOV = (LAST1 + LAST2) * FF2 / MOLV
INONE = AAO + BBO*T1 + CCO*T21 + DDO*T31 + EEO*T41
INTWO = FFO*T51 + GGO*T61 + HHO * T71
CPGIV = (INONE + INTWO ) * FF2 / MOLV
COMMENT LEAST SQUARE INERT SPECIFIC HEAT - NITROGEN
OUTONE= AAI +BBI*T0 +CCI*T20 +DDI*T30 +EEI *T40
OUTTWO= FFI*T50 +GGI*T60 +HHI*T70 +JJI*T80
CPGOI = (OUTONE + OUTTWO)*RU / MOLI
FIRST = AAI +BBI*T1 +CCI*T21 +DDI*T31 +EEI*T41
SECOND= FFI*T51 +GGI*T61 +HHI*T71 +JJI*T81
CPGII = (FIRST + SECOND ) * RU / MOLI
OUTPUT PI, TI, UI, CI, MI, MUI, PO, TO, UO, CO, MO, MUO, ...
S.G.J,RCRIT,DIRDX,PD,TD,TIME1,TIMEO,MIV,MOV,MII,MOI,...
JI,JO,GIN,GOUT,RHOI ,RHO0 ,CIV,COV,CII,COI,BVO,BIV,BII,BIO,HBMIV,...
HBMOV,HBMII,HBMOI,ENEGYI,ENEGYO,ENEGYT,FRCTCV,MTOTAL
END
END
TERMINAL
END
END

```

APPENDIX A. ENERGY EQUATION EXPANSION

Expansion of the term

$$\left(h + \frac{u^2}{2}\right) dG_x \quad (A.1)$$

is done in the following manner

$$\left(h + \frac{u^2}{2}\right) dG_x = \left(x_i^i h_i^i + x_v^i h_v^i + x_c^i h_c^i + \left(\frac{u^i}{2}\right)^2\right) (J^0 - J^i) \frac{dx}{a} \quad (A.2)$$

and results in the following individual terms,

$$\begin{aligned} \left(h + \frac{u^2}{2}\right) dG_x = & \left[\left(x_i^i h_i^i\right) J^0 + \left(x_v^i h_v^i\right) J^0 + \left(x_c^i h_c^i\right) J^0 + \left(\frac{u^i}{2}\right)^2 J^0 \right] \frac{dx}{a} \\ & - \left[\left(x_i^i h_i^i\right) J^i + \left(x_v^i h_v^i\right) J^i + \left(x_c^i h_c^i\right) J^i + \left(\frac{u^i}{2}\right)^2 J^i \right] \frac{dx}{a}. \end{aligned} \quad (A.3)$$

The solution of the mass diffusion equation presented in Eq. (A.2) implies the following assumptions about the mass transfer process:

1. Vapor which leaves control volume never returns; therefore, axial mass flux changes due to the vapor diffusion only.
2. Inert which enters control volume never leaves; therefore, axial mass flux changes due to inert diffusion only.
3. Condensed vapor is not handled and therefore never leaves the control volume.

Based on these assumptions the following terms in Eq. (A.3) disappear and are annotated in that equation appropriately. The result becomes

$$h + \frac{u^2}{2} dG_x = x_i^i h_i^i J^0 - x_v^i h_v^i J^i + J^0 \frac{u_x^2}{2} - J^i \frac{u_x^2}{2} \frac{dx}{a} \quad (A.4)$$

which is Eq. (35) in the main body of the paper.

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