

Implementation of Multiphase Species Transport into VERA-CS for Molten Salt Reactor Analysis

A Thesis Presented for the
Master of Science
Degree

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dedication...

Acknowledgments

I would like to thank...

Abstract

Abstract text goes here...

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Chapter 1

Introduction

TODO:

- Talk about the purpose of this project "To model gas sparging and noble gas removal."
- Talk about the economic and process advantages of using MSRs over other power options.
- Talk about CTF a little bit.
- Talk about what code I wrote and what code Bob wrote

Recent commercial interest in molten salt reactors (MSRs) creates the need for a deep understanding of fission product behavior. Some of the major features that make MSRs so appealing include: simple fuel cycle, fuel handling, waste disposal, versatility and economic benefits [1]. The molten salt reactor experiment (MSRE) is an 8-MW(th) nuclear reactor that was operated at the Oak Ridge Nation Laboratory (ORNL) from 1965-1969. The goal of the MSRE was to demonstrate the technical validity of such a reactor at a time when the global supply of uranium was still unknown. This reactor was successfully operated using both ^{235}U and ^{233}U [2].

The majority of MSR designs include having fissile material dissolved and flowing about a circulating loop. This greatly differs from traditional light water reactors (LWRs) where fissile material is maintained in a fixed solid form. Fissile material is dissolved in either a chloride or fluoride based salt and is often referred to as the solvent or carrier salt. Fluoride

salts generally used in applications where the reactor runs in the thermal region, chloride in the fast.

MSRs produce the unique challenge of allowing fission products to flow throughout the system. Fission products exist in multiple phases (gas, liquid, solid) with each phase interacting with various process equipment contained in the flow loop [3]. In order to accurately model a dynamic and steady-state fission product behavior all three phase fields must be resolved.

Fission products of main concern for this report and can be broken down in the three general categories for MSRs.

- Salt seekers
- Noble metals
- Noble gases

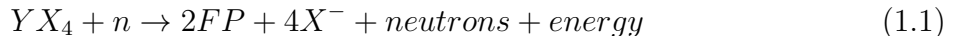
Salt seekers are fission products that will form stable ionic compounds with the carrier salt of interest (XF, XCl) where X is the fission products. Noble metals are fission products which will undergo redox reactions in solution to form solid elemental metals which can plate out in the system. Noble gases are fission products which will be in the gaseous state which are slightly soluble in the carrier salt and will be processed in an off-gas system [3].

Volatile fission products are a subclass of fission products that can include fission products from both noble metals and gases. These are known as volatile because their behavior is either: non-ideal, tend to change rapidly or unpredictable. With the term non-ideal meaning they have a noticeable impact on system behavior and cannot be ignored. These impacts include but not limited to: depositing on process equipment, neutron economy, forming collides and other undesired compounds.

1.1 Fission product elements

Although it is possible to generate all the elements on the Periodic Table we will only focus on a portion of fission products which are known to be volatile. Table 1.1 shows common

fission products in their respective categories based on MSRE experience [3]. Elements that have been removed in previous simulation efforts are listed in Table 1.2 [4]. A visual representation of elemental grouping on the periodic table is shown in Figure 1.1. In general, the nuclear reaction for a given fissionable isotope show in equation



Where Y is the fissionable isotope, X is the salt of interest (Cl or F) and FP are the fission products produced.

Table 1.1: Common fission products

Group	Element
Salt seekers	Rb, Sc, Sr, Ba, Y, Zr, Lanthanides
Noble metals	Nb^a , Mo, Tc, Ru, Rh, Pb, Ag, Sb, Te^b , I^b
Noble gases	Xe, Kr

^a Niobium is borderline and depends on redox condition of the salt

^b Iodine can form iodides and remain in the salt however it is included because of its tellurium predecessor [3]

Table 1.2: Common fission products removed from salt

Group	Element
Volatile gases	Xe, Kr
Noble metals	Se, Nb, Mo, Tc, Ru, Rh, Pb, Ag, Sb, Te
Seminoble metals	Zr, Cd, In, Sn
Volatile fluorides	Br, I
Rate earth elements	Y, La, Ce, Pr, Nd, Pm, Sm, Gd, Eu
Discard	Rb, Sr, Cs, Ba

1.1.1 Salt seekers

Salt seekers for stable fluoride or chloride compounds which are soluble in the carrier salt. These compounds are almost completely found in the molten fuel [5]. Stability of salt seekers

Periodic Table of the Elements

Legend:

- Volatile gases (Blue)
- Noble metals (Red)
- Seminoble metals (Green)
- Rare earth elements (Purple)
- Volatile fluorides (Yellow)
- Discard (Orange)

Figure 1.1: Periodic table with highlighted fission products.

is approximated by energy of formation. Compounds that have a more negative energy of formation will be more stable than those same elements forming other compounds. Many of the salt seeker fission products are rare earth elements with high neutron capture cross sections [6]. Neutron economy can be increased if these elements are separated.

1.1.2 Noble metals

Noble metals are born as ions from fission and decay of their precursors. They are unstable in the fuel salt and do not live as ions very long. Once they are born they quickly undergo reduction reactions and are homogeneously dispersed in the salt. This group of fission products tend to deposit on surfaces inside the flow loop, which can include: heat exchanger, pipes, reactor vessel and moderator. Noble metals also deposit on liquid-gas interfaces such as bubble surfaces and display some properties of surface active agents [7].

1.1.3 Noble gases

Fission product noble gases Xe and Kr form no compounds in a MSR and are sparingly soluble in the carrier salt. Because of this, noble gases tend to collect in any void fractions contained in the flow loop. Many present and past MSR designs utilize this fact and include gas stripping processes which entrained bubbles in the carrier salt. Process equipment may also be permeable to noble gases. In the case of the MSRE, moderator graphite was permeable and influence steady-state and transient noble gas behavior [5].

1.2 Historical MSR designs

Talk about the background of MSR designs

1.2.1 Molten Salt Reactor experiment

The MSRE was an experiment conducted in the 1960s at ORNL to deduce the validity of molten salt reactors. This was a fluid fueled 8-MW thermal nuclear reactor operating with the following materials represented in Table [2].

Insert table of MSRE material properties

Process description

During operation, molten salt is continuously circulated about a primary loop containing: the reactor vessel, fuel pump, and heat exchanger. This primary loop contained molten salt with the properties described in Table and a depiction of the process flow diagram is shown in Figure.

Salt enters the reactor vessel through holes at the top portion of the reactor. The holes impart a spiraling flow which moves down the sides of the reactor and up through the bottom head. Salt then flows up the moderator channel tubes shown in Figure 3. While the fuel salt is flowing up the channels, graphite moderates the neutrons, inducing fission and power generation. Upon exiting the core, the molten salt then enters the pump bowl shown in Figure 4.

Salt enters the fuel pump via the suction port at the bottom of the pump. The pump bowl had three main functions: sample collection, working pump for flow and off noble gas removal. The pump bowl had a head space which was constantly purged using a cover gas. Upon discharge, a portion of salt was redirected back into the head space of the pump bowl. This salt was forced through a perforated ring which allowed gas to be removed from the salt via the cover gas. After discharge, the salt flows through a heat exchanger which exits back into the reactor vessel and the process is repeated [2].

Figure of Process flow diagram

Figure of MSRE fuel channels

Figure of MSRE fuel pump

1.2.2 Molten Salt Demonstration Reactor

The molten salt demonstration reactor (MSDR) was a 750-MW thermal semi-commercial-scale nuclear reactor based off of technology demonstrated by the MSRE. This system utilized three different salts, the properties are shown in Table 4 [8].

Table of MSDR salt properties

Process description

During operation, salt is continuously circulated about a loop similar to that of the MSRE. The main difference that is of primary concern for this report is the way in which fission product gases are removed. A simplified flow diagram for the MSDR is shown in Figure 5.

Salt enters through the bottom of the reactor vessel at a temperature of 1050F. This concept involves moderating the neutrons using the same process in the MSRE, however the channels created by graphite matrix are non-uniform in the radial direction. This is done to ensure that the temperature rise in each channel is uniform through the core. Another key difference between the MSRE and MSDR core is the use of axial and radial graphite reflectors. The reflector has a twofold purpose, to conserve neutrons by reducing leakage and to shield the radiation reaching the vessel wall. Salt exits the top of the reactor at 1250F and enters the primary salt pump [8].

Unlike the MSRE fuel pump, gas separation does not happen in the primary salt pump. A portion (10%) of the pump discharge is redirected to a bypass line leading the salt back into the pump inlet. This bypass line contains both a gas stripper and bubble generator used to purge fission product gas from the system. The primary fuel pump discharges directly into the primary heat exchanger. This heat exchanger is a shell and tube design made with Hastelloy N material. After the heat exchanger, the fluid reenters the reactor vessel and the process is repeated.

Figure of flow diagram

1.2.3 Molten Salt Breeder Reactor

The molten salt breeder reactor (MSBR) was a conceptual design for a 1000-MW(e) single fluid molten salt reactor power plant. This MSR design operates on the Th-233U fuel cycle with both fissile and fertile materials mixed in a single fluid. The MSBR utilized two different salts in its design, their properties are summarized in Table 5 [9].

Process description

Chapter 2

Governing Equations

The governing species transport equations are implemented into a coding structure based on a finite volume discretization. First the integral volume formulation of the species transport equation is derived. Next volumetric source terms for isotopic species, boundary conditions and phase coupling are discussed. Finally, the interfacial area tacking method is derived.

2.1 Conservation of species for multi-phase flow

Consider the fixed control volume for two phase flow show in figure [2.1](#).

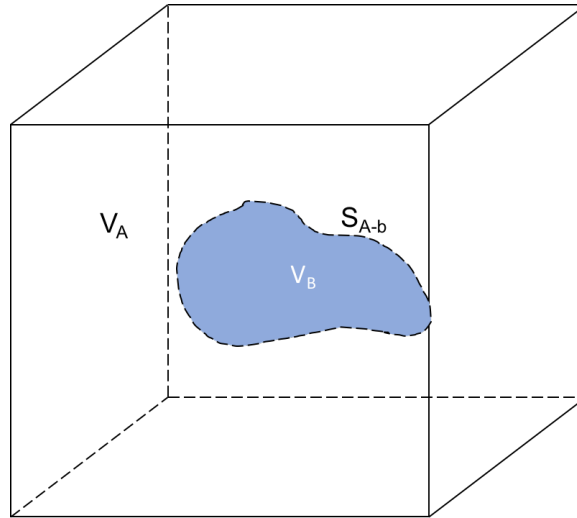


Figure 2.1: General control volume.

To derive the conservation of species relation we will first start with the relation for a system with a single phase. Let C be the conserved quantity of interest, amount per unit volume and let F be the flux, amount per unit area per time, passing through the unit normal surface of V . If the quantity C is being generated in control volume V then let its generation rate be denoted by C_V . Equation 2.3 represents the conservation of species in a fixed control volume.

$$\frac{\partial}{\partial t} \iiint_V C dV = - \iint_S n \cdot F dS + \iiint_V C_V dV \quad (2.1)$$

The differential operator in the first term of equation 2.3 can be brought inside the integral by applying Leibniz integral rule shown below.

$$\frac{\partial}{\partial t} \iiint_V C dV = \iiint_V \frac{\partial C}{\partial t} dV \quad (2.2)$$

This simplifies equation 2.3 to

$$\iiint_V \frac{\partial C}{\partial t} dV = - \iint_S n \cdot F dS + \iiint_V C_V dV \quad (2.3)$$

Let a phase be a region where C is a continuous function and interfaces are surfaces which can introduce discontinuities in C . Using equation 2.3, Leibniz integral rule is applied to the time derivative of each phase volume separately.

$$\frac{\partial}{\partial t} \iiint_{V_A} C dV = \iiint_{V_A} \frac{\partial C}{\partial t} dV + \iint_{S_I} C_A n_I \cdot v_I dS \quad (2.4)$$

$$\frac{\partial}{\partial t} \iiint_{V_B} C dV = \iiint_{V_B} \frac{\partial C}{\partial t} dV - \iint_{S_I} C_B n_I \cdot v_I dS \quad (2.5)$$

The last term in equations 2.4 and 2.5 take into account the velocity of the phase interface. In equation, this contribution is subtracted due to the unit normal point in the opposite direction. These two equations can be added together to represent the entire volume.

$$\iiint_V \frac{\partial C}{\partial t} dV = - \iint_S n \cdot F dS + \iiint_V C_V dV + \iint_{S_I} (C_A - C_B) n_I \cdot v_I dS \quad (2.6)$$

The last term in equation 2.6 is only present when the interface is moving and C is discontinuous. If a source term is present in the interface then the rate of formation per unit area of interface is C_S .

$$\iiint_V \frac{\partial C}{\partial t} dV = - \iint_S n \cdot F dS + \iiint_V C_V dV + \iint_{S_I} (C_A - C_B) n_I \cdot v_I dS + \iint_{S_I} C_S dS \quad (2.7)$$

When more than two phases are present, then the last two terms in equation 2.7 are represented as summations for all phases present. The integral formulation at an interface can also be represented by equation 2.8 [10].

$$\iint_S [(F - CV_I)_B - (F - CV_I)_A] dS = \iint_S C_S dS \quad (2.8)$$

Where the term $F - CV_I$ is the flux relative to the interface. For an arbitrary number of phases, species can be represented as a balance over each phase volume.

$$\iiint_{V_k} \frac{\partial C_k}{\partial t} dV = - \iint_S n \cdot F_k dS + \iiint_V C_{V,k} dV + \iint_{S_j} C_{S_k} dS \quad (2.9)$$

These set of equations are the fundamental relations regarding the conservation of species for a multi-phase system. In the case of a multi-component system, these same relations apply, however care must be taken when developing inner species interactions and phase migration.

2.2 Understanding Volumetric Source Terms

To understand the behavior for fission products it is first necessary to understand the source and sink terms for each product of interest. For a general reactor design these terms are represented in 2.1[11].

To understand the fate of volatile fission products in a MSR we must first derive a rate balance for each species of interest. Molten salts are characterized by having a melting point with reactors operating at temperatures well above liquidus temperatures. Because of this,

Table 2.1: Source and sink terms for chemical species and elemental isotopes

Source/Sink	Mechanisms involved
Direct from fission	Neutron flux, fission yield
Decay from parent atom	Decay constant
Transmutation	Neutron flux, microscopic
Phase/material migration	mass transfer, diffusion theory
Removal/addition system	Removal efficiency, addition rate
Chemical reaction	Reaction rate, thermodynamic equilibrium

it is assumed that all chemical reaction occurring in the salt happens instantaneously [6][7]. This also leads to the next assumption, that the salt is in a pseudo equilibrium state at almost all times. This allows for the calculation of thermophysical properties with the use of Gibbs free energy minimization.

2.2.1 Nuclear interactions

Because volumetric generation rates depend on nuclear reactions, it is important to first understand the mechanisms governing the physical interaction of particles and isotopes.

2.2.2 Importance of decay chains

Most fission products are atomically unstable and will decay into other elements based on half-lives and decay chains. These other elements may not be of the same fission products grouping. This greatly complicates fission product behavior and will influence the ultimate disposition. Consider the following decay scheme [7]:

$$\rightarrow Kr \rightarrow Rb \rightarrow Sr \rightarrow Y \rightarrow Zr \rightarrow Nb \rightarrow Mo \rightarrow \quad (2.10)$$

In this scheme Kr is a noble gas, Rb, Sr, Y, Zr are salt seekers, Mo is a noble metal with Nb being either a noble metal or salt seeker depending on redox condition of the carrier salt. This demonstrates the need to understand fission product decay chains. An understanding of half-lives relative to process cycle times is also needed. For example, if one of the precursors is removed from the system then so will all other elements. However, if removal time is short

compared to half-life then the chain is more likely to proceed and produce the elements further down the decay chain.

2.2.3 Direct from fission

Generation rate from fission is a function of neutron flux and fission yield shown in 2.11 [11].

$$rate = \gamma_i \Sigma_f \phi \quad (2.11)$$

Where γ_i , Σ_f and ϕ are fission yield, macroscopic fission cross section and neutron flux. The majority of generation from this term will be in the liquid salt phase. The key to understanding where this term will exist one must follow the dissolved salt. If the salt has a tendency to migrate into any process equipment for example a moderator, then the moderator material will have a fission source term. 3

2.2.4 Generation from decay

Generation rate from precursor decay is a function of decay constant and isotope number density, shown in equation 2.12 [11].

$$rate = \sum_{n=1}^N \lambda_i N_i \quad (2.12)$$

Where λ_i and N_i are decay constant and atomic number densities respectively. The decay constant is a natural constant meaning it is constant and only dependent on the isotope of interest. Nuclear decay can be both a source and sink term. If the isotope of interest is not stable then it will decay into another isotope, making it a sink. If the isotope is being generated from the decay of its parent it becomes a source term.

2.2.5 Generation from transmutation

Generation from transmutation is a function of neutron flux, number density and microscopic cross section, shown in 2.13 [11].

$$rate = \sum_{n=1}^N \sigma_i N_i \phi \quad (2.13)$$

Where σ_f , N_i , and ϕ are microscopic cross section, atomic number density and neutron flux. The Microscopic cross section is the probability of neutron-nuclear reaction for the nucleus i. Just like generation from decay, a summation is needed to account for all isotopes that can transmutate into isotope i or leave from isotope i transmuting into another isotope.

2.2.6 System removal and addition

This term is depended on the MSR design and must be evaluated for each design case. A simple example of removal rate from salt is shown in equation 2.14.

$$rate = S_{eff} N_i \quad (2.14)$$

Where S_{eff} and N_i are system removal efficiency and atomic number density. In this case system removal is defined by the atomic number density of isotope i. In general the system removal coefficient can be defined in a number of ways (i.e. volumetric or mass flow rate) so the appropriate conversions must be taken.

2.3 Boundary Conditions and Phase Coupling

For this work boundary conditions are defined as the mathematical formulation of physical phenomena that occur across phase/material boundaries in the solution domain. This can include both from phase migration (i.e. species dissolving or absorbing out of solution) and from material migration such as species plating out to a solid surface and or material migrating from liquid to solid surfaces. For any boundary (liquid-gas, liquid-solid, solid-gas) equation 2.8 is valid. In the absence of bulk movement across the boundary the normal component of the velocity in either phase is equal to the normal component of the interfacial velocity [10]. This simplifies the flux term F to only the diffusive flux component.

$$J_{in_2} - J_{in_1} = C_{S_{in}} \quad (2.15)$$

If there are no surface source terms at the surface then the two diffusive fluxes are equation to one another.

For binary and mixtures Fick's Law can be used when determining the species diffusive flux. Fick's Law describes the flux as a relation of a diffusion coefficient multiplied by the gradient of species concentration across a spacial length shown in table 2.2 [10].

Table 2.2: Fick's Law for various units

Reference velocity	Diffusive flux
\mathbf{v}_{mass}	$J = -\rho D_{AB} \nabla \omega_A$
\mathbf{v}_{molar}	$J = -C D_{AB} \nabla x_A$

For multicomponent mixtures a pseudobinary approximation can be used. In the assumption, a mixture of species is dissolved in a mixture where their concentrations dilute and it is assumed that they only interact with the solvent they are dissolved in.

2.3.1 Two-phase interface

In two-phase systems, the transfer of a species will continue along an interface until an equilibrium is reached. One common mechanism which describes this process is commonly known as two-film theory or two-resistance theory. Transport across an interface can be broken down into three steps.

1. Transport of species from bulk of phase 1 to phase 1 interface
2. Transport across the interface
3. Transport from phase 2 interface to phase 2 bulk

The two-resistance theory assumes that the rate for the overall transfer is determined from rate at which a species diffused from bulk to interface and from interface to bulk. In other words, the resistance transport across an interface is negligible [12].

At phase interfaces, a local equilibrium does not imply equal concentrations on both sides of the interface, as shown in figure 2.2. The two concentration are however, related to one another by the partition coefficient [10]. The partition coefficient $K_{P,i}$ is calculated based

on the relative solubility of species i in the two phases. For a liquid-gas interface, Henry's law can be used.

$$C_{i,1} = K_{P,i} C_{i,2} \quad (2.16)$$

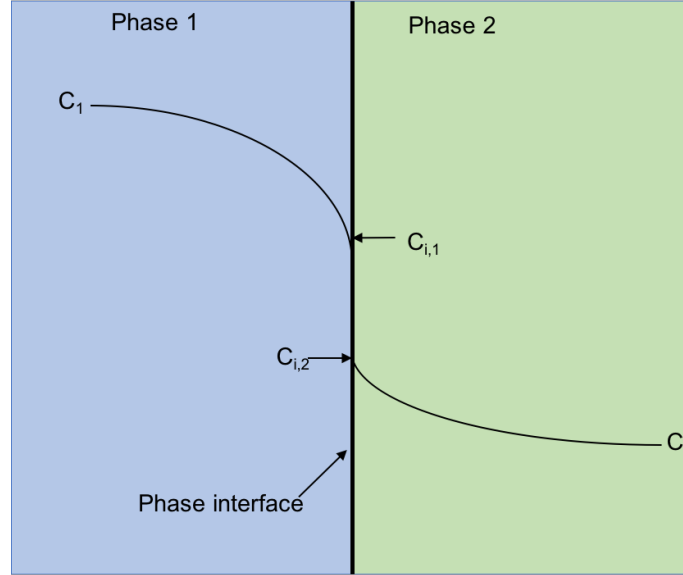


Figure 2.2: Concentration profile across an interface

In situations where there is no phase change (i.e. no bulk flow across the interface) a convection boundary condition can be applied [10].

$$J_{in,2} = J_{in,1} = k_2(C_{in,2} - C_{bulk}) = k_1(C_{bulk} - C_{in,1}) \quad (2.17)$$

Equation 2.17 states that the flux across a boundary is proportional to the difference in concentration between the bulk fluid in phase k and the interface multiplied by the mass transfer coefficient k_{ci} . It is important to note that the driving force for species transport is the concentration only in the phase in question. Instead of using individual mass transfer coefficients, equation 2.17 can also be represented using overall mass transfer coefficients K_i [13].

$$J_{in,2} = J_{in,1} = K_2(C_{e,2} - C_{bulk}) = K_1(C_{bulk} - C_{e,1}) \quad (2.18)$$

$C_{e,2}$ and $C_{e,1}$ represent the equilibrium concentration in either phase. Using equations 2.16, 2.17 and 2.18 the following expression is obtained to relation single-phase and two-phase mass transfer coefficients for a liquid-gas system.

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{m}{k_L} \quad (2.19)$$

$$\frac{1}{K_L} = \frac{1}{k_L} + \frac{1}{mk_G} \quad (2.20)$$

Where m is derived using Henry's law. For processes in which $m \gg 1$, $\frac{1}{mk_G}$ approaches zero and mass transfer is liquid-phase controlled. On the other hand, if $m \ll 1$, $\frac{1}{mk_G}$ becomes very large, making the system gas-phase controlled. For systems which obey Henry's Law, the over all mass transfer coefficient can be represented by

$$\frac{1}{K_L} = \frac{1}{k_L} + \frac{HRT}{k_G} \quad (2.21)$$

Therefore, if the Henry's law constant is very small i.e. the chemical species is sparsely soluble in the liquid, then the contribution from k_G is small and can be ignored.

2.4 Mass transfer coefficients

Mass transfer coefficients is of great importance to the understanding of interface mass transport. There are many difference ways in which mass transfer coefficients can be derived. For simple situations mass transfer coefficients can be derived using first principles [14]. However in industrial applications most of these coefficients are empirically defined from experimental data. In many situations a number of corrections may exist and one must be careful to use the appropriate coefficients. The Perrys's Chemical Engineers' Handbook [14] states the following heuristics to aid in choosing the appropriate coefficients.

1. Mass-transfer coefficients are derived from models. The must be employed in a similar model. For instance, if k is defined for a difference in concentration, it should only be used with an arithmetic concentration difference.

2. Semi-empirical correlations are often better than purely empirical or purely theoretical
3. Correlations with wide data sets
4. The analogy between heat and mass transfers holds over wider ranges than mass and momentum transfer.
5. More recent data is preferred over older data.
6. Complicated geometries requires the use of volumetric mass transfer coefficients.

2.4.1 Stagnant-film model

This approach assumes the steady state unidirectional diffusion through a stagnant film adjacent to the surface. The process of mass transfer is driven by molecular diffusion across the film thickness. Film thickness depends on depends on the Reynolds and Schmidt number. Using Fick's law, the mass transfer coefficient is proportional to the the diffusion coefficient over the film thickness [14]. For example, the liquid side mass transfer coefficient is represented by equation 2.22

$$k_L = \frac{D}{\delta_L} \quad (2.22)$$

2.4.2 Penetration theory

Penetration model was first proposed by R. Higbie in 1935 [15] to predict the mass transfer in a packed tower [14]. In this model, liquid flows across packing in laminar flow and is remixed in a transient fashion as you move across the packing material. The time average mass transfer coefficient is given by

$$k_L = 2\sqrt{\frac{D_L}{\pi t}} \quad (2.23)$$

Where t is the contact time which is not known in many cases.

2.4.3 Surface renewal theory

Danckwerts extended Penetration theory to what is known as Surface renewal theory [14]. Surface renewal theory allows for the continuous replacement of the liquid to the interior surface. The liquid is exposed to gas for finite lengths of time before being replaced with fresh fluid. Equation 2.24 represents the mass transfer coefficient.

$$k_L = \sqrt{D_L s} \quad (2.24)$$

Where s is the fraction rate of surface renewal.

2.4.4 Mass transfer correlations

The rate of mass transfer is often described by the Sherwood number which is analogous to the Nusselt number for heat transfer. The Sherwood number (Sh) is a dimensionless number defined as the convective mass flux over the diffusion flux at the interface.

$$Sh = \frac{h}{D/L} = \frac{\text{Convective mass transfer}}{\text{Diffusive mass transfer}} \quad (2.25)$$

In terms of dimensionless numbers, the Sherwood number can also be defined as a function of Reynolds number (Re) and Schmidt number (Sc). The Reynolds number represents the inertial forces over the viscous forces, with the Schmidt number corresponding to the viscous diffusion rate over the mass diffusion rate.

$$Re = \frac{\rho v L}{\mu} = \frac{\text{Inertial forces}}{\text{Viscous forces}} \quad (2.26)$$

$$Sc = \frac{\mu}{\rho D} = \frac{\text{Viscous diffusion}}{\text{Mass diffusion}} \quad (2.27)$$

There are many correlations for calculating the Sherwood number, all being problem specific. Another aspect to take into consideration is the fact that both equations 2.25 and 2.27 require the diffusion coefficient. For single small bubbles (modeled as solid spheres) of gas in dilute liquid systems the Sherwood correlation is given by [14]

$$Sh = \frac{kd_b}{D} = 1.0(ReSc)^{1/3} \quad d_b < 0.1\text{cm} \quad (2.28)$$

$$Sh = \frac{kd_b}{D} = 1.13(ReSc)^{1/2} \quad d_b > 0.5\text{cm} \quad (2.29)$$

During MSRE operations, the bubble size rang considered was 0.0127cm - 0.0508 cm [16], well in the range of equation 2.28.

2.5 Interfacial area tracking

The interfacial area plays a critical role in the calculation of species migration between two phases. These areas can remain relatively constant or (in the case of liquid-gas phase) be highly variable. Take for instance the diffusion of gas initially dissolved in the liquid phase into a rising bubble. As the the bubble rises the dissolved gas migrates into the bubble increases the number of moles the bubble contains. Also, as the bubble rises the effect of hydrostatic pressure diminishes. Therefor, as the bubble rises, its interfacial area increases. This is because pressure is inversely correlated to gas volume, so as the bubbles surrounding pressure decreases, its volume increases. For mass, as the bubble travels up the number of moles increase expanding the bubble volume.

Equations of state (EOS) describe the relations of four variables have on a gas phase substance. These include: pressure, temperature, volume and mass or moles. One of the most widely utilized EOS is the ideal gas law, shown in equation 2.30. The ideal gas law is valid for systems of low pressure, high specific volume, and no molecular interactions. There are other EOS which one can use, such as Van der Waals and Peng-Robinson which account for molecular interactions and other situations for which the ideal gas law falls short.

TODO: Link in what is said in chapter one about low OP pressure and how noble gases including He act as ideal gases. Talk about how to came up with the assumes you made.

For a bubble suspended in solution, its volume is calculated using the ideal gas law.

$$PV = nRT \quad (2.30)$$

P is pressure, V is volume, n is moles, T is temperature, and R is the universal gas constant. With all of the properties just mentioned to be represented as pertaining to the bubble i.e. T , P are the temperature and pressure inside the bubble.

Assuming the bubble is small and of spherical shape, the volume is calculated by,

$$V = \frac{\pi d^3}{6} \quad (2.31)$$

Where d is bubble diameter. Plugging into the idea gas law,

$$P \frac{\pi d^3}{6} = nRT \quad (2.32)$$

For static bubbles for which the forces are uniform across its surface, the Young-Laplace equation 2.33 is used to calculate the pressure inside of the gas bubble [10].

$$P_b = P_l + \frac{4\sigma_l}{d} \quad (2.33)$$

Where P_b , P_l , σ_l and d are bubble pressure, liquid pressure, surface tension, and bubble diameter. The bubbles are considered to be in thermal equilibrium with the surrounding fluid, meaning $T_b = T_l$. Plugging in equation 2.33 into 2.32 yields.

$$\left[P_l + \frac{4\sigma_l}{d} \right] \frac{\pi d^3}{6} = nRT_l \quad (2.34)$$

In equation 2.34 we are solving for bubble diameter. To do this, liquid pressure, temperature, and surface tension are acquired from the CTF solution domain. In order to calculate the number of moles a single gas bubble, a mole balance is preformed across each finite cell volume. Figure 2.3 shows a distribution of bubbles in a cell volume.

The number of moles, represented by n , is the summation of all chemical/elemental species in a the bubble. For a system for which we are trying to remove Xenon gas using Helium as our sparging gas, n could be a collection of Helium and Xenon gas. The number of moles in a single bubble is calculated by dividing the total moles of gas in the cell by the number of bubbles.

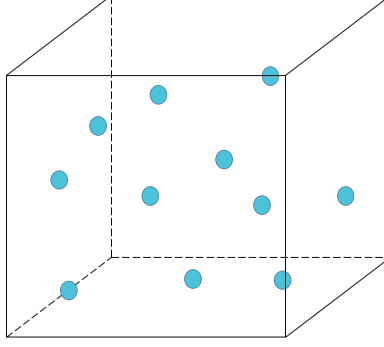


Figure 2.3: Bubbles dispersed in cell volume.

$$n_{bubble} = \frac{1}{\#of\ bubbles} \sum_{j=1}^k n_j \quad (2.35)$$

The number of bubbles determined from a species transport solve. Because the void fraction in the MSRE is so low ($>1.0\%$) [16], bubble interactions are neglected. Bubble diameter is solved using the assumption what all bubbles in the cell volume are the same size.

Two solution methods are employed to solve for bubble diameter. The first involves solving the non-linear equation 2.34 using Newtons Method, which will be discussed later. The second involves making the assumption $P_b \approx P_l$, this allows for the direct calculation of bubble diameter.

$$D = \left(\frac{6nRT_l}{\pi P_l} \right)^{1/3} \quad (2.36)$$

To justify this assumption, the contribution of bubble pressure due to surface tension must be low. Looking at equation 2.33, $4\sigma_l/d \rightarrow \infty$ as $d \rightarrow 0$. As the bubble gets smaller, the contribution from surface tension increases. The range of bubble sizes considered in the MSRE was between $0.0127 - 0.0508$ cm [16]. Figure 2.4 shows the contribution of surface tension to the bubble pressure for a range of bubbles considered in the MSRE.

From figure 2.4 as expected the contribution from surface tension is highest for smaller bubbles. As temperature increases surface tension slightly decreases leading to a smaller pressure contribution. For a system pressure of 1 and 2 atm, the maximum contribution to the bubble pressure would be 6.54% and 3.38% respectively.

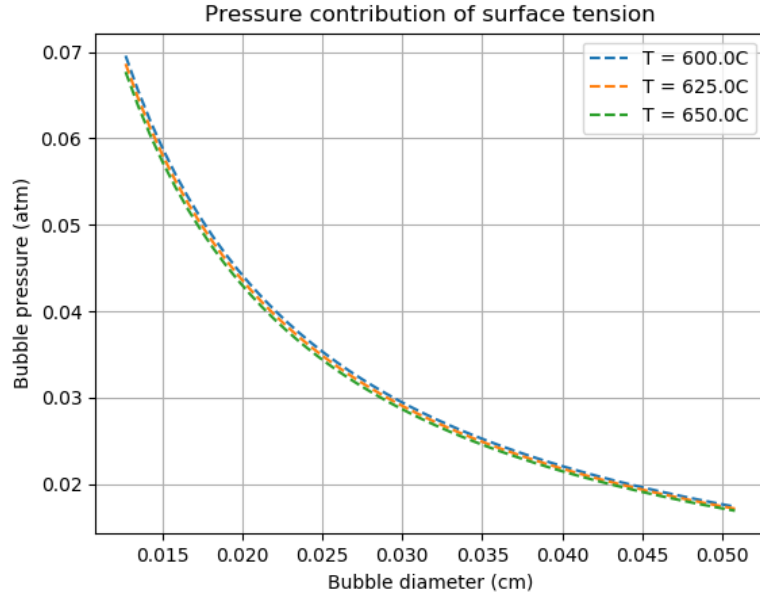


Figure 2.4: Pressure contribution of surface tension.

There are a number of boundary conditions required to solve the interfacial area. These conditions include inlet: temperature, pressure, number of bubbles, gas molar flow rate and bubble diameter. Together temperature, pressure, and bubble diameter are utilized in calculating the number of moles in a single bubble. This information, combined with the inlet gas flow rate is used to calculate the inlet number of bubbles.

Chapter 3

Behavior of Volatile Fission Products

3.1 Noble Gases

Volatile gases are elements or compounds which exist in the gaseous state and include both fission products Xe and Kr and other fission products. In a fluoride system both Br and I can form volatile fluorides. Noble gases Xe and Kr are only sparsely soluble in the molten salt and can be seen from the Henry's law constant for each $2.75\text{e}-9$ and $8.0\text{e}-9-9.0\text{e}-9$ respectively, with units moles per cc of salt per atmosphere [11]. Because of this low solubility, Xe and Kr tend to leave the salt and enter any circulating voids. During MSRE operation circulating voids existed under normal operating conditions with values ranging from 0.02 to 0.04 vol. %. Significant changes in void fraction could be influenced by temperature, overpressure, and fuel-pump level [16]. Noble gases also diffuse into process material. During MSRE operations, a graphite moderator was utilized in the reactor core. This graphite had a porosity which allowed noble gases to migrate inside, this migration is non-negligible when compared to other material migration mechanisms. As short-lived noble gases diffuse into the graphite, they decay or undergo transmutation. Once this process occurs, daughter products remain in the graphite [17].

3.1.1 Effect of circulating voids

Transport of volatile gases to circulating voids is an attractive mechanism for removal in MSR. These circulating voids can then undergo gas removal operations followed by an off-gas processing system. Usually, off-gas removal systems utilize a charcoal decay method which generates a holdup time allowing for gases to decay into stable isotopes. As the equilibrium, noble gas concentration increases in the circulating voids, it is to be expected that removal of said gases should increase. This effective removal process is controlled by the surface area of the circulating voids [18].

Salt density was also affected by circulating voids. As void fractions in the reactor increase this decreased the amount of fissile material. This would then cause a decrease in reactivity. During MSRE operations a 1% change in density would cause a 0.18% or 0.45% change in reactivity for ^{235}U and ^{233}U operations, respectively. Redox condition of the salt can also have an effect on void behavior through changes in surface tension and viscosity [19].

3.1.2 Cover gas solubility

During MSRE operations two cover gases were used as a transfer medium for fission product gas removal, helium and argon. A model was developed to describe ^{135}Xe behavior, however when argon was substituted for helium as the cover gas, variation of steady-state xenon poisoning was observed [16]. This was due to the relative differences in cover gas solubility. Argon is less soluble in the MSRE carrier salt than helium.

Bubble life can widely vary depending on liquid pressure and cover gas solubility. When pressure increases void fractions decrease due to compressibility and gas solubility. In these high-pressure regions, gas can transfer from the bubbles into the solution and back into the bubbles in low-pressure zones. This is due to cover gas solubility and bubble diameter. Figures 3.1 and 3.2 show the relative differences between argon and helium for the MSRE salt.

Figure 3.1 shows the void fraction as a function of time while varying pressure. In this case the initial pressure and void fractions are 20 psia and 1.5 vol% respectively. At time zero the liquid is instantly pressurized to 70 psia then linearly decreases to 20 psia after 25

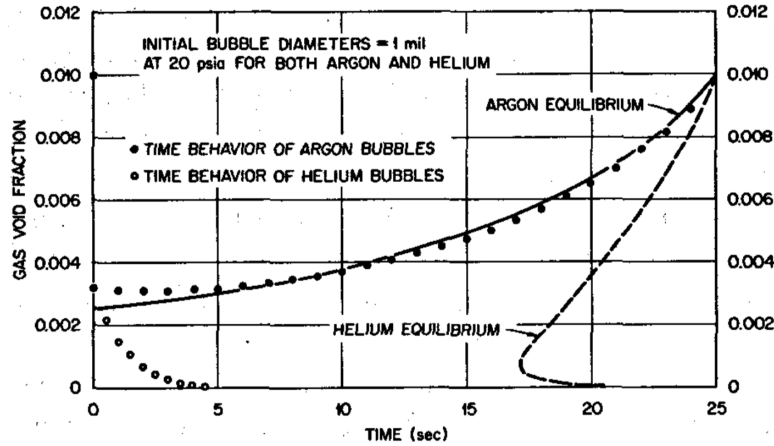


Figure 3.1: Time dependent liquid pressure effects on gas void fraction.

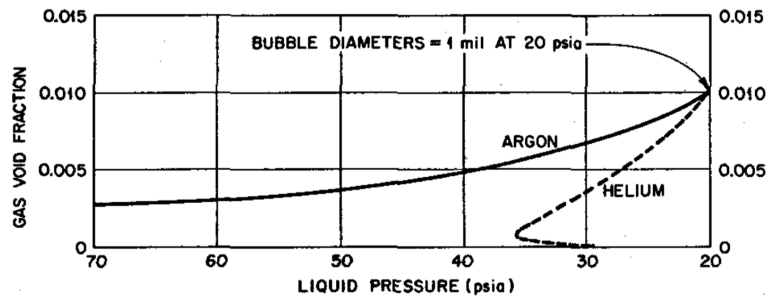


Figure 3.2: Equilibrium void fraction vs. liquid pressure.

seconds. Figure 3.2 shows the equilibrium void fraction vs liquid pressure. This figure shows the impact gas solubility can have on void fraction. Higher gas solubility means that under increased pressure the entire bubble can collapse thus allowing any isotope dissolved in the cover gas to redistribute into the carrier salt. Larger helium bubble also tended to retain their identity around the MSRE salt loop [20].

3.1.3 Bubble nucleation

TODO: Talk about bubble nucleation stuff

3.1.4 Noble gass transport

Mass transfer to moderator

Depending on reactor design, a moderator might be utilized in slowing down neutrons to induce thermal fissions. This moderator can be directly exposed to the circulating fuel salt, and therefore be subject to mass transfer to its surface along with subsequent diffusion into the material. It is important to note that all species included in the circulating salt are subject to mass transport on and into the moderator. This includes: fission products, fissile material and carrier salt. Three contributing factors that influence this rate include Reynolds number, moderator porosity and diffusion coefficients. As porosity and diffusion coefficient decrease, absorption rates into the moderator decrease. Typically, as Reynolds number increases mass transfer rates increase [21].

Pressure changes will not move salt into or out of moderator pores with any appreciable amount, so long as the pores are relatively small. Gas however will, and the rate will vary depending on the nature of the pressure change and the extent of pressure increase over the time interval. The amount of gas in the moderator is a function of the partial pressure in the carrier salt [x+16].

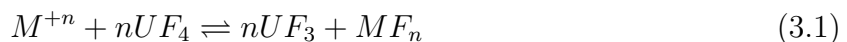
Generally, when one approaches transport from bulk fluid to an interface, boundary layer theory is applied. In this approach, the velocity fields are assumed to be in the laminar flow regime for distances very close to the solid interface. As the distance approaches z_0 shown in previously in figure ?? the fluid velocity approaches zero for a no slip boundary condition or non-zero for a slip boundary condition.

Mass transfer to circulating voids

TODO: Talk about how this section relates to experience in the MSRE. Like what I did in the section before this.

3.2 Noble Metals

The noble metals represent a class of fission products that are reduced by the fuel salt resulting in their existence to be in the solid metallic state. These reduction reactions are fast and as soon as the noble metals are born they quickly undergo reaction to become neutral metallic nanoparticles. Reactions of noble metals occur with the fissionable isotope in the fuel salt or components of vessel via the sample reaction shown in equation 3.1. For a structural metal, shown in 3.2.



In equation 3.1 fission product M is being reduced by UF_4 and in equation 3.2, M is being reduced by a structural metal E . Structural metal E will most likely form an ionic compound with free anions from the carrier salt.

These solid particles will have properties much similar to surface active agents which tend to gather around liquid-gas interfaces. During MSRE operations, these particles were also found to deposit in the off-gas system and pump bowl. It has also been seen that these noble metals tend to accumulate on vessel and heat exchanger surfaces [7].

3.2.1 Thermodynamic background

Oxidation and reduction reactions occur within the molten salt with fission products, fissile material and the metal container. These reactions go on to produce corrosion products and noble metals. A number of fission products may exist as noble metals or as salt seekers and their fate depends upon the redox condition of the salt.

Redox reactions involve the transfer of electron between reacting species. The species that receives electrons is reduced and the species that donates the electrons is oxidized. The redox condition is often used in referring to a systems propensity to reduce or oxidize a given species. During MSRE operations this term was used when referring to a fission

products tendency to reduce to their metallic state or for the corrosion of container metals [22]. Controlling these reactions (conditioning the salt) is accomplished by controlling the salts tendency to reduce. For either fluoride or chloride based salts, this is done by controlling the potential of diatomic gases anion.

As mentioned in section 2.2, because the reactor operates at such a high temperature, a pseudo equilibrium assumption can be made about the salt. This means that thermodynamic equilibrium is set and reaction equilibrium concentrations can be calculated. Some noble metal reactions almost reach completion while others do not. The ones that do not are known as semi noble metals and their reactivity will be dependent on the redox condition of the salt. In many previous MSR reports, redox condition was a loose term used to describe an elements propensity to undergo redox reactions. Redox condition of the salt is correlated to the chemical potential of the anion either Cl⁻ or F⁻ of the carrier salt [22].

For a given reversible chemical reaction,



the law of mass action says that,

$$K_a = \prod a_i^{v_i} = \frac{a_C^{v_C} a_D^{v_D}}{a_A^{v_A} a_B^{v_B}} \quad (3.4)$$

therefor at equilibrium and standard state the term on the right-hand side will equal a constant (K_a) where a_i is activity and v_i is stoichiometric coefficient. Chemical activity for the liquid phase can be defined in terms of a substances activity coefficient (γ) and molar fraction (x).

$$a_i = \gamma_i x_i \quad (3.5)$$

For an ideal solution, the activity coefficient is equal to one and for the gas phase, mole fraction can be replaced with partial pressure. The reaction quotient is related to the Gibbs energy of reaction by,

$$K_a = \exp\left(\frac{-\Delta G_{rxn}^o}{RT}\right) \quad (3.6)$$

The change in Gibbs energy with reaction is defined as,

$$\Delta G_{rxn}^o(T, P) = \Delta G_f(products) - \Delta G_f(reactants) \quad (3.7)$$

The summation of the Gibbs energy of formation for products minus reactants. Gibbs energy is a thermodynamic property which is defined as,

$$G = H - TS \quad (3.8)$$

where H is enthalpy, T is temperature and S is entropy. The change in Gibbs energy is equal to the maximum non-expansion work accompanying a process at constant temperature and pressure. When solutions undergo reactions, the extent is driven toward equilibrium by minimizing the Gibbs energy. This means that for a multicomponent mixture undergoing reactions, the equilibrium species concentrations can be calculated by minimizing the total Gibbs energy of the system.

In a classical thermodynamic chemical potential is defined as the change in Gibbs energy with number of moles.

$$\Delta \bar{G}_i^o = \mu_i = \frac{\partial(nG)}{\partial n_i} \quad (3.9)$$

When examining a chemical reaction, the potential of a particular species can be solved for by combining the relations for equilibrium constant and the definition of activity. For example, take reaction shown in equation 3.3. The law of mass action shows.

$$\exp\left(\frac{-\Delta G_{rxn}^o}{RT}\right) = \frac{a_C^{v_C} a_D^{v_D}}{a_A^{v_A} a_B^{v_B}} \quad (3.10)$$

The chemical potential for reactant A is,

$$\Delta \bar{G}_i^o = RT \ln(a_A) = \frac{1}{v_A} \left[RT \ln\left(\frac{a_C^{v_C} a_D^{v_D}}{a_B^{v_B}}\right) + \Delta G_{rxn} \right] \quad (3.11)$$

TODO: Talk about the significance of what you just talked about. Seems kinda out of place unless you tie it together.

3.2.2 Nanopartical nucleation

As nuclear operation processes throughout the lifetime of the plant, fission product will accumulate and reach a point where their concentrations become supersaturated. The same concept of fission gas nucleation applies to nanoparticles. When the species concentration reaches supersaturation, nucleation can occur. Homogeneous nucleation occurs when a cluster of particles uniformly forms in solution within the liquid phase. Heterogeneous nucleation forms at nucleation sites (phase boundaries, impurities).

Homogeneous nucleation can be examined thermodynamically by analyzing the total Gibbs energy of the particle [23]. The total Gibbs energy is the sum of the surface and bulk energy. For spherical particles, the total Gibbs energy is given by 3.12.

$$\Delta G = 4\pi r^2 \gamma + \frac{4}{3}\pi^3 \left[\frac{-k_B T \ln(C/C_o)}{v} \right] \quad (3.12)$$

where, γ , T , k_B , C , C_o , v and r are surface energy, temperature, Boltzmann's constant, solute concentration, solute solubility, molar volume and particle radius, respectively. Because the surface energy is always positive and the solid energy always negative, a maximum Gibbs energy can be found by taking the derivative of equation 3.12 with respect to r and setting it equal to zero. This results in the critical size, r_{crit} and energy G_{crit} [23].

$$r_{crit} = \frac{2\gamma v}{k_B T \ln(C/C_o)} \quad (3.13)$$

$$\Delta G_{crit}^{homo} = \frac{4}{3}\pi r_{crit}^2 \gamma \quad (3.14)$$

Critical energy is the barrier energy or the minimum energy required for particles to remain stable in solution. Critical size is the minimum radius for a particle to survive. The rate of nucleation per unit volume is given by 3.15 [24] with A being a pre-exponential factor.

$$\frac{dN}{dt} = A \exp \left[\frac{16\pi\gamma^3 v^3}{3k_B^3 T^3 (\ln(C/C_o))^2} \right] \quad (3.15)$$

From equation 3.15, it can be seen that supersaturation has the largest effect on nucleation rate. If impurities of another phase are present, the energy required for nucleation is decreased. The critical energy required for heterogeneous nucleation is represented by equation 3.16. Where ϕ is a factor dependent on contact angle [23].

$$\Delta G_{crit}^{hetero} = \phi \Delta G_{crit}^{homo} \quad (3.16)$$

$$\phi = \frac{(2 + \cos \theta)(1 - \cos \theta)^2}{4} \quad (3.17)$$

Nanoparticle growth is often divided into two steps, diffusion to particle surface and surface deposition reaction [24]. Rate of disposition on particle surface can be either determined by the diffusion of particulates to the nanoparticle surface, by surface reaction or a combination.

3.2.3 Noble metal transport

One of the key requirements for understanding noble metal transport is to first understand their behavior relative to the fluid velocity field. The homogeneous equilibrium model is a simple mixture model which describes the multiphase model as a pseudo single-phase mixture in thermodynamic equilibrium. This model includes assumptions much like the ones which were used earlier to describe two-phase liquid bubble transport. The primary being that the relative velocities between each phase are zero and each phase is in thermodynamic equilibrium with another.

Many different surface environments exist in a molten salt loop, which include; moderator, heat exchanger, reactor wall, piping/process equipment and liquid-gas interfaces. Many of these surfaces may not be in thermodynamic equilibrium with the bulk fluid, creating temperature gradients which can affect the amount of noble metal which can deposit. One example of this is in the heat exchanger where bulk fluid temperature is changing as a function

of heat exchanger length and fluid velocity. Solubility, which is a function of temperature, begins to change which can lead to a supersaturated state of the liquid solution, leading to increased noble metal deposition. Other processes which can affect surface deposition rates include fluid turbulence, torturous paths and surface area for transfer.

For noble metal deposition on surfaces, the same convention in which the boundary layer is ignored and a linear convection boundary condition is utilized, equation 2.17. The trick for using this assumption is knowing the mass transfer coefficient and the surface concentration. Surface concentration can only be assessed if certain assumptions are used. These assumptions deal with the noble metals propensity to stick and stay on the surface and diffuse into the material. A common assumption is to treat the surface material as an infinite sink, making the concentration at the surface zero. This assumption can be used when solving a steady state problem where the surface concentration is unknown. In a time dependent problem, the surface concentration can be assumed to be equal to zero or a given constant. Then for all times greater the surface concentration would be the integral of the flux from zero to the current time or the previous time step.

An interesting note that comes into play when discussing mass transfer in a saturated system is the affect heterogeneous nucleation has on transfer coefficient. Depending on how the mass transfer coefficient is obtained, nucleation may not be included in the transfer rate. This must then be added to the migration model to obtain a more accurate model. However, if the liquid solution never reaches a point of super saturation, then nucleation does not occur.

3.2.4 Noble metal behavior

Observations made during the MSRE impart great insight into the general behavior of noble metals in a molten salt environment. During operations, noble metals played a role in many key processes which effected system wide behavior. The behavior includes; deposition on liquid-gas interfaces, plating to container surfaces, and entrapment in the off-gas system.

Liquid-gas interactions

As previously noted, noble metals have a tendency to migrate to liquid gas interfaces. This tendency to collect on liquid-gas interfaces follows the same physical model as was surface deposition, however the question remains in finding the surface concentration. During MSRE operation an analytical model was developed for determining migration of noble metals [7]. From these models, as well as experimental results, it was found that noble metals did not have a tendency to stay on the bubble surface once they became attached.

Solid surface deposition

Chapter 4

CTF Methodology

TODO: Give introduction to CTF

4.1 Governing Equations

CTF works on a two-fluid model with three separate fluid fields: liquid film, liquid droplets, and vapor. Each phase is field uses three conservation equations with each phase being modeled with its one mass, momentum and energy equations. CTF simplifies the conservation equations using the sub-channel approach. This approach considers two flow directions, axial and lateral flow. Axial flow denotes the main flow direction where lateral flow represents any orthogonal direction to axial flow. This approach is suitable for situations where flow is dominated by a single direction. For more information on CTF please refer to [1].

4.1.1 Mass conservation

The conservation of mass for each field k is represented in Cartesian form in equation 4.1

$$\frac{\partial}{\partial t} (\alpha_k \rho_k) + \frac{\partial}{\partial x} (\alpha_k \rho_k u_k) + \frac{\partial}{\partial y} (\alpha_k \rho_k v_k) + \frac{\partial}{\partial z} (\alpha_k \rho_k w_k) = L_k + M_e^{T''' } \quad (4.1)$$

The first term on the left hand side represents the change in density with time, followed by convection terms. On the right hand side L_k is the inter-phase mass transfer in and out of

phase k and can represent evaporation/ condensation or entrainment/de-entrainment. $M_e^{T'''}$ is the mass transfer from turbulent mixing and void drift only in the lateral direction which is modeled using simple turbulent diffusion and void drift models. Equation 4.1 represented in sub-channel form is shown in equation 4.2.

$$\frac{\partial}{\partial t} (\alpha_k \rho_k) + \frac{\partial}{\partial x} (\alpha_k \rho_k u_k) + \sum_{k=1}^{nk} (\alpha_v \rho_v w_v)_k = L_k + \sum_{k=1}^{nk} \left(M_v^{T'''} \right)_k \quad (4.2)$$

Where w_k is the lateral flow velocity and is summed over all connected lateral cells.

4.1.2 Momentum conservation

4.1.3 Energy conservation

4.2 Solution Methods

4.3 Fluid Properties

Chapter 5

Implementation of Species Transport

5.1 Volume Averaging

5.2 Discretization

5.3 Solution Methods

5.4 Verification Problems

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Appendices

A Summary of Equations

some text here

A.1 Cartesian

some equations here

A.2 Cylindrical

some equations also here

B Summary of Stuff

some text here

B.1 More Things

some equations here

B.2 Other Aspects

some equations also here

Vita

Vita goes here. The vita should be a brief biography about the author written in third person and paragraph format. It should not be the author's resume or CV.