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PARAMETRIC STUDIES OF OFF-GAS RELEASE DURING IN SITU VITRIFICATION

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ABSTRACT

Off-gases are released from underground sources during the In Situ Vitrification (ISV) process. Most of these gases will be generated beyond the melt front where advancing high temperatures will cause pyrolysis and vaporization of organic and volatile materials. Some of these gases will enter the bottom of the melt pool and propagate upwards to the surface where they will enter the ISV confinement hood. A computer code called OGRE (Off-Gas RElease) has been written to model bubble-rise physics in the melt pool for given volumetric gas flux rates into the bottom of the pool. The models incorporated into OGRE have previously been reported. The purpose of the present document is to report the results of a series of parametric studies performed with OGRE. The numerical studies involve the variation of seventeen parameters for each of the two different inlet bubble-size models. Results indicate that while predictions appear qualitatively reasonable, additional development of the agglomeration and drift flux models is needed. This development will require experimental data for bubble formation and terminal velocity.

CONTENTS

ABSTRACT	ii
NOMENCLATURE	vi
1. INTRODUCTION	1
2. PARAMETRIC STUDY BASE CASES	2
3. PARAMETRIC STUDIES	8
3.1 Variation of Volumetric Inflow at Melt Pool Boundary	8
3.2 Terminal Velocity Variation	12
3.3 Variation of Agglomeration Model Coefficient	12
3.4 Variation of Agglomeration Model Exponent	17
3.5 Variation of Average Gas Rise Velocity Model Exponent	17
3.6 Variation of the Critical Weber Number for Bubble Breakup	20
3.7 Variation of a Linear Temperature Rise in the Liquid Phase	26
3.8 Variation of a Parabolic Temperature Rise in the Liquid Phase	26
3.9 Variation of a Linear Temperature Drop in the Liquid Phase	31
3.10 Variation of a Parabolic Temperature Drop in the Liquid Phase	31
3.11 Spatial Nodalization Variation	31
3.12 Temporal Nodalization Variation	38
3.13 Variation of the Liquid Phase Velocity	38
3.14 Variation of the Liquid Phase Surface Tension	38
3.15 Variation of the Liquid Phase Density	46
3.16 Confinement Hood Pressure Variation	46
3.17 Variation of the Pore Radius at the Melt Pool Inlet Boundary	51

4. CONCLUSIONS	54
REFERENCES	56
APPENDIX A--INPUT DECK FOR THE BASE CASE ONE CALCULATION	A-1
APPENDIX B--DERIVATION OF THE EFFECT OF HOOD PRESSURE ON OFF-GAS RELEASE	B-1
APPENDIX C--SAMPLE PRESSURE SPIKE CALCULATION	C-1

FIGURES

1. Base case calculation for Case One	5
2. Base case calculation for Case Two	6
3. Gas inflow variation at melt front for Case One	10
4. Gas inflow variation at melt front for Case Two	11
5. Fixed bubble terminal velocity variation for Case One	13
6. Fixed bubble terminal velocity variation for Case Two	14
7. Agglomeration model coefficient "a" variation for Case One	15
8. Agglomeration model coefficient "a" variation for Case Two	16
9. Agglomeration model exponent "b" variation for Case One	18
10. Agglomeration model exponent "b" variation for Case Two	19
11. Drift flux model exponent "i" variation for Case One	21
12. Drift flux model exponent "i" variation for Case Two	22
13. Bubble breakup model variation for Case One	24
14. Bubble breakup model variation for Case Two	25
15. Linear temperature rise variation for Case One	27
16. Linear temperature rise variation for Case Two	28
17. Parabolic temperature rise variation for Case One	29
18. Parabolic temperature rise variation for Case Two	30

19. Linear temperature drop variation for Case One	32
20. Linear temperature drop variation for Case Two	33
21. Parabolic temperature drop variation for Case One	34
22. Parabolic temperature drop variation for Case Two	35
23. Special nodalization variation for Case One	36
24. Special nodalization variation for Case Two	37
25. Temporal nodalization variation for Case One	39
26. Temporal nodalization variation for Case Two	40
27. Melt velocity variation for Case One	41
28. Melt velocity variation for Case Two	42
29. Melt surface tension variation for Case One	44
30. Melt surface tension variation for Case Two	45
31. Melt density variation for Case One	47
32. Melt density variation for Case Two	48
33. Hood pressure variation for Case One	49
34. Hood pressure variation for Case Two	50
35. Melt front pore radius variation for Case One	52
36. Melt front pore radius variation for Case Two	53

TABLES

2.1 Base case values for the parametric studies	4
C-1 Parametric values	C-2

NOMENCLATURE

<u>Symbol</u>	<u>Description of Symbol</u>
a	Cross sectional area for gas flow (m^2)
D_m	Depth of melt/solid interface (m)
D_s	Subsidence depth of the top melt surface (m)
g	Gravitational acceleration (m/s^2)
N_p	Number of pores at the melt front
P_c	Capillary pressure between the gas and melt (liquid) phases (Pascals)
P_g	Pressure in the gas phase (Pascals)
P_l	Pressure in the melt (liquid) phase (Pascals)
Q_0	Volumetric flow rate through an effective orifice (m^3/s)
q_g	Mass flux of gas at the melt/solid interface (kg/m^2-s)
R	Gas constant (m^2/s^2-K)
R_b	Effective bubble radius (m)
S	Average vertical gas velocity (m/s)
S_∞	Terminal rise velocity (m/s)
T	Temperature of the liquid phase (K)
v_l	Vertical liquid velocity (m/s)
We_{crit}	Critical Weber number

Greek

α	Volumetric concentration of gas (void fraction)
μ_l	Dynamic viscosity of the liquid (kg/m-s)
ω	Relaxation parameter
ρ_g	Gas density (kg/m ³)
ρ_l	Liquid density (kg/m ³)
σ	Surface tension (kg/s ²)

Subscripts

b	Bubble, bottom
c	Capillary
g	Gas
∞	Terminal (steady state)
l	Liquid
m	Melt
0	Initial
s	Subsidence surface
t	Top

Superscripts

i	Agglomeration exponent
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1. INTRODUCTION

During the In Situ Vittrification (ISV) process, high temperatures will be experienced by buried waste materials ahead of the advancing melt front. These high temperatures will cause vaporization and pyrolysis of volatile and organic wastes ahead of the melt zone. The sharply increased local pressures associated with these thermodynamic and chemical changes will drive the gas phase products away from their sources. Some of these gases will penetrate the melt pool and rise toward the ground surface where they may enter the ISV confinement hood. The models that attempt to simulate the rise, agglomeration, and breakup of these gas bubbles in the melt pool are coded in the program called OGRE (Off-Gas RElease).¹

There are a total of seventeen parameters associated with the numerical procedures, initial and boundary conditions, and bubble-size models contained in OGRE. In addition, there are two different bubble-size models coded into OGRE, each of which is designed to determine the inlet bubble sizes of gases moving into the liquid phase. The objectives of the present study are to vary each of the 17 parameters for the two bubble-size models to determine off-gas response to the parameters and assess the suitability of present models in OGRE for modeling the transient migration of off-gases through the melt zone. In this way, the importance of each parameter may be separately assessed.

The organization of the report is as follows. Section 2 describes the inlet bubble-size models and the two base cases used in this study. Section 3 describes the results of the numerical studies for each of the parameters varied. Section 4 summarizes conclusions and indicates further research that should be pursued to help in model development.

2. PARAMETRIC STUDY BASE CASES

The parametric studies reported herein are derived from two similar base cases, each of which is based on a particular inlet bubble-size model. The transport equation used in OGRE is dependent on the terminal bubble rise velocity which in turn is dependent on the bubble size.¹ As reported in Reference 1, there are two models for the inlet bubble size for gases that enter the melt zone. The first model specifies a bubble size radius which is dependent upon the volumetric flow rate of gas entering the melt and assumes that gas effectively enters through an orifice.¹ The model equation is given by

$$R_b (D_m) = 0.648 \left(\frac{Q_o^2}{g} \right)^{1/5} \quad (2.1)$$

where R_b is the bubble radius, D_m is the depth of the melt pool, Q_o is the volumetric flow rate through one effective orifice, and g is the acceleration due to gravity. Equation (2.1) is more appropriate when off-gases are produced on a large scale or by a sudden surge such as when a drum is breached by the melt front.

The second model is based on the pore size of a porous media such as a plate at the bottom of a column of liquid with orifices drilled into it and through which gas is forced. The analogy for the ISV process is the layer of porous material adjacent to the melt front through which the gases must pass. The second model for the inlet bubble size is given by

$$R_b (D_m) = \left[\frac{\sigma R_p}{g(\rho_l - \rho_g)} \right]^{1/3} \quad (2.2)$$

where σ is the surface tension of the liquid phase, R_p is an average pore radius of the porous medium, and ρ_l and ρ_g are liquid and gas densities, respectively. Equation (2.2) is appropriate for determining the inlet bubble

size when the bubbles are formed in the porous soil layer prior to entering the melt zone.

The base case situations are constructed by simulating an hypothesized ISV pool two meters deep and five meters in diameter. Properties used for the liquid phase are taken from measured values of soil and mixtures involving silicon dioxide.^{1,2,3} (Improved values for these properties may be necessary for more accurate simulations). The maximum bubble size allowed for bubble agglomeration is set by specifying a critical Weber number.¹ For all cases in the present study, except for the case where the Weber number is varied, a relatively high value of critical Weber number (5000) is specified, effectively eliminating any bubble breakup.

The total volumetric gas inflow (gas source) rate used for base case one is $236 \text{ m}^3/\text{s}$ (500 CFM), a value based on an average off-gas production rate calculation.⁴ The input deck for base case one is given in Appendix A. The total volumetric inflow rate for base case two is lower than for base case one. Also, since the bubbles for base case two are smaller and move more slowly than for base case one, larger time steps are used for base case two than for base case one. Table 2.1 lists the settings for the model parameters, initial and boundary conditions, and numerical parameters for the two base cases. The models associated with the parameters listed in Table 2.1 are fully described in Reference 1. Each parameter is later varied independently to assess the variation of the model results to that parameter. Note that the vertical temperature variation of the liquid phase must be specified. For the base cases, no variation in temperature is assumed, as indicated. For the parametric studies, the temperature is assumed to either increase or decrease with depth in either a parabolic or linear fashion. Figures 1 and 2 show the transient release rates for base cases one and two, respectively. As can be seen, the gas flow rates increase asymptotically with time to values of $0.36 \text{ m}^3/\text{s}$ and $0.075 \text{ m}^3/\text{s}$, in times of 30 and 100 seconds, respectively, for the two base cases.

With the increasing or decreasing, linear or quadratic variation of temperature in the melt pool, Table 2.1 indicates the seventeen parameters

Table 2.1. Base case values for the parametric studies

Parameter	Value for Case One	Value for Case Two
Gas source ($\text{kg/m}^2\text{-s}$)	3.5766e-3	7.45125e-4
Terminal velocity (m/s)	computed, not set (approx. 0.1)	computed, not set (approx. 0.1)
Agglomeration coefficient "a"	8.0	8.0
Agglomeration exponent "b"	2.0	2.0
Drift flux exponent "i"	3.0	3.0
Critical Weber number	5000.0	5000.0
Linear temperature change (K)	0.0	0.0
Parabolic temperature change (K)	0.0	0.0
Delta x (m)	0.1	0.1
Delta t (s)	0.1	0.2
Melt velocity (m/s)	0.0	0.0
Melt surface tension (kg/s^2)	0.2731	0.2731
Melt density (kg/m^3)	2700.0	2700.0
Hood pressure (Pa)	1.0e+5	1.0e+5
Port radius (m)	4.11008e-2	4.11008e-2

Figure 1. Base case calculation for Case One

Figure 2. Base case calculation for Case Two

that are varied about the two base cases that form the envelope for the present set of parametric studies. A set of forty runs is made while varying each parameter listed, one at a time, for each of the two base cases. The following section reports the results for the various parametric studies.

3. PARAMETRIC STUDIES

This section reports the results for seventeen parametric studies. Each parametric study consists of individually varying one parameter for each of the two base cases as given in Section 2, while holding the other parameters constant at the conditions indicated in Table 2.1. Forty variations of the parameters are made while recording the transient effects on the gas release rate. Results are plotted using contour and surface maps.

In the following sections, those studies wherein one of the 17 parameters is varied from base case one values will be referred to as case one results for that parameter. Those based on base case two will be referred to as case two results. For each parametric study, results are presented first for case one and then for case two. Both two- and three-dimensional plots are shown. For the 3D plots, the gas release rate is always shown as the vertical (surface map) coordinate, while the parameter being varied and time are represented by the coordinates of the plane below. The same information is provided in the 2D plot where the contours are easier to discern than they are in the 3D plot.

It is noted that for the conditions listed in Table 2.1, inlet bubble radii of approximately 1.5 and 0.75 cm are generated for base cases one and two, respectively.

3.1 Variation of Volumetric Inflow at Melt Pool Boundary

The volumetric flow of off-gases into the bottom of the melt pool is varied for this study. This is accomplished by varying the velocity of the incoming gases, as the total inlet pore area is held constant. An increase in the local inlet flow velocity causes the local volumetric flow rate Q_0 to increase. Examination of Equations (2.1) and (2.2) indicates that the inlet bubble size for case one will be affected by varying Q_0 , while inlet bubble sizes for case two will not.

Figure 3 presents results for case one. As the volumetric inflow (gas source) rate increases, the asymptotic gas release rate increases, as expected, while the time required to reach steady state decreases. The reason for the decrease in the time it takes to achieve steady state with increasing gas source is that as the inlet bubble size increases, buoyancy forces on the bubble increase, accelerating the process. Figure 2.2 in Reference 1 generally supports this conclusion.

Case two results are presented in Figure 4. A rise in gas release rate, similar to case one results, is recorded here as the gas source rate increases, as expected. However, in contrast to the results for case one, the time required to achieve steady state increases with increasing gas inflow. This can be explained as follows. Since the inlet bubble size remains the same for case two, and since the terminal velocity is directly related to bubble size, no change in terminal velocity occurs as gas inflow increases as it does for case one. On the other hand, other effects become important. The empirically based equation for the average gas rise velocity is given as¹

$$\bar{S} = S_{\infty} (1 - \alpha)^{i-1} + v_l \quad (3.1)$$

where S_{∞} is the terminal velocity, α is the void fraction, 'i' is an empirical constant (set to $i = 3$), and v_l is the liquid phase velocity. While an increase in terminal velocity will increase the average gas velocity, an increase in void fraction α does just the opposite. The increase in void fraction for case two is apparently the reason that the average gas velocity decreases as the gas inflow and, hence, the void fraction increase. Of course, as the average gas velocity decreases, the time required to achieve steady state increases.

The contrasting results for the two cases emphasize the importance of using the appropriate inlet bubble model for the simulation. Additional experimental data is required to help determine which bubble size model should be used for particular situations.

Figure 3. Gas inflow at melt front variation for Case One

Figure 4. Gas inflow at melt front variation for Case Two

3.2 Terminal Velocity Variation

The terminal velocity is a quantity that is computed in OGRE based on the values of other parameters.¹ For this parametric study, however, the terminal velocity is specified as a given value for each run. All bubbles, regardless of size are required to travel with the same terminal velocity. Figures 5 and 6 present results for case one and case two, respectively. As shown, the asymptotic values for gas release increase as the terminal velocity increases, while the time required to achieve steady state decreases, as expected. It is also obvious that the value for the terminal velocity has a dramatic effect on the time required to achieve steady state, while the effect on the asymptotic release rate value is not so important.

3.3 Variation of Agglomeration Model Coefficient

Bubble growth in the liquid phase results from two contributory effects. The first effect is due to the decrease in hydrostatic pressure as the bubble rises. The second is due to agglomeration of neighboring bubbles as they rise through the liquid phase. The phenomenological model used to account for agglomeration in OGRE is¹:

$$V_{ba}(x) = \left\{ 1 + a \left[1 - (x - D_s) / (D_m - D_s) \right]^b \right\} V_b(D_m), \quad D_m \leq x \leq D_s \quad (3.2)$$

where V_{ba} is the bubble volume due to agglomeration, 'a' is an empirical coefficient, D_m and D_s are the melt pool and subsidence depths, respectively, x is distance from the ground level (positive upward), 'b' is an empirical exponent, and V_b is the effective bubble volume. The coefficient 'a' represents the ratio of the size of a bubble at the top of the pool versus its size at the bottom.

The present parametric study varies the value of the model coefficient 'a' in Equation (3.2) above. It should be noted that the terminal velocities for this and all following studies are computed by OGRE based on various parameters as indicated in Reference 1. Figures 7 and 8 illustrate the effects of the variation of the coefficient 'a' on the gas release rates for

Figure 5. Fixed bubble terminal velocity variation for Case One

Figure 6. Fixed bubble terminal velocity variation for Case Two

Figure 7. Agglomeration model coefficient "a" variation for Case One

Figure 8. Agglomeration model coefficient "a" variation for Case Two

cases one and two, respectively. While no effect is apparent on the final release rate for either case, the time required to achieve steady state is increased as coefficient 'a' is decreased. This result is due to the fact that larger bubbles, resulting from an increase in 'a', accelerate faster due to an increase in buoyancy force as discussed in Section 3.1.

3.4 Variation of Agglomeration Model Exponent

The subject of this parametric study is the variation of the model exponent 'b' in the agglomeration model represented by Equation (3.2) above. For larger values of 'b', the agglomeration process is delayed and can be forced to occur very near to the top boundary of the melt pool. For small values of the exponent, the process is enhanced, causing bubbles to agglomerate earlier. This response is illustrated in the numerical data plotted in Figures 9 and 10 for cases one and two, respectively. As 'b' diminishes, agglomeration occurs earlier, producing larger bubbles which rise faster and reach steady state earlier.

A problem with the agglomeration model not highlighted by the above parametric study is the fact that the model represents a distribution of average bubble volume for the steady state case. However, when it is used in a transient calculation, the presence of the factor $V_b(D_m)$ in (3.2) produces unphysical results. For example, consider a step change in the inlet gas flow at the bottom of the melt pool caused, for instance, by suddenly breaching a closed drum. According to the agglomeration model, Equation (3.2), the agglomeration of bubbles everywhere in the melt pool is directly and instantaneously affected by the volume of bubbles $V_b(D_m)$ entering the melt pool. This, of course, is unphysical since the bubbles must travel from the inlet boundary at a finite velocity before they can combine in other regions of the pool. Further development or replacement of this model is required.

3.5 Variation of Average Gas Rise Velocity Model Exponent

The equation for the average gas rise velocity $\bar{S}$, given by Equation (2.3), is derived from the drift flux model for two phase flow.¹ The

Figure 9. Agglomeration model exponent "b" variation for Case Two

Figure 10. Agglomeration model exponent " b " variation for Case Two

exponent 'i' in Equation (2.3) is the subject of the present parametric study. The exponent regulates the influence of the void fraction α on the terminal velocity S_{∞} in determining the average gas rise velocity. For larger values of 'i', an increasing void fraction will slow the gas flow rate more so than for smaller values of 'i'. This effect can be seen in Figures 11 and 12 which give results for cases one and two for this study. The steady state gas release rates remain unaffected by the variation of this parameter.

A problem not illuminated by the present parametric study is the interaction of the average gas rise velocity $\bar{S}$ and the void fraction α present in the drift flux model. Equation (2.3) shows that as the void fraction increases, the average gas rise velocity will decrease for values of the exponent 'i' greater than 1. For a transient calculation, this relationship can cause a negative feedback loop that paralyzes the computation. For instance, if a sudden increase in the gas flow rate is experienced at the inlet to a cell (perhaps a barrel is breached in the melt pool), the void fraction increases. This causes a decrease in the gas rise velocity which further increases the void fraction, since more gas remains in the cell. The cycle is repeated until the void fraction reaches a value of one where no liquid phase is present, clearly an unphysical situation.

The drift flux model was designed and tuned for water as the liquid phase and it may have to be modified for application to the ISV process. One approach may be to adjust the terminal velocity model to account properly for high void fractions. Another approach would be to increase the number of bubble sizes directly accounted for, as suggested in the implementation plan,⁵ rather than using one average size.

3.6 Variation of the Critical Weber Number for Bubble Breakup

The model that represents the opposing trend to bubble agglomeration is the bubble breakup model. A maximum bubble radius criterion is used to model the physically maximum size a bubble can have before it breaks into smaller bubbles.¹ The maximum bubble radius criterion is given by

Figure 11. Drift flux model exponent " i " variation for Case One

Figure 12. Drift flux model exponent "i" variation for Case Two

$$R_b \max = \frac{\sigma We_{crit}}{2 \rho_l (\bar{S} - V_l)^2} \quad (3.3)$$

where σ is the liquid phase surface tension, We_{crit} is the critical Weber number for bubble breakup, and ρ_l and V_l are liquid phase density and velocity. From (3.3), it can be seen that the maximum allowed bubble size increases with critical Weber number, but decreases as the average gas rise velocity $\bar{S}$ increases.

Since the critical Weber number is set to the large value of 5000 for all parametric studies except this one, the bubble breakup model is effectively turned off for those studies. For this study, We_{crit} is varied between values of 10 and 210. Figures 13 and 14 present results for cases one and two for the variation of critical Weber number.

A significant problem with the interaction of the agglomeration and breakup models is illustrated by Figure 13. The smooth region in the surface map is the region where We_{crit} is high enough that all bubbles are smaller than the maximum size dictated by (3.3). For smaller values of We_{crit} , however, the interaction between the agglomeration and breakup models becomes apparent. The agglomeration model first determines that the average bubble size can be relatively large based on Equation (3.2). If the average bubble rise velocity $\bar{S}$ is slow enough, the maximum bubble radius criterion, Equation (2.5), will be met, avoiding any bubble breakup. The terminal velocity will then be computed based on the new larger average bubble size, increasing the terminal velocity. This will, in turn, increase as shown by Equation (2.3). Then, on the next time step, the larger value will cause a smaller maximum bubble size to be allowed as given by (3.3). If this smaller bubble size limit is small enough, the breakup model takes effect, lowering the average bubble size. Having come full circle, the agglomeration will again increase the bubble size, starting a new cycle. The result is the oscillatory behavior exhibited in Figure 13. This unfriendly interaction between the bubble agglomeration and breakup models will need to be addressed to prevent this oscillatory behavior.

Figures 13. Bubble breakup model variation for Case One

Figure 14. Bubble breakup model variation for Case Two

It is clear that the agglomeration model is inadequate for transient activity (Section 3.4) and will need improvement. Furthermore, adequate data is required to obtain an appropriate value for We_{crit} for the breakup model.

The results for case two do not show oscillatory behavior since the critical Weber number is high enough to prevent the breakup model from actuating.

3.7 Variation of a Linear Temperature Rise in the Liquid Phase

The two base cases assume uniform temperature distributions from the bottom to the top of the melt pool. This parametric study assumes that the temperature linearly increases from the bottom to the top of the melt pool. The total temperature variation ranges from zero to 500K. There are two effects that arise from a spatial temperature increase in the melt pool. The first effect is an increase in specific volume of the gas bubbles as they approach the surface of the melt pool due to both a change in temperature and a decrease in hydrostatic pressure. The second effect is due to the decrease in viscosity as the temperature increases. This effect is felt through the determination of the terminal velocity. These effects tend to increase the gas release rate as well as lower the time required to achieve steady state. Figures 15 and 16 illustrate these trends for cases one and two, respectively.

3.8 Variation of a Parabolic Temperature Rise in the Liquid Phase

In this study, the temperature of the melt pool is varied such that the temperatures at the top and bottom of the melt pool are the same, but the distribution in between follows a parabolic curve with the maximum being in the middle. The amount of the difference between the boundaries and the center of the pool is the parameter that is varied in this study. The results, presented in Figures 17 and 18, indicate that the steady state value for the gas release is reached more quickly the higher the temperature difference between the center and boundaries. The temperature variation, however, does not affect the final level of gas release rate.

Figure 15. Linear temperature rise variation for Case One

Figure 17. Parabolic temperature rise variation for Case One

Figure 18. Parabolic temperature rise variation for Case Two

3.9 Variation of a Linear Temperature Drop in the Liquid Phase

This parameter study is similar to that of section 3.7 except that the temperature decreases from the bottom of the melt pool to the top. The amount of the drop is varied from zero to 200 K. The results, as expected, are the reverse of those for the linear temperature rise study. Figures 19 and 20 present the numerical data for cases one and two, respectively, showing that as the temperature drop increases, the asymptotic gas release rate decreases and the time required to achieve steady state increases. The reasons for this behavior are the decreasing specific volume and increasing viscosity as the temperature difference grows.

3.10 Variation of a Parabolic Temperature Drop in the Liquid Phase

For this study, the temperatures of the melt pool surface and bottom are kept equal but with a parabolic drop of temperature in the center of the pool (the inverse of the study in Section 3.8). As expected, the gas release rate diminishes and the time to achieve steady state enhanced as the difference between the boundary and center temperatures is increased as shown in Figures 21 and 22.

3.11 Spatial Nodalization Variation

The one-dimensional cell height is varied in this study to determine the effects on the transient portion of the base cases. Figures 23 and 24 illustrate the effects of varying cell height for cases one and two, respectively. As can be seen, for both cases, the effect of increasing the cell height is to increase the time required to achieve steady state gas release, although the steady state levels remain unaffected. It appears that further reduction of the transient time would be achieved by further refinement of the mesh.

Figure 19. Linear temperature drop variation for Case One

Figure 20. Linear temperature drop variation for Case Two

Figure 21. Parabolic temperature drop variation for Case One

Figure 22. Parabolic temperature drop variation for Case Two

Figure 23. Special nodalization variation for Case One

Figure 24. Special nodalization variation for Case Two

3.12 Temporal Nodalization Variation

The size of the temporal step in the transient calculation is varied in this parametric study. Figures 25 and 26, which plot results for cases one and two, respectively, indicate that variation of the time step size has virtually no effect on the transient or the gas release rate.

3.13 Variation of the Liquid Phase Velocity

The two base cases assume that the liquid phase in the melt zone is stationary. If the viscosities and temperature gradients are high enough, however, natural convection cells may be formed in the melt pool. This would mean either an enhancement or inhibition of the buoyancy driven upward velocity of the gas bubbles depending on the location of the bubbles in the convection cells. This parametric study varies the velocity of the liquid phase in the melt pool from negative (downward) to positive (upward). Figures 27 and 28 show the results for the two cases for the negative to positive variation of the liquid phase velocity. As the velocity becomes more negative, the time to reach steady state is increased, as expected, since the downward velocity inhibits bubble progression. The opposite effect is seen to occur for an increasingly positive liquid phase velocity. The effects are more pronounced for case two than for case one since the bubbles for case two are smaller and more easily affected by liquid phase movement.

It remains to be determined if any natural convection cells will be generated in the melt pool and how important their influence will be on off-gas release rate.

3.14 Variation of the Liquid Phase Surface Tension

The role of the liquid phase surface tension in the overall off-gas release model is several-fold. First, it affects the gas phase pressure since it appears in the expression for capillary pressure which is summed with the liquid phase pressure to obtain the gas phase pressure¹:

Figure 25. Temporal nodalization variation for Case One

Figure 26. Temporal nodalization variation for Case Two

Figure 27. Melt velocity variation for Case One

Figure 28. Melt velocity variation for Case Two

$$P_g = P_l + P_c = P_l + \frac{2\sigma}{R_b} \quad (3.4)$$

Here, P_l is the liquid phase pressure, P_c is the capillary pressure and σ is the surface tension.

The second effect appears in the breakup model in the expression for the maximum bubble radius. Since the bubble breakup model is effectively turned off for this parametric study, this second effect is not present. The third place where the surface tension appears is in the terminal velocity model.¹ The terminal velocity model involves five different expressions for S_∞ for various ranges of bubble radius. It has been determined, however, that neither of the two expressions for S_∞ that involve surface tension are used for the range of parameters employed for cases one and two.

The final appearance of surface tension in the off-gas release model is in the expression for inlet bubble size for base case two, Equation (2.2). This appearance clearly will have an effect on case two results since the bubble size has been shown to be important in results for previous parametric studies.

Figures 29 and 30 present results for cases one and two, respectively, for the variation of liquid phase surface tension. There apparently is little or no effect due to the change in gas phase pressure (first effect) from varying σ for case one for the range considered. Examination of Figure 30 for case two, however, shows a significant change in time required to reach steady state as σ is decreased. The results for case one would indicate that the effects seen for case two are due entirely to the influence that the variation of σ has on the inlet bubble size. The results for case two, in fact, are consistent with the known effect that an increase in bubble size has on the transient: the larger the bubble, the faster steady state is reached. Therefore, the results for case two are attributed to an increasing bubble size as σ is increased.

Figure 29. Melt surface tension variation for Case One

Figure 30. Melt surface tension variation for Case Two

3.15 Variation of the Liquid Phase Density

The density of the liquid phase determines the hydrostatic pressure distribution in the melt pool. Variation of the liquid phase density is the subject of this parametric study. Figures 31 and 32 show the effect of varying the density for cases one and two. Both cases show similar trends. That is, as the liquid density increases, the bubbles seem to increase in size and velocity, thus increasing the gas release rate. However, one would expect the bubbles to decrease in size when the liquid phase density increases, since the gas phase density also increases [Equation (3.4) plus the ideal gas law]. In fact, what is happening is that the inlet volumetric gas flow at the bottom of the melt pool remains constant while the liquid phase density and hence the gas phase density change. This change in gas density results in a change in the mass flow rate for the gas since the inlet volumetric flow rate is held constant. Thus, the major effect seen in the figures for this study is the change in mass flow rate, which means an accelerated increase in the size of the ascending bubbles as the liquid phase density increases to accommodate the increase in gas phase mass. The conclusion drawn from this study is that the inlet boundary gas flow should be specified in terms of mass rather than volumetric flow rate.

3.16 Confinement Hood Pressure Variation

The parameter varied for this study is the boundary pressure at the top of the melt pool, that is, the pressure in the ISV confinement hood adjacent to the melt. Increasing the hood pressure is expected to inhibit the emergence of the off-gas into the hood. The analytical basis for this expectation is detailed in Appendix B. A sample calculation of the influence of a hypothetical pressure spike to the gas release rate is given in Appendix C. The results for the variation of hood pressure for cases one and two are plotted in Figures 33 and 34. As shown, an increase in the hood pressure does increase, slightly, the time required to reach steady state. Also, a slight decrease in the gas release rate occurs as the hood pressure increases, as expected.

Figure 31. Melt density variation for Case One

Figure 32. Melt density variation for Case Two

Figure 33. Hood pressure variation for Case One

Figure 34. Hood pressure variation for Case Two

3.17 Variation of the Pore Radius at the Melt Pool Inlet Boundary

The final parametric study investigates the effects of changing the radii of the effective pores at the inlet boundary of the melt pool. The expected result is that for smaller pore sizes, smaller bubbles are formed. Smaller bubbles rise more slowly resulting in lower rates of gas release and longer times required to achieve steady state. Figures 35 and 36 provide the results for cases one and two, respectively. The results are as expected.

Figure 35. Melt front pore radius variation for Case One

Figure 36. Melt front pore radius variation for Case Two

4. CONCLUSIONS

A summary of the important conclusions that have emerged as a result of the present parametric studies using the OGRE code are the following:

1. Experimental data are required to characterize the pore sizes of the porous layer adjacent to the melt front and to help determine which inlet bubble size model or models are appropriate to characterize the sizes of the bubbles generated as the off-gases enter the melt pool,
2. An improved model is needed for agglomeration that is more appropriate for the transient calculations and that will work well with the bubble breakup model(s),
3. An improved model for the gas rise rate for high void fractions is needed since extrapolating the current drift flux model to large void fractions appears to be inappropriate,
4. Experimental data are needed to determine appropriate critical Weber numbers for bubble breakup models which may apply to different flow regimes or for different ranges of flow parameters,
5. Experimental or numerical data are needed to accurately specify the distribution of temperature in the melt pool,
6. Further information is required to determine whether natural convection cells will be present in the ISV melt pool and what their strength and influence will be,
7. Experimental data are needed to accurately characterize the liquid phase surface tension and density for the ranges of thermodynamic conditions that will be present in the melt pool,

8. As the volumetric inflow (gas source) rate increases, the asymptotic gas release rate increases while time required to reach steady state decreases,
9. As terminal velocity increases, the time required to reach a steady state release dramatically decreases while the effect on the asymptotic release rate is not so important,
10. A spatial temperature increase from the bottom to the top of the melt pool tends to increase the gas release rate as well as lower the time required to achieve steady state, whereas a spatial temperature decrease has the opposite effect, and
11. Typical operating pressures in the ISV confinement hood have a negligible effect on off-gas release.

REFERENCES

1. R. J. MacKinnon and V. A. Mousseau, "OGRE/MOD1: A Computer Model for Predicting Off-Gas Release from In Situ Vitrification Melts," EGG-WM-9041, July 1990.
2. J. L. Buelt (et. al.), "In Situ Vitrification of Transuranic Waste: An Updated Systems Evaluation and Applications Assessment," PNL-4800 Suppl.1 UC-70, Pacific Northwest Laboratory, March 1987.
3. J. J. Bikerman, "Surface Chemistry Theory and Applications," Academic Press Inc., New York, 1958.
4. C. E. Slater, R. W. Johnson, and R. J. MacKinnon, "Off-Gas Release Rate Calculations for the Large Scale Test in Pit 9," Engineering Design File, ERP-ISV-038.
5. R. J. MacKinnon (et. al.), "In Situ Vitrification Model Development and Implementation Plan," EGG-WM-9036, August 1990.

APPENDIX A
INPUT DECK FOR THE BASE CASE ONE CALCULATION

'c'

'c'

'c'

GEOMETRY'

20

1.00d-1

.0d+0

100000

-1

9.8d+0

4.11008d-2

11

1

'c'

'c'

'c'

1.00d-1

600

600

15

100000

100000

-1

-1

'c'

'c'

'c'

287.0d+0

1.0d+5

2700.0d+0

1773.0d+0

10.0d+0

0.2731d+0

0.0d+0

'c'

'c'

'c'

1.0d-10

5.0d+3

2.0d+0

8.0d+0

3.0d+0

'c'

'c'

'c'

0.0d+0

1.0d-3

0.0d+0

'c'

* ncells - number of real cells in the simulation
* dx - cell length
* diamc - diameter of the control volume
* nhiac0 - the initial highest active cell
* lwact0 - the initial lowest active cell
* grav - acceleration due to gravity
* porrad - radius of the pores in front of the melt
* ntdpcl - cell number of TDP data output
* nclskp - # of cells between surface plot output

TIME CONTROL'

* dt - time step
* mxyc - maximum number of time steps
* nprint - number of cycles between printed output
* nplot - number of cycles between plotting output
* ncycsb - the # cyc. before the surface moves 1 cell
* ncycft - the # cycl before the front moves 1 cell
* ndbstt - cycle number to start debug output
* ndbstp - cycle number to stop debug output

FLUID PROPERTIES'

* rair - gas constant for air from IGL
* p0 - ambient pressure above the melt
* rhofo - the density of the melt pool
* t0 - the temperature of the melt pool
* viscf0 - the viscosity of the melt pool
* sigfo - the surface tensions of the melt pool
* vmelt - vertical velocity of the melt pool

CORRELATION COEFFICIENT NAD POWERS'

* timcon - the time for bubble volume change
* wecrit - the critical Weber number
* powagg - the power that sets the agglom curve
* grwfrr - the bubble agglom growth fraction
* power - Wallis (4.14) n

INITIALIZATIONS'

* void0 - initial void fraction
* volb0 - initial average bubble volume
* vbss0 - initial bubble velocity

'c
'c'

INFLOW CONDITIONS'

51
0.33d+0
1000000
-1
1000000
1.0d-6
4.8d-2
6.0d-2
6.0d-2
2.5d-1
2.5d-1
2.5d-1

* ncelin - cell to inject void at
* voidin - amount of void to inject
* nccin - cycle number to inject void on
* nsttgm - cycle to start gas inflow
* nstpgm - cycle to stop gas inflow
* gamfrt - the void source at the front
* vbbs - bubble velocity at the melt front
* vbbs0 - bubble velocity at the melt front
* vbbs1 - bubble velocity at the melt front
* voidbs - void fraction at the melt front
* voidbs0 - void fraction at the melt front
* voidbs1 - void fraction at the melt front

'c'
'c'
'c'

CODE FLAGS'

1
1
2.5d-1
2
1.0d-1
2
0
1
0
1.0d+2
1
10

* nbub0 - bub init flag (1) uniform (0) gradient
* ncvbss - bub vel flag (1) computed (0) vbinp
* vbinp - bubble terminal velocity.
* norfis - orifice flag (1) computed (0) radbt0
* radbt0 - bubble radius at melt bottom
* injmtd - injection method flag values 1-5
* nsorce - void source flag (1) cell (0) flux
* nvisc - viscosity flag (1) computed (0) viscf0
* ntemp - temperature flag (2) par (1) lin (0) const
* tmpcrv - use depends on ntemp
* nstud0 - starting number of parametric studies
* nstud1 - stopping number of parametric studies

APPENDIX B

DERIVATION OF THE EFFECT OF HOOD PRESSURE ON OFF-GAS RELEASE

From the conservation of mass, the mass flow rate of gas into the bottom of the melt must equal the mass flow rate of gas out the top of the melt at steady-state. This means that

$$(\rho Sa)_t = (\rho Sa)_b .$$

Therefore, we can solve for the volume flow rate at the top yielding

$$(Sa)_t = (\rho_b/\rho_t)(Sa)_b .$$

From the perfect gas law we know that

$$\rho_b = P_b/(RT) \text{ and } \rho_t = P_t/(RT)$$

where T is the constant melt temperature for this problem. We can solve for P_b in terms of P_t from the hydrostatic head giving

$$P_b = P_t + \rho_l D_m g .$$

Now solving for the ratio ρ_b/ρ_t we get

$$\rho_b/\rho_t = P_b/P_t = (P_t + \rho_l D_m g)/P_t = 1 + [(\rho_l D_m g)/P_t] .$$

Therefore, we can write

$$(Sa)_t = \{1 + [(\rho_l D_m g)/P_t]\} (Sa)_b$$

This result shows that as the hood pressure (P_t) goes down, the release rate $(Sa)_t$ goes up.

APPENDIX C

SAMPLE PRESSURE SPIKE CALCULATION

From Appendix B we know that the hood pressure's effect on release rate is

$$(Sa)_t = [1 + (\rho_l D_m g / P_t)] (Sa)_b$$

Now consider the following table of numbers that correspond to the "base case" calculation.

Table C-1. Parametric values

Parameter Name	Parameter Symbol	Parameter Value
Gas flow	$(Sa)_b$	0.236 (m ³ /S)
Liquid Density	ρ_l	2700.0 (kg/m ³)
Melt Pool Depth	D_m	2.0 (m)
Gravitational acceleration	g	9.8 (m/s ²)
Hood Pressure	P_t	1.0e+5 (Pa)

Substituting these values into the above equation we get

$$(Sa)_t = 0.3608912 \text{ (m}^2\text{/s)} .$$

Now, consider a 6 in H₂O pressure spike in the hood. Converting this to Pascals yields

$$6(\text{in}) * .0254(\text{m/in}) = .1524(\text{m}) .$$

Hence,

$$dP = \rho_l g D_m = 1000 \text{ (kg/m}^3\text{)} * 9.8 \text{ (m/s}^2\text{)} * 0.1524(\text{m}) = 1493.52 \text{ (Pa)} .$$

The pressure in the hood becomes $1.0\text{e}+5 + 1493.52 = 101493.52 \text{ Pa}$.

Recomputing $(Sa)_t$, using the new hood pressure, we get

$$(Sa)_t = 0.3590533 \text{ (m}^3\text{/s)},$$

which is a change of only 0.5% in the volumetric flow rate of gas at the top melt pool boundary.

END

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