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A CALCULATIONAL MODEL FOR CONDENSATION OF WATER VAPOR DURING AN UNDERGROUND NUCLEAR DETONATION

Richard J. Knox

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LAWRENCE LIVERMORE LABORATORY
University of California, Livermore, California, 94550

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A CALCULATIONAL MODEL FOR CONDENSATION OF WATER VAPOR DURING AN UNDERGROUND NUCLEAR DETONATION

Abstract

An empirally derived mathematical model has been developed to calculate the pressure and temperature history during condensation of water vapor in an underground-nuclear-explosion cavity. The condensation process is non-isothermal. Use has been made of the Clapeyron-Clausius equation as a basis for development of the model. Analytic fits to the vapor pressure and the latent heat of vaporization for saturated-water vapor, together with an estimated value for the heat-transfer coefficient, have been used

to describe the phenomena. The calculated pressure-history during condensation has been determined to be exponential, with a time constant somewhat less than that observed during the cooling of the superheated steam from the explosion. The behavior of the calculated condensation-pressure compares well with the observed-pressure record (until just prior to cavity collapse) for a particular nuclear-detonation event for which we have data.

The Conventional Cavity Pressure-Temperature History Formulation

Olsen¹ has devised a simplified model for cavity cooling based on the time-dependent Newtonian cooling process. Upon termination of cavity growth, the vaporized rock must condense in a very short time (on the order of a few tenths of seconds) in contrast with the longer term cooling (tens of minutes) of the water vapor. The longer term cooling of this superheated steam has been modeled by Olsen¹ using the Newtonian decay

algorithm (see Appendix) given by:

$$\frac{T - T_{\infty}}{T_0 - T_{\infty}} = e^{-(hA/c_v n)t}, \quad (1)$$

where

t = time in minutes,

T = temperature at time t in kelvins. Also, $T = T_0$ at $t = 0$ (derived from

$\frac{P_0 V}{nR}$, where P_0 = overburden pressure) and

$T = T_{\infty}$ at $t = \infty$ (ambient temperature of cavity wall is assumed constant).

h = surface heat transfer coefficient ($\text{cal/cm}^2 \cdot \text{sec} \cdot \text{K}$),

A = surface area of cavity in cm^2

R = 0.08314 liter $\cdot$ bar/mole $\cdot$ K (gas constant)

n = total moles of water vapor

V = cavity volume in liters

c_v = molar heat capacity of the steam at constant volume ($\text{cal/mole} \cdot \text{K}$)

Assuming that the behavior of the steam follows the ideal gas law, the pressure is derivable from the expression

$$P = \frac{nRT}{V} \quad (2)$$

Olsen was able to achieve a good fit to the pressure history for a particular underground nuclear event for which the following values were used:

$\rho = 1.9 \text{ g/cm}^3$ = overburden density

$h = 0.012 \text{ cal/cm}^2 \cdot \text{sec} \cdot \text{K}$

$Y = 6.5$ kilotons = device yield

$d = 240$ meters = depth of burial

$c_v = 6.5 \text{ cal/mole} \cdot \text{K}$

$W = 0.12$ weight fraction of water at the shot point.

It is for this same event that an attempt is made in this paper to also calculate the condensation-pressure history. Initially, Olsen used both

a fixed value for c_v (i.e., $c_v = 6.5 \text{ cal/mole} \cdot \text{K}$), which was treated as the average over the entire temperature range, and a cavity radius formula independent of the in situ water content. However, adjusting the value of the heat transfer coefficient* (i.e., $h = 0.012 \text{ cal/cm}^2 \cdot \text{sec} \cdot \text{K}$), produces a good fit between the calculated and observed pressure data until shortly before cavity collapse. The result of that fit is displayed in Fig. 1. Figure 2 depicts the corresponding calculated pressure vs temperature curve.

Olsen² later made a study of pressure decay in several underground events using a modified form of the Newtonian equation in order to account for the effect of rock strength on the initial pressure. For this purpose, an "excess pressure" coefficient was implemented, permitting calculated cavity pressures to exceed overburden pressure. In several cases, one or more parameters in the equation had to be altered to obtain a consistent fit. However, the value of $h = 0.012 \text{ cal/cm}^2 \cdot \text{sec} \cdot \text{K}$ seemed to be about the best value for the transfer coefficient.

* For convective transfer with superheated steam in contact with a solid, h is nominally in the range of 0.002-0.005 $\text{cal/cm}^2 \cdot \text{sec} \cdot \text{K}$ (Ref. 5).

Fig. 1. Olsen's¹ exponential fit to the observed pressure decay, displayed linearly and semi-logarithmically. Both c_v and h are constant ($c_v = 6.5$ cal/mole and $h = 0.012$ cal/cm²·sec·K).

Fig. 2. Pressure vs temperature curve resulting from the ideal-gas-law assumption for the calculated fit of Fig. 1.

Improvements to the Cavity-History Formulation

A code (called DCAVSTM³) has recently been written for the Hewlett-Packard* HP-9821A computer and for Lawrence Livermore Laboratory's (LLL) CDC-7600 that calculates a cavity's entire pressure-temperature history through condensation. This code employs the original Newtonian cooling calculation with minor improvements and includes the late-time development of the vapor condensation phase. The DCAVSTM code calculates the temperature and pressure histories prior to condensation using a modified Newtonian equation. Also, the code includes:

- A temperature-dependent c_v
- A cavity radius with dependence on water content
- A temperature-dependent heat-transfer coefficient.

Olsen's latest technique² uses Higgins and Butkovich's⁴ revised cavity-radius (R_c) formula which includes the effects of water content,

i.e.,

$$R_c = \frac{100Y^{1/3}}{[\rho d]^{\alpha}} \quad (3)$$

where

R_c = cavity radius expressed in meters

Y = yield in kilotons

ρ = density in gram/cm³

d = depth of burial in meters

and

$$\alpha = 0.3262 - 0.3326W + 0.7857W^2 - 0.9778W^3.$$

The total moles of water in the cavity (n_0) is given by

$$n_0 = \frac{WY}{18} (7 \times 10^8) \quad (4)$$

assuming 7×10^8 grams of rock is vaporized and melted by the detonation.⁵

The cavity growth is assumed to terminate when the gas pressure is equal to or slightly greater than the overburden pressure (P_0 , in bars) which is given by:

$$P_0 = 1 \times 10^{-4} \rho g d \quad (5)$$

where $g = 980 \text{ cm/sec}^2$ (acceleration of gravity). The expression for P_0 assumes an "excess overburden" coefficient of unity.

In terms of the units mentioned, the initial temperature T_0 is derivable using Eqs. 2 through 5.

* Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Energy Research & Development Administration to the exclusion of others that may be suitable.

Fig. 3. Smoothed function representing the dependence of the empirical parameter, α , as a function of weight-fraction water. See Butkovich's cavity-radius formula.⁵

That is,

$$T_0 = 1.2955 \times 10^{-7} \frac{\rho g d R_c^3}{W Y}, \quad (6)$$

and for

$$T_\infty = 300K,$$

the temperature expression takes

the form

$$T = (T_0 - T_\infty) e^{-1938.81ht / (c_v W Y^{1/3} [\rho d]^2 \alpha)} + T_\infty \quad (7)$$

or

$$T = K_1 e^{-K_2 t} + 300, \quad (8)$$

where the coefficients of the above equation are

$$K_1 = 1.2955 \times 10^{-7} \frac{\rho g d R_c^3}{W Y} - 300 \quad (9)$$

and

$$K_2 = 1938.81h / (c_v WY^{1/3} [wd]^{2a}) \quad (10)$$

The pressure can then be derived by assuming the ideal gas law,

$$P = \left(\frac{n_0 R}{V} \right) T, \quad (11)$$

where

$$R = 0.08314 \text{ liter} \cdot \text{bar} / \text{mole} \cdot \text{K} \\ (\text{gas constant})$$

and

$$V = \text{cavity volume in liters;}$$

or

$$P = \left(771.9 \frac{WY}{R_c} \right) T = K_3 T. \quad (12)$$

Using Eq. (8) as the expression for temperature we obtain

$$P = K_3 \left(K_1 e^{-K_2 t} + 300 \right) \\ = A_1 e^{-K_2 t} + B_1. \quad (13)$$

Olsen² implemented c_v as a function of vapor temperature according to the empirical equation:

$$c_v = 5.913 - 54.32/T + 8.009 \times 10^{-4} T + 6.404 \times 10^{-7} T^2. \quad (14)$$

(See Figs. 4 and 5). This had the effect of decreasing the pressure decay at early times and increasing it at late times. Although the overall deviation was not major, introduction

of a variable c_v did not improve the fitting properties (see Fig. 6) for comparison with measured data. However, Olsen had reason to believe an improvement was evident in calculations at high yields and considerable depth of burial, but was not able to make a comparison of results for the case of a variable c_v with any "observed" data.

Since there was probably more uncertainty in the value of the heat-transfer coefficient and in the determination of the water content (W) in the cavity region during this era than in other geologic quantities, we attempted several fits to the observed pressure data by independent variation of the water content ($W \pm 4\%$) and heat transfer coefficient ($h \pm 50\%$), all of which proved to be unsuccessful. However, an improved fit was accomplished by introducing a simple dependence for the heat transfer coefficient upon water vapor temperatures (see Fig. 7):

$$h = h_0 (1 + \delta T), \quad (15)$$

$$\text{where} \\ h_0 = 0.0068 \text{ cal/cm}^2 \cdot \text{sec} \cdot \text{K}^{-1}, \\ \delta = 6.087 \times 10^{-4} \text{ K}^{-1}.$$

The associated temperature history is given in Fig. 8.

Fig. 4. Empirical fit to the specific heat of superheated steam (low-temperature range).

Fig. 5. Empirical fit to the specific heat of superheated steam (high temperature range).

Fig. 6. Calculated pressure decay for the example data with a constant $h = 0.012 \text{ cal/cm}^2 \cdot \text{sec} \cdot \text{K}$ showing the failure of a temperature-dependent c_v alone to improve fitting properties. This fit also used the water-dependent cavity-radius formula.

Fig. 7. Improved calculated fit to the observed decay displayed linearly and semilogarithmically. Fit uses the same conditions as Fig. 6 but includes a temperature-dependent heat-transfer coefficient.

Fig. 8. Calculated temperature curves using the improved fitting parameters of Fig. 7.

Temperature and Pressure at Incipient Condensation

An analytic description of tabular vapor pressure data for water is essential for the calculation of both the temperature and pressure at the instant condensation begins. From theoretical considerations, it may be shown that the vapor pressure of water can be approximately fitted to a simple exponential equation of the form

$$P = c_1 e^{-c_2/T} \quad (16)$$

Using tabular vapor pressure data, the constants c_1 and c_2 take the values of

$$c_1 = 3.32431 \times 10^5$$

(for P in bars)

and

$$c_2 = 4.73976 \times 10^3.$$

The fit using these constants is shown in Fig. 9.

Condensation begins at the point (P^*, T^*) where the cavity pressure decay with temperature intersects the vapor-pressure (V-P) curve for water. That is,

$$P_{\text{cavity}} = \frac{n_0 R}{V} T = K_3 T = c_1 e^{-c_2/T} \quad (17)$$

vapor pressure

where K_3 was defined in the previous section to be

$$K_3 = 771.9 \frac{\text{WY}}{\text{R}^3} \quad (18)$$

The quantity K_3 is known and the constants c_1 and c_2 are determined from the functional fit; however, $K_3 T = c_1 e^{-c_2/T}$ is not directly solvable for T . Analytically, it requires a special technique because of the non-linearity. We have developed a recursive method called the "method of approaching tangents". It gives rapid convergence in a very few iterations and may be done without the aid of computers.

Referring to Fig. 10 for identification of the subscripted variables ($P_1, T_1; P_2, T_2$; etc.), a tangent to the V-P curve can be drawn through the critical point (not shown in Fig. 10). The cavity pressure decay curve intersects this tangent at a coordinate in P-T space (P_1, T_1). The equation of this tangent line (called "tangent line No. 1" in Fig. 10) is given by:

$$P - P_c = \left(\frac{dP}{dT} \right)_{T_c} (T - T_c) \quad (19)$$

where

$$T_c = 647.18\text{K (critical temperature),}$$

$$P_c = 220.61 \text{ bars (critical pressure),}$$

Fig. 9. Fit of $P = 3.32431 \times 10^5 e^{-4.73976 \times 10^3/T}$ to tabular vapor pressure data of water.

and the slope of the (V-P) curve is determined to be

$$\left(\frac{dP}{dT}\right)_{T_c} = \frac{c_1 c_2}{T_c^2} e^{-c_2/T_c} = A. \quad (20)$$

At the intersection of this tangent line with the decaying volatility-pressure curve, we obtain the temperature

$$T = \frac{P_1}{K_3}. \quad (21)$$

The corresponding pressure at that intersection is derivable using Eqs. 19, 20 and 21, as follows:

$$P_1 = P = \frac{P_c - AT_c}{\left(1 - \frac{A}{K_3}\right)}. \quad (22)$$

If this pressure value P_1 is translated horizontally to the V-P curve, it corresponds to a temperature (T_1) at that intersection. Whereupon, making

Fig. 10. Illustration of recursive calculational technique by which the intersection of the ideal-gas function and the vapor pressure for water is determined.

use of the V-P equation [Eq. (17)],

$$T_1 = \frac{c_2}{\frac{c_1}{\ln \frac{1}{P_1}}} \quad (23)$$

T_1 is thus the first estimate of the incipient condensation temperature.

The next estimate is made, similarly, by construction of a second tangent passing through point (P_1, T_1) and repeating Eqs. (20, 22 and 23) where, in equation (20), we substitute T_1 for T_c and calculate

a new A . This value of A together with T_1 and P_1 (which is now being substituted for P_c) are then used in the right member of Eq. (22).

A new pressure, P_2 , is then calculated with Eq. (22). This pressure (P_2) is used in Eq. (23) to arrive at a second estimate (T_2). Figure 10 thus indicates graphically how this solution converges. A calculation of T and P at the beginning of condensation is given in the following section for the example data.

Calculation of the Time of Incipient Condensation

The time at which condensation begins is calculable from

$$P = A_1 e^{-K_2 t} + B_1 \quad (24)$$

where

$$A_1 = K_3 K_1$$

and

$$B_1 = T_\infty K_3 = 300 K_3$$

(Average values of $c_v = 6.3$ and $h = 0.0085$ were selected to calculate K_2 during the condensation phase.)

Therefore,

$$A_1 e^{-K_2 t} = P - B_1$$

which leads to:

$$t = t^* = \frac{1}{K_2} \ln \frac{A_1}{P - B_1} \quad (25)$$

where t is expressed in minutes.

Olsen's original fit to the pressure decay was:

$$P = 36.7 e^{-0.36 t} + 7.8 \quad (26)$$

from which

$$A_1 = 36.7,$$

$$K_2 = 0.36,$$

and $B_1 = 7.8$.

Using the method described, the pressure at condensation was determined from the intersection of Olsen's ideal-gas function with the V-P curve (see Fig. 11). That is,

$$P = P^* = 12.06 \text{ bars}$$

and

$$\begin{aligned} t^* &= \frac{1}{0.36} \ln \frac{36.7}{12.06 - 7.8} \\ &= 5.98 \text{ minutes} \end{aligned}$$

Fig. 11. Intersection of Olsen's original ideal-gas fit and the vapor pressure curve for water.

This time agrees reasonably well with the estimate of 6.5 minutes that Olsen made from the observed pressure data.

A second calculation of this time has been made using the modified formation. The value K_2 is now a function of temperature since

$$h = 0.0068 (1 + 6.087 \times 10^{-4} T) \quad (27)$$

and

$$c_v = 1.687 \times 10^{-3} T + 5.52 \quad (28)$$

are both functions of temperature. An excellent fit for c_v over the entire temperature range for condensing steam is shown in Fig. 12.

The quantities K_1 and K_3 also differ from Olsen's coefficients because of the different formula used for cavity radius. The condensation

Fig. 12. Straight-line approximation vs specific heat of condensing steam.

pressure and temperature P^* and T^* are calculated to be

$$P^* = 9.64 \text{ bars}$$

and $T^* = 453.6 \text{ K}$.

The value of t^* is similarly arrived

at as

$$t^* = 7.76 \text{ minutes.}$$

This time of condensation can be observed (in Fig. 7) as the point where the observed pressure begins to fall away from that calculated.

Calculation of Time Duration and Heat Lost During Condensation

The condensation of the cavity vapor is not an isothermal process because it is not isobaric. We assume the process is slow enough so that the water vapor remains in equilibrium with the condensing liquid. This "saturated" vapor must follow the vapor pressure curve as it condenses. Initially, heat is lost to the walls at a rate of

$$\frac{\Delta q}{\Delta t} = h^* A (T^* - T) \quad (28)$$

where

$\frac{\Delta q}{\Delta t}$ is expressed in Cal/sec
 T^* = temperature at incipient condensation

and h^* = the heat transfer coefficient during condensation.

Olsen¹ suggested "dropwise" condensation as a probable mode due to the value of h^* (i.e., $h^* = 1.31 \text{ cal/cm}^2 \cdot \text{sec} \cdot \text{K}$) he inferred from his calculations on the observed data. However, upon reviewing these calculations we have arrived at a value of h^* lower by a factor of 20 (i.e., $h^* = 0.07 \text{ cal/cm}^2 \cdot \text{sec} \cdot \text{K}$) than originally computed. "Filmwise"⁶ condensation is typified by values of h^* in this range, assuming heat transport to be dominated by convection.

The total heat lost throughout the entire condensation phase has to be less than $n_0 \lambda_p$ where

n_0 = original moles of vapor.
 λ_p = the latent heat of vaporization at the triple point

since the latent heat of the phase transformation is a maximum at the triple point (see Fig. 13). Thus, the minimum duration time of condensation can be estimated from

$$\frac{n_0 \lambda_p}{60 \Delta t} = h^* A (T^* - T_\infty) \quad (29)$$

$$\Delta t = \frac{n_0 \lambda_p}{60 h^* A (T^* - T_\infty)} \quad (30)$$

where Δt is expressed in minutes. For our example data this value comes out to be approximately 4.4 minutes.

The DCAVSTM code calculates this time more accurately by computing a running sum of the total heat lost at each time step to provide an integrated maximum heat loss value,

$$Q_{\max} = \sum \left(\frac{\Delta q}{\Delta t} \right) \Delta t \quad (31)$$

at

$$T = T_\infty = 300\text{K}$$

from which

$$\Delta t = \frac{Q_{\max}}{60 h^* A (T^* - T_\infty)} \quad (32)$$

The code calculates this value to be approximately 3.8 minutes.

For the event we considered, condensation occurred at a calculated temperature of 453K. Using the latent heat of vaporization of water at that temperature (see Fig. 13) we can calculate the approximate heat loss by two other methods.

(1) If we assume the process is isothermal with

$$\lambda(T^*) = 8661 \text{ cal/mole}$$

and

$$n_0 = 3.033 \times 10^7 \text{ moles of vapor}$$

the latent heat evolved at that temperature is

$$H_1 = n_0 \lambda(T^*) = 3.033 \times 10^7 \times 8661 = 2.63 \times 10^{11} \text{ cal.}$$

Fig. 13. Exponential fit to the latent heat of vaporization for water.

The path traversed over the PVT surface for water is A-B (see Fig. 14). The path from B to C is traversed while cooling the saturated water from 453K to 300K; it is

$$\begin{aligned} H_2 &= n_0 \Delta T_{c_p} = 3.033 \times 10^7 \times \\ &153 \times (1 \text{ cal/g} \cdot \text{K}) \\ &= 4.64 \times 10^9 \text{ cal} \end{aligned}$$

where 1 cal/g·K is the specific heat of water.

Finally, the total heat lost is

$$\begin{aligned} Q &= H_1 + H_2 \\ &= 2.68 \times 10^{11} \text{ cal.} \end{aligned} \quad (33)$$

(2) Use of standard mechanical-engineering "steam tables" is valid whether or not the process is

Fig. 14. PVT surface for water, showing possible paths during condensation.

isothermal since internal energy values are required only at the initial and final states. At point A ($T^* = 453\text{K}$ and $P^* = 9.64$ bars) the cavity is filled with saturated vapor. The specific internal energy of the saturated vapor is found to be

$$u_1 = 11102.22 \text{ cal/mole.}$$

After complete condensation,

$$T_{\text{final}} = T_{\infty} = 300\text{K},$$

and

$$P_{\text{final}} = 0.034 \text{ bars.}$$

The specific internal energy of the saturated liquid is

$$u_f = 476.31 \text{ cal/mole.}$$

Applying the first law of thermodynamics,

$$Q - W = \Delta U$$

where $W = 0$ (since no work is being done by the system, i.e., the gas in the cavity)

$$Q = U_f - U_1 = n_0(u_f - u_1)$$

$$Q = -3.033 \times 10^7 \\ \times (11102.22 - 476.31)$$

$$Q = -3.22 \times 10^{11} \text{ cal.}$$

(The minus sign signifies that energy is lost by the system.)

The condensation code (DCAVSTM) calculated a total value of $Q = 2.81 \times 10^{11}$ calories for the example data. It is interesting to note that this energy is somewhat less than 5% of the total device energy of 6.5×10^{12} calories. A summary of all output results for the cavity calculation is given in Table 1.

Table 1. Code-calculated results relating to H_2O condensation for the example event

Time of incipient condensation	7.76 minutes
Pressure at condensation	9.64 bars
Temperature at condensation	453.6 K
Total heat lost during condensation	2.81×10^{11} calories
Total time of condensation ($T \equiv T_{\infty}$)	6.3 minutes

Calculation of the Pressure-Temperature History During Condensation

The Clapeyron-Clausius equation⁷ is applicable during condensation. It is obtained as

$$\frac{dP}{dT} = \frac{\lambda}{T\Delta v} \quad (34)$$

where

$$\Delta v = v_{\text{gas}} - v_{\text{liquid}}$$

This expression is the difference between specific volumes of the two phases present. Since v_{liquid} is very small in comparison with the gas volume v_{gas} and for a typical cavity of volume V , we may make the following approximation

$$\Delta v \approx v_{\text{gas}} \approx \frac{V}{n}$$

where

n = number of moles of vapor present. Thus, we may rewrite equation (34) as

$$\frac{dP}{dT} = \frac{\lambda n}{TV} \quad (35)$$

which may be recognized as the slope of the vapor pressure curve at a given temperature. The number of moles of vapor is then calculable from this expression as

$$n = \frac{TV}{\lambda} \frac{dP}{dT} \quad (36)$$

From Eq. (20) we found that

$$\frac{dP}{dT} = \frac{c_1 c_2}{T_2} e^{-c_2/T} \quad (37)$$

In addition, λ has been well fitted to the analytic exponential form (see Fig. 13):

$$\lambda(T) = D_1 e^{E_1/T} + D_2 e^{E_2/T} \quad (38)$$

where $\lambda(T)$ is expressed in cal/mole.

The equation 35 becomes

$$n(T) = \frac{V c_1 c_2 e^{-c_2/T}}{T (D_1 e^{E_1/T} + D_2 e^{E_2/T})} \quad (39)$$

where, for water vapor, the values of each of the fitting coefficients are:

$$c_1 = 3.32431 \times 10^5$$

$$c_2 = 4.73976 \times 10^3$$

$$D_1 = 1.381 \times 10^4$$

$$E_1 = -9.063 \times 10^{-4}$$

$$D_2 = -1.619$$

$$E_2 = 1.261 \times 10^{-2}$$

and $n(T)$ is expressed in moles.

The calculation of the pressure and temperature history during the phase change is performed by means of an iterative calculation. Beginning with a time t^* (time of incipient condensation) and $n(t^*)$ (original moles of vapor) we calculate $\lambda(T^*)$ by use of Eq. 38.

Then,

$$P(T^*) = c_1 e^{-c_2/T^*} \quad (40)$$

The heat-loss rate to the cavity wall is

$$q(t^*) = h^*A(T^* - T_\infty). \quad (41)$$

We then increment the time to

$$t_1 = t^* + \Delta t \quad (42)$$

and calculate

$$n(t_1) = n(t^*) - \frac{q(t^*)}{\lambda(T^*)} \Delta t \quad (43)$$

from which a new temperature T_1 is iteratively calculated using the Clapeyron-Clausius equation. The calculation then recycles back to the computation of $\lambda(T_1)$, $P(T_1)$, $q(t_1)$, t_2 and $n(t_2)$, etc.

Figure 15 gives a comparison of the observed data with the computed pressure history after condensation begins. Figure 16 shows the comparison over the entire range. Agreement here is fairly good. Figure 17 depicts the calculated temperature profile. A mark on the axis at 7.76 minutes denotes the calculated occurrence of incipient condensation.

Although no CO_2 was measured for the event of the example data, we have neglected throughout this development the influence of its presence (or any other noncondensibles) in the cavity. Carbon dioxide remains a noncondensable during the

H_2O condensation regime because of its relatively low boiling point of 194.7K and critical temperature of 304.28K. The ambient wall temperatures hover in the neighborhood of 300K. However, the CO_2 does somewhat increase the total pressure according to Dalton's law of partial pressures. Since virtually no CO_2 would dissolve in the near boiling water puddle, the final cavity pressure should essentially become that of the residual carbon dioxide.

It is not clear what coupling effects significant concentrations of CO_2 (> 5%) would have on the cavity temperature during the H_2O condensation phase since the process would then become a three-phase system. Whether the CO_2 continues to cool independently according to the Newtonian prescription and to what extent it might retard the heat transfer to the walls remains to be investigated. The calculational technique described here is felt to provide a valid approximation for CO_2 concentrations less than 5%.*

* Shot-point environments having greater than 5% by weight CO_2 are generally deemed undesirable.

Fig. 15. Comparison of calculated condensation pressure history with the observed pressure, using improved Newtonian equation.

Fig. 16. Comparison of entire calculated pressure history with the observed pressure, using improved Newtonian equation.

Fig. 17. Associated-temperature calculation using improved Newtonian equation.

Conclusion

It has been demonstrated, at least for a particular event, that the application of the Clapeyron-Clausius equation may be used to describe the pressure and temperature decay during condensation of water vapor released by an underground nuclear event. The calculated pressure has been found to approximate well the observed pressure during this time regime.

Unfortunately, due to difficulties with survival of pressure transducers, we have had relatively few cavity-pressure measurements extending over the entire condensation regime.

Accurate water-content analysis and working-point density measurements together with the fielding of several redundant pressure sensors would greatly facilitate observation of the condensation history.

It might be worthwhile to conduct laboratory experiments to measure the convective heat coefficient between saturated water vapor and a variety of Nevada Test Site (NTS) soils under a controlled temperature and pressure environment. This would shed light on the greatest factor of uncertainty in this type of calculation.

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Appendix: Derivation of the Newtonian Cooling Equation

ISOTHERMAL WALL

A nonrigorous development can be described by a heat balance equation for the amount of heat given up to the walls by the cavity gas and the heat transferred by convection; namely

$$\rho V c_v \frac{dT}{dt} = -hA(T - T_\infty).$$

If we define $m = \frac{hA}{\rho V c_v}$ and $n = \rho V$

then

$$\frac{dT}{dt} = -m(T - T_\infty).$$

Upon integration

$$\ln \frac{c_1}{T_\infty - T} = mt$$

where c_1 is an arbitrary constant.

Initial conditions are

$$t = 0$$

$$T = T_0.$$

Therefore,

$$c_1 = T_\infty - T_0,$$

resulting in

$$\frac{T - T_\infty}{T_0 - T_\infty} = e^{-\left(\frac{hA}{c_v n}\right)t}.$$

NONISOTHERMAL WALL

If we allow the wall temperature to rise from T_∞ to some maximum value T_f with exponential time constant B , we may formulate a non-constant expression for the wall temperature T_w (see Fig. A-1),

$$T_w = T_{wall} = T_\infty + T_f(1 - e^{-Bt}).$$

Then, using

$$\rho V c_v \frac{dT}{dt} = -hA(T - T_w),$$

and again defining

$$m = \frac{hA}{\rho V c_v},$$

we obtain

$$\frac{dT}{dt} = m(T_\infty + T_f) - mT_f e^{-Bt} - mT,$$

a first order differential equation whose solution we will simply state as

$$T = \frac{c_1 e^{-mt} + m^2 T_f e^{-Bt}}{mB - m^2} + (T_\infty + T_f) \quad (A-1)$$

where c_1 is the constant of integration at time $t = 0$ and $T = T_0$. Whereupon

$$c_1 = [mB - m^2][T_0 - (T_\infty + T_f)] - m^2 T_f.$$

Equation (A-1) now becomes

$$T = \frac{[m(B - m)(T_0 - [T_\infty + T_f]) - m^2 T_f] e^{-mt} + m T_f e^{-Bt}}{(B - m)} + (T_\infty + T_f).$$

Fig. A-1. Wall temperature vs time.

Finally, we arrive at an expression for cavity temperature with a non-isothermal wall:

$$T = \left[T_0 - (T_\infty + T_f) - \frac{mT_f}{(B-m)} \right] e^{-mt} + \frac{mT_f}{(B-m)} e^{-Bt} + (T_\infty + T_f)$$

for $B \neq m$.

It should be noted, by the way, that if $B = 0$ and $T_f = T_\infty$, the solution

properly degenerates into the isothermal-wall solution. That is,

$$\begin{aligned} c_1 &= -m^2[T_0 - 2T_\infty] - m^2T_\infty \\ &= m^2[T_\infty - T_0] . \end{aligned}$$

Then, upon substitution into Eq. (A-1) we arrive at the isothermal expression:

$$T = (T_0 - T_\infty)e^{-mt} + T_\infty .$$