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APPENDIX F
HEAT TRANSFER MODEL DERIVATION
METHANE EXPLOSION

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METHANE EXPLOSION

Under the conditions of a postulated methane explosion within the panel, the temperature of the gas is raised by the combustion process to an initial value $T_{g\,init}$ with time $t = 0$ corresponding to initial conditions in the panel. Subsequently, the gas temperature in the panel decreases as heat is transferred to the surrounding salt and to the two explosion-isolation walls in the air-intake and air-exhaust drifts of each panel.

At time $t = 0$ the pressure in the panel is P_{init} based on panel closure due to creep and the elevation in pressure resulting from the explosion. Thus, the rise time of the temperature is not considered in the model.

At time $t = 0$, the volume of the panel is V_{init} and is assumed to remain constant throughout the cooling of the gas in the panel because of the short duration of the explosion. This means that the effect of creep on the panel volume is assumed negligible during the postulated explosion. The initial volume is given by:

$$V_{init} = V_{panel} - V_{waste} - V_{creep}$$

where

V_{init} = Initial volume
V_{panel} = Volume of the panel
V_{waste} = Volume of the waste
V_{creep} = Volume reduction due to creep

and is taken as given at the start of the heat transfer analysis and assumed to remain constant during the transfer of heat to the panel walls, roof, and floor.

F.1.0 Heat Balance

Assuming a constant volume is equivalent to stating that any creep closure of the panel volume during the explosion and subsequent cooling can be neglected.

$$\frac{dQ_{volume\ of\ gas}}{dt} = qA_{walls,\ floor,\ roof}$$

where $Q_{volume\ of\ gas}$ represents the heat contained in the hot gases subsequent to an explosion, q is the heat flux rate at the boundaries of the panel volume, and $A_{walls,\ floor,\ roof}$ is the surface area of the panel volume.

Following D'Appolonia (1978) it is conservatively assumed that the heat transfer to the surrounding walls, floor, roof, is related to the rate of change of enthalpy of the reaction products gas. Thus, the heat content of the room is given by:

$$\frac{dQ_{volume\ of\ gas}}{dt} = nC_p \frac{dT_g}{dt}$$

where n is the number of moles of gas in the room subsequent to the explosion, T_g is the gas temperature, and C_p is the heat content of the gas at constant pressure.[1] Thus,

$$nC_p \frac{dT_g}{dt} = qA_{walls,\ floor,\ roof} \tag{1}$$
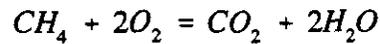
F.2.0 Moles of Gas

The gas in the panel subsequent to the explosion is a mixture of the combustion products of the explosive gas which is taken to be a mixture of methane, CH_4 and air. Because methane can explode with other than a stoichiometric air/methane mixture (i.e., the methane concentration in air for an explosion to occur is a range as opposed to a single value), it is impossible to determine the number of moles of combustion product gas precisely. Thus, it is assumed that the explosion occurs with a stoichiometric air/methane mixture.

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[1]The specific heat at constant volume is used even though the explosion or rapid combustion of the methane-air mixture occurs at constant volume because the rate of change of enthalpy as opposed to internal energy has been used.
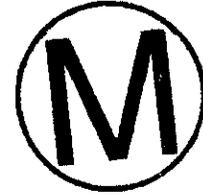
F.2.1 Mixture

The stoichiometric reaction for methane is (Bodartha, 1980):

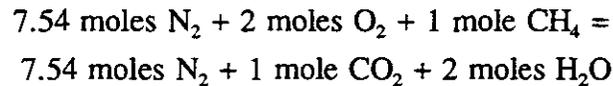$$CH_4 + 2O_2 = CO_2 + 2H_2O$$

with the moles of air given by:

$$n_{air} = 4.77(2) = 9.54 \; mole \; air/mole \; methane$$

or 9.54 moles of air are required to provide 2 moles of oxygen. Using a ratio of 9.54 moles of air per mole of methane, the total moles of gas at the time of the explosion would be:

$$n = (9.54 + 1)n_{CH4}$$

The number of moles of nitrogen in the air and in the combustion products gas is 3.77(2) = 7.54 moles/mole of methane (Bodartha, 1980). Thus,

$$7.54 \; moles \; N_2 + 2 \; moles \; O_2 + 1 \; mole \; CH_4 =$$
$$7.54 \; moles \; N_2 + 1 \; mole \; CO_2 + 2 \; moles \; H_2O$$

On a molar basis the reaction products are 71.5% nitrogen, 9.5% carbon dioxide, and 19% water vapor. This compares with a reaction product that is 72.9% nitrogen, 11.6% carbon dioxide and 15.5% water vapor when propane is burned at a stoichiometric ratio (D'Appolonia, 1978). Also, 10.54 moles of the methane-air mixture produces 10.54 moles of reaction products. Thus, the number of moles of air/methane prior to the explosion is the same as the number of moles of the product gas and the above relation for n will be used to compute the heat content in a panel prior to cooling.

$$n_{gas} = 10.54 \; n_{CH4} \tag{2}$$

Substituting (2) into (1),

$$10.54 \; n_{CH4} \; C_p \; \frac{dT_g}{dt} = qA_{walls, \, floor, \, roof}$$

or

$$\frac{dT_g}{dt} = \frac{qA_{walls,\ floor,\ roof}}{10.54\ n_{CH4}\ C_p}$$ (3)

is the differential equation for the time rate of change of the gas temperature in the panel following an explosion.

F.2.2 Specific Heat

The specific heat, Cp, of the combustion products of the explosion is required by equation (3). In general, the specific heat is a function of temperature over large temperature ranges. Figure C-1 shows plots of specific heats of the combustion products of stoichiometric propane-air mixtures and methane-air mixtures based on data from D'Appolonia (1978) and Reid, et al., (1977). The curves for propane-air mixtures are shown for comparison between the Reid, et al. data and the D'Appolonia data.

For an explosion temperature on the order of 2400 degrees kelvin ($^\circ$K), and using an average of the wall temperature and gas temperature to evaluate the specific heat, the temperature dependence curve will be evaluated in the region of 1400 $^\circ$K which is about the maximum useful temperature for the Reid, et al. data.

As shown on Figure F-1, the Reid et al. (1977) and D'Appolonia (1978) data agree well up to a temperature of approximately 1400 $^\circ$K. At the greater temperatures Reid et al. (1977), and other data indicate a decrease in specific heat with greater temperatures which is not consistent with expectation.

Figure F-2 shows a comparison of Reid et al. (1977) and the D'Appolonia (1978) data multiplied by 0.961, the ratio of specific heats for a methane-air mixture to a propane-air mixture at 300 $^\circ$K. Below 1400 $^\circ$K the agreement is very good. Above 1400 $^\circ$K the curve based on the D'Appolonia data remains valid. Therefore, the specific heat of the combustion products formed from a stoichiometric methane air mixture as a function of temperature is[2]

$$C_p = 1.29 \times 10^{-3}\ T + 7.3353 - \frac{32682}{T^2}$$ (4)

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[2]Equation (4) was obtained by multiplying Equation (9) of Appendix B of D'Appolonia [1978] by 0.961.
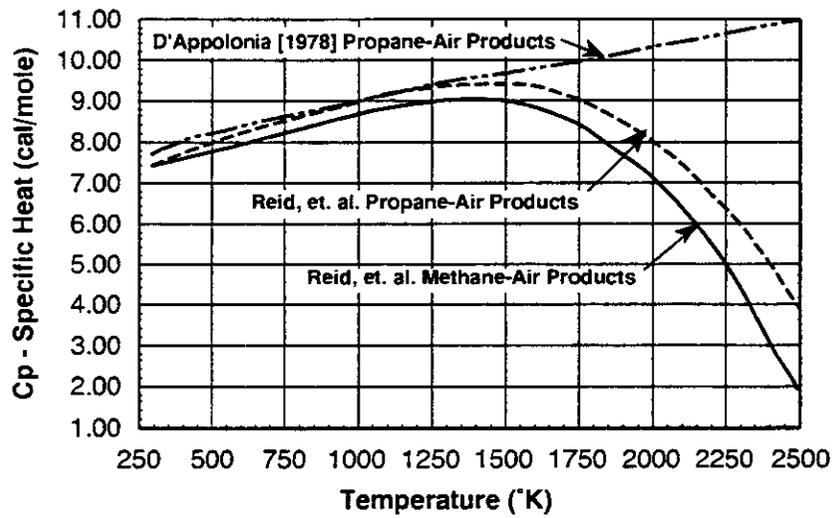
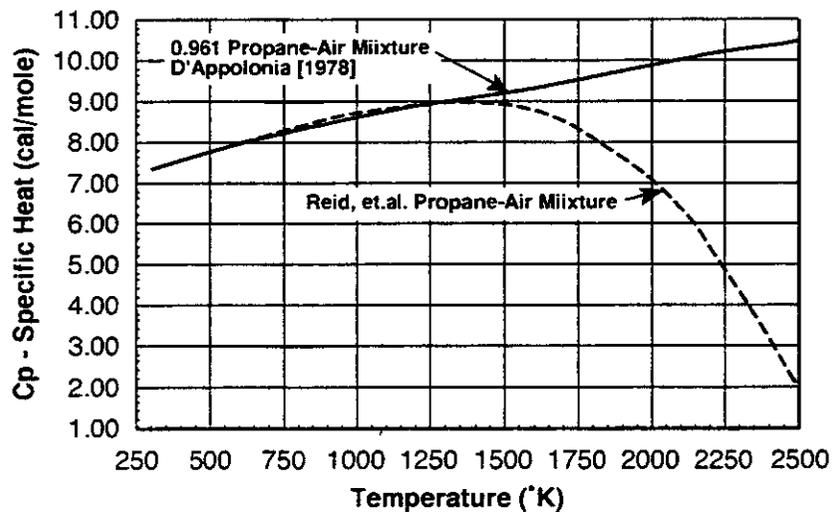**Figure F-1**
Specific Heat as a Function of Temperature

Figure F-2

Specific Heat for Methane-Air Stochiometric Mixture

F.3.0 Heat Transfer to the Walls, Floor, Etc._____

Heat is transferred from the gas to the surrounding walls, floor and roof of the panel rooms by both convection and radiation. Heat is then transferred into the walls, floor, roof, via conduction. Thus, the rate of heat conduction into the salt or the wall is governed by the rate at which heat can be conducted into the solids.

F.3.1 Radiation Heat Transfer

Heat transferred from the gas to the walls, floor, roof, is given by:

$$q_{rs} = \sigma\left(T_g^4 - T_w^4\right)$$

where q_{rs} is the heat flux to the walls, floor, roof, σ is the Stefan-Boltzmann constant $(1.35 \times 10^{-12}$ cal/cm^2-sec-$^\circ$K), and T_w is the temperature of the walls, floor, and roof.

The majority of the surface area of the panel available for heat transfer via both radiation and convection is salt. However, a small portion of the total area will be the inner face of the explosion-isolation wall (or construction-isolation well). Because the wall, floor, roof temperature is controlled by the time dependent conduction of heat into either the walls, floor, roof or the wall faces, and the diffusivities and conductivities of the salt and wall, floor, roof material may be different, the radiation heat transfer is divided into two components.

The radiative heat transfer to the salt (T_{ws}) is:

$$q_{rs} = \sigma\left(T_g^4 - T_{ws}^4\right)$$

and the radiative heat transfer to the explosion-isolation wall (T_{wb}) is:

$$q_{rb} = \sigma\left(T_g^4 - T_{wb}^4\right)$$

The combined radiative heat transfer to the walls, floors, roof is:

$$Q_r = q_{rs}A_s + q_{rb}A_b$$

or

$$Q_r = \sigma\left(A_s\left[T_g^4 - T_{ws}^4\right] + A_b\left[T_g^4 - T_{wb}^4\right]\right) \tag{5}$$

where A_b = Area of the walls, and A_s = area of the salt.

Equation (5) comprises the radiation portion of the right hand side of the differential equation, (3), for the rate of gas temperature in the panel.

F.3.2 Convection Heat Transfer

In addition to radiation, heat is transferred to the walls, floor, roof, and explosion-isolation walls by natural convection. In subsequent discussion, walls denote all exposed surface area of salt within a panel. Explosion-isolation walls denote the surface area of the expendable walls placed in the sealed air-intake and air-exhaust drifts of the panel.

F.3.2.1 Heat Transfer from Gas to the Walls

In addition to radiation, heat is transferred to the walls, floor, roof, and explosion-isolation walls via natural convection. The heat flux due to convection (q_c) is given by:

$$q_c = h\left(T_b - T_w\right)$$

where h = Film coefficient.

As for the case of radiation, the majority of heat transfer by convection will occur to the surrounding salt. However, a portion will be transferred to the explosion-isolation wall. Because the temperature of the explosion-isolation wall may be different from the temperature of the salt, the convective heat transfer is divided into the two components analogous to the radiation heat transfer. For the salt, the convection heat transfer is:

$$q_{cs} = h\left(T_g - T_{ws}\right)$$

and for the explosion-isolation walls:
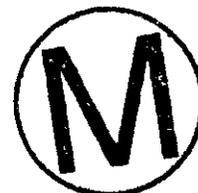
$$q_{cb} = h\left(T_g - T_{wb}\right)$$

The combined radiative heat transfer (Q_c) to the walls, floors, roof, and explosion-isolation walls is:

$$q_{cb} = h\left(T_g - T_{wb}\right)$$

The combined radiative heat transfer (Q_c) to the walls, floors, roof, and explosion-isolation walls is:
assuming that the heat transfer coefficient does not change with location or material.

$$Q_c = q_{c\ NaCl}\ A_s + q_{cb}A_b$$

Theoretically the convective heat transfer coefficient is different for the face of the explosion-isolation walls, which are vertical compared with the heat transfer coefficient for the roof and floor faces of the panel which are horizontal. Neglecting the difference in heat transfer coefficient due to geometric differences, the above two equations for the heat flow to the walls, floor, roof, and explosion-isolation walls can be combined to give

$$Q_c = h\left(A_s\left[T_g - T_{ws}\right] + A_b\left[T_g - T_{wb}\right]\right) \tag{6}$$

Equation (6) gives the convective heat transfer portion of the right hand side of Equation (3). Combining (3), (5) and (6),

$$\frac{dT_g}{dt} = -\frac{Q_c + Q_r}{10.54\ n_{CH4}\ C_p} \tag{7}$$

where the negative sign indicates that Q_c and Q_r represent heat transferred out of the system consisting of the gas in the room. These same quantities then represent heat transferred into the surrounding salt and explosion-isolation wall.

F.3.2.2 Convection Coefficient

Assuming the convection coefficient is the same at all surfaces and following the methods developed in D'Appolonia (1978), with all units in the centimeter-gram-second (cm-g-sec) system of units,

$$N_u = 0.13[P_r G_r]^{1/3}$$

where P_r is the Prandtl number and G_r is the Grashof number. The Prandtl number is essentially *constant and is taken as 0.71 regardless of pressure and temperature*. The Grashof number is given by

$$G_r = \frac{g\beta L^3(T_g - T_w)}{v^2}$$

where g is the acceleration of gravity, β is the volume coefficient of thermal expansion and v is the kinematic viscosity of the gas. For ideal gases,

$$\beta = \frac{1}{T_g}$$

and the kinematic viscosity is given by

$$v = \frac{\mu}{\rho}$$

where μ is the absolute viscosity ρ = mass density. Substituting for n and β in the expression for the Grashof number,

$$G_r = \frac{g\rho^2 L^3(T_g - T_w)}{T_m \mu^2}$$

where

$$T_m = \frac{T_g + T_w}{2}$$

is the average of the gas and surface temperature.

Substituting for the Grashof number and Prandtl number in the expression for the Nusselt number,

$$N_u = 0.13\left(0.71\frac{g\rho^2 L^3[Tg-T_w]}{T_m\mu^2}\right)^{1/3}$$

$$N_u = 0.146L\left(\frac{g\rho^2}{\mu^2}\left[\frac{T_g-T_w}{T_g+T_w}\right]\right)^{1/3}$$

and substituting for the Nusselt number in the expression for the convection coefficient,

$$h = 0.146k_g\left(\frac{g\rho^2}{\mu^2}\left[\frac{T_g-T_w}{T_g+T_w}\right]\right)^{1/3}$$

Since the thermal conductivity of the gas is given by[3]

$$k_g = 6.4\ x\ 10^{-5}\left(\frac{T_m}{300}\right)^{.75}$$

$$h = 9.34\ x\ 10^{-6}\left(\frac{T_g+T_w}{600}\right)^{.75}\left(\frac{g\rho^2}{\mu^2}\left[\frac{T_g-T_w}{T_g+T_w}\right]\right)^{1/3} \qquad (8)$$

Figure F-3 shows h as a function of surface temperature based on a gas temperature of 2400°K and density and viscosity consistent with conditions at the time of an explosion.

Assuming that no additional gas is generated subsequent to the explosion, the density of the gas after the explosion is the same as before the explosion since mass is conserved. Thus, the gas density after the explosion is the molecular weight of n moles of methane plus 9.54n moles of air divided by the initial volume,

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[3]D'Appolonia [1978].
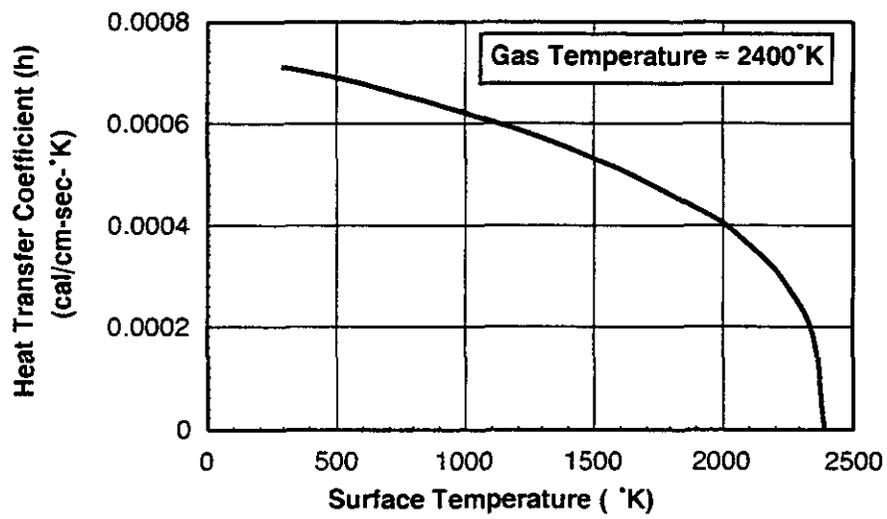
Figure F-3

Convection Heat Transfer Coefficient Versus Temperature

$$\rho = n\left(\frac{M_{w\ CH4} + 9.54M_{w\ air}}{V_{init}}\right)$$

$$\rho = n\left(\frac{16 + 9.54(29)}{V_{init}}\right)$$

$$\rho = \frac{292.66n}{V_{init}} \tag{9}$$

$$\mu = 1.85 \times 10^{-4}\left(\frac{T_m}{300}\right)^{0.67} \tag{10}$$

and the viscosity is given by (D'Appolonia, 1978), where the viscosity is evaluated at the average of the surface and gas temperatures.

Because there will be two different surface temperatures, one corresponding to the salt, and one for the explosion-isolation wall, there will be different convective heat transfer coefficients as well.

F.3.3 Conduction Into the Walls, Floor, Roof, and Explosion-Isolation Walls

The temperature which controls the heat transfer from the gas via radiation and convection is controlled by the rate at which heat is conducted into the walls, roof, floor, and explosion-isolation walls. The diffusion of heat into the walls, floor, roof, and explosion-isolation walls is assumed to be governed by a one-dimensional, semi-infinite thermal diffusion model. If the temperature penetrates the explosion-isolation walls, the model is changed to be thermal diffusion across a slab of finite thickness with an ambient gas temperature on the side in the isolation zone.

Thermal diffusion into the walls, floor, roof, and explosion-isolation walls is governed by the partial differential equation,

$$\alpha \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}$$

where α is the thermal diffusivity, T is the temperature, x is the distance into the wall, floors, roof, or explosion-isolation walls, and t is time. At x = 0 the flow of heat into the walls, floor, roof, or explosion-isolation walls is governed by the boundary condition,

$$-k \frac{\partial T}{\partial x} = q_{in}$$

where q_{in} is the heat flux into the walls, etc. from the gas via convection and radiation and k is the thermal conductivity. Because the thermal diffusivity and conductivity for salt is different from that of the explosion-isolation wall, two conduction models are required.

F.3.3.1 Heat Conduction to the Salt

The first involves the heat transferred from the gas to the salt and is governed by the partial differential equation,

$$\alpha_s \frac{\partial^2 T_s}{\partial x^2} = \frac{\partial T_s}{\partial t} \tag{11i}$$

where α_s is the thermal diffusivity of salt which is a function of temperature. Figure F-3 shows plots of thermal diffusivity for halite, anhydrite, argillaceous halite and polyhalite (Krieg, 1983). Figure F-4 also shows data from D'Appolonia (1978) that used the relation

$$\alpha_s = \frac{10}{T_s}$$

for salt. The D'Appolonia temperature dependence yields slightly higher values compared with the Waste Isolation Pilot Plant (WIPP) data, but indicates a consistency in the data. For purposes of the post-explosion heat transfer analysis the temperature dependent data for salt has been used.
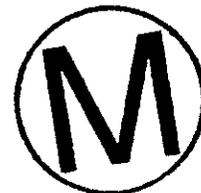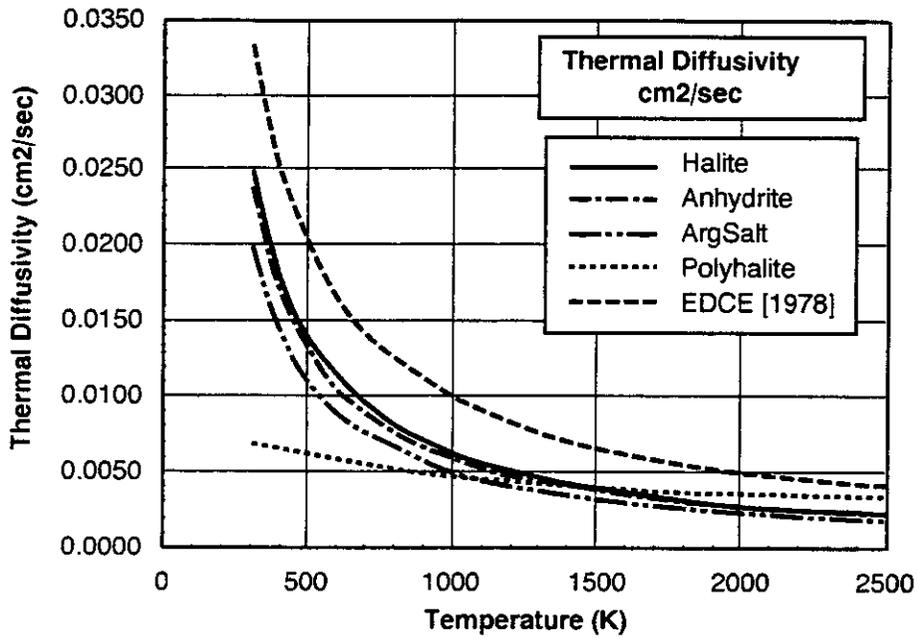
Figure F-4
Thermal Diffusivity of WIPP Geologic Materials

$$\alpha_s = 0.025 \left[\frac{300}{T_s} \right]^{1.14} \tag{12i}$$

The boundary condition at the surface of the salt is:

$$-k_s \frac{\partial T_s}{\partial x} = q_{sr} + q_{sc} \tag{13i}$$

where k_s is the thermal conductivity of the salt. Figure F-4 shows plots of thermal conductivities for the same materials as a function of temperature. Again, the thermal conductivity from D'Appolonia (1978):

$$k_s = \frac{4.5}{T_s}$$

is also shown on Figure F-5 to check the consistency of the WIPP data. Again, the thermal conductivity for halite was used for the post-explosion heat transfer analysis.

$$k_s = 0.012 \left[\frac{300}{T_s} \right]^{1.14} \tag{14i}$$

The terms q_{sr} and q_{sc} in (13i) couple the heat conduction into the salt with the rate of cooling of the gas via equations (7) through (10). In addition to the boundary conditions given by (12i), initial conditions at time $t = 0$ are required. It is assumed that at $t = 0$ the salt is at the ambient temperature in the panel, T_{amb}. Equations (11i) through (14i) with the initial conditions form the complete problem for the temperature in the salt as a function of time as the gas cools following the explosion.

F.3.3.2 Heat Conduction to the Explosion-Isolation Walls

The second model involves the heat transferred from the gas to the explosion-isolation walls and is governed by the partial differential equation,

$$\alpha_b \frac{\partial^2 T_b}{\partial x^2} = \frac{\partial T_b}{\partial t} \tag{11ii}$$