Review of the ALOHA Code Pool Evaporation Model (U)

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REVIEW OF THE ALOHA CODE POOL EVAPORATION MODEL (U)

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Abstract

The ALOHA computer code determines the evaporative mass transfer rate from a liquid pool by solving the conservation of mass and energy equations associated with the pool. As part of the solution of the conservation of energy equation, the heat flux from the ground to the pool is calculated. The model used in the ALOHA code is based on the solution of the temperature profile for a one-dimensional semi-infinite slab. This model is only valid for cases in which the boundary condition (pool temperature) is held constant. Thus, when the pool material temperature is not constant, the ALOHA ground-to-pool heat flux calculation may result in a non-conservative evaporation rate.

The analytical solution for the temperature profile of a one-dimensional semi-infinite slab with a time-dependent boundary condition requires *a priori* knowledge of the boundary condition. Lacking such knowledge, a time-dependent finite-difference solution for the ground temperature profile was developed. The temperature gradient, and thus the ground-to-pool heat flux, at the ground-pool interface is determined from the results of the finite-difference solution.

The evaporation rates over the conditions sampled using the ALOHA ground-to-pool heat flux model were up to 15% lower than those generated when the finite-difference model to calculate ground-to-pool heat flux.

Overall ALOHA code estimates may compensate by judicious selection of input parameters and assumptions. Application to safety analyses thus must be performed cautiously to ensure that the estimated chemical source term and its attendant downwind concentrations are bounding.

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INTRODUCTION

The ALOHA computer code, Version 5.1 (NOAA 1992) is used in chemical source term / consequence calculations as part of safety and accident analyses that support Savannah River Site Safety Analysis Report, Basis for Interim Operation, Preliminary Hazard Analysis, and Emergency Management Hazards Assessment documentation. As such, a review of the source term and dispersion models contained in the ALOHA code was required to ascertain the applicability of the models to accident analysis calculations. During the course of the review of the pool evaporation model, an error was discovered in the ground-to-pool heat flux model. A new ground-to-pool heat flux model was developed to address the discovered deficiency. A series of test cases were run to determine the impact of the error on the pool evaporation rate.

POOL EVAPORATION ALGORITHM

The ALOHA computer code determines the evaporative mass transfer from a liquid pool by solving the conservation of mass and energy equations associated with the pool. The heat transfer mechanisms accounted for in the algorithm include solar flux, net longwave radiation flux between the pool and the atmosphere, ground-to-pool heat flux, atmosphere-to-pool sensible heat flux, and evaporative heat flux.

The solar flux is calculated as a function of Julian day, time of day, longitude, and latitude as prescribed by Raphael (1962). The Stefan-Boltzman radiation law (White 1984) is used to calculate the net longwave radiation flux. Atmosphere-to-pool sensible heat flux is determined using the mass transfer-heat transfer analogy (Incropera and DeWitt 1985) in conjunction with the evaporative mass transfer rate. The evaporative heat flux is calculated based on the evaporative mass transfer rate and the pool material's heat of vaporization. Ground-to-pool heat flux is calculated using Fourier's law of heat conduction, with the ground temperature profile characterized by one-dimensional, constant temperature boundary, constant temperature initial condition, semi-infinite slab heat conduction. Brighton's solution of the advection-diffusion equation (Brighton 1985) is used to model the evaporative mass transfer from the pool. Reynolds (1992) provides a detailed overview of these models as used in the ALOHA pool evaporation algorithm.

GROUND-TO-POOL HEAT FLUX MODELS

The ground-to-pool heat flux is calculated in the ALOHA code by

$$F_G = \frac{\chi k_G}{\sqrt{\pi \alpha_G}} \frac{(T_G - T_p)}{\sqrt{t}} \quad t > 0 \quad (1)$$

where:

- F_G - ground-to-pool heat flux
- χ - ground roughness factor
- k_G - ground thermal conductivity
- α_G - ground thermal diffusivity
- T_G - initial ground temperature
- T_p - pool temperature
- t - time from initial pool formation

The solution for the ground temperature profile associated with equation (1) is

$$T(x, t) = (T_p - T_G) \left[1 - \frac{2}{\sqrt{\pi}} \int_0^\eta e^{-\eta'^2} d\eta' \right] + T_G \quad \text{for } t > 0 \quad (2a)$$

$$\eta = \frac{x}{2\sqrt{\alpha_G t}} \quad (2b)$$

where:

- η - similarity variable
- x - distance into the ground from the pool-ground interface

Equations (1) and (2) are valid only if the pool temperature remains constant (White 1984). The ground temperature profile for the time-dependent boundary condition case is given in Ozisik (1980)

$$T(x, t) = \frac{2T_G}{\sqrt{\pi}} \int_\eta^\infty e^{-\eta'^2} f\left(t - \frac{x^2}{4\alpha_G \eta'^2}\right) d\eta' \quad \text{for } t > 0 \quad (3a)$$

where η is now defined as

$$\eta = \frac{x}{2\sqrt{\alpha_G(t - \tau)}} \quad (3b)$$

with:

- τ - a time-independent dummy variable introduced as a result of using Duhamel's Theorem to solve for the temperature profile

It is apparent by inspection that equations (3a-b) are not equivalent to equations (2a-b), and, therefore, the ground-to-pool heat flux calculated using equations (1a-b) is not appropriate for cases where the pool temperature varies with time.

An analytical solution of equations (3a-b) cannot be found without *a priori* knowledge of the boundary condition (pool temperature). Lacking such knowledge, a finite-difference solution for the ground temperature profile was developed.

The one-dimension heat conduction equation

$$\frac{\partial T(x,t)}{\partial t} = \alpha_g \frac{\partial^2 T(x,t)}{\partial x^2} \quad (4)$$

is expressed in finite difference form, using the Forward-Time Centered-Space method (Anderson, *et al.* 1984), and arranged to solve for the updated temperature

$$T_n^{i+1} = T_n^i + \frac{\alpha_g \Delta t}{(\Delta x)^2} [T_{n+1}^i - 2T_n^i + T_{n-1}^i] \quad (5)$$

$$\text{for } \begin{cases} i = 1, 2, \dots, \infty \\ n = 2, 3, \dots, N-2, N-1 \end{cases}$$

with:

- i - time step index
- n - grid point index
- N - grid point index at ∞
- Δt - time-step
- Δx - grid spacing

Equation (5) is first-order accurate with truncation error of $O[\Delta t, (\Delta x)^2]$ and is stable when the following Courant-Friedrichs-Lewy (CFL) condition is met

$$0 \leq \frac{\alpha \Delta t}{(\Delta x)^2} \leq \frac{1}{2} \quad (6)$$

The boundary condition at the pool-ground interface ($n=1$) is prescribed by the pool conservation of energy solution (*i.e.* the pool temperature); the boundary condition at infinity ($n=N$) is equal to the initial ground temperature.

For the purpose of the finite-difference solution, "infinity" is defined as a spatial location where the temperature does not vary over the time period of interest. As an estimate, the penetration depth, δ , associated with the constant-temperature boundary solution is used to calculate the distance between the pool-ground interface grid point ($n=1$) and the infinity grid point ($n=N$)

$$\delta = 3.64 \sqrt{\alpha_g t} \quad (7a)$$

where

$$\left| \frac{T(\delta, t) - T_g}{T_p(t=0) - T_g} \right| = 0.01 \quad (7b)$$

A *post priori* comparison of the temperature at the infinity grid point to the constraint of equation (7b) is made to verify that the constant-temperature-at-infinity boundary condition was maintained.

The relationship between the time step and grid spacing is prescribed by the stability criterion. Choosing the CFL condition that minimizes the truncation error and the deviation from the exact amplification factor (Anderson, *et al.* 1984), the time step as a function of grid spacing is given by

$$\Delta t = \frac{(\Delta x)^2}{6\alpha_G} \quad (8)$$

Note that the time step and grid spacing must not only meet the CFL condition, but must also be small enough such that the truncation error has a minimum impact upon the solution.

EVALUATION OF GROUND-TO-POOL HEAT FLUX MODELING ON EVAPORATIVE MASS TRANSFER RATE

A series of test cases was performed in which benzene evaporation rates were calculated using both the original and finite-difference based ground-to-pool heat flux models. The air, initial pool, and initial ground temperatures were varied between 10 °C and 40 °C. Figure 1 presents the results of those calculations.

Figure 1. Benzene Evaporation Rate Results

In Cases 1, 2, and 3 the original ALOHA pool evaporation model consistently underpredicted the evaporation rate from the pool (with respect to the pool evaporation rate results as calculated using the finite-difference based ground-to-pool heat flux model) by up to 15%. The initial ground temperatures in these cases were equal to or less than the initial pool temperatures. In Case 4, the original ALOHA pool evaporation model predicted higher evaporation rates (by up to 6%) in the first 180 seconds; over the remaining duration it underpredicted by up to 11%. The initial ground temperature was higher than the initial pool temperature in this case.

A possible way to compensate for the non-conservatism in the ALOHA-calculated source term is to adjust one or more of the input parameters such that the source term is "artificially" increased. For example, if the air, initial pool, and initial ground temperatures in Case 1 are all increased by 5 °C, the evaporation rate calculated by the ALOHA model is increased to the extent that it bounds the evaporation rate as calculated by the modified model at 10 °C. Another compensatory measure would be to use an alternative method to calculate the source term, and use the ALOHA code only for calculating downwind concentrations.

CONCLUSIONS

The ALOHA code pool evaporation model contains an error in its ground-to-pool heat flux model. Based on the test cases evaluated, this error results in evaporation rates that are in general lower than those predicted when employing a ground-to-pool heat flux model that accounts for the error. Overall ALOHA code estimates may compensate by judicious selection of input parameters and assumptions. Application to safety analyses thus must be performed cautiously to ensure that the estimated chemical source term and its attendant downwind concentrations are bounding.

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