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DEVELOPMENT OF A THERMAL TRANSIENT CALCULATIONAL TOOL FOR HIGH LEVEL WASTE TANKS

by

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ABSTRACT

Thermal design constraints exist on the processing operations in the High Level Waste (HLW) tanks of the Savannah River Site (SRS). A FORTRAN computer code was developed to provide a simple, fast, and reasonably accurate analysis tool for plant operation design. The code computes a lumped transient temperature for the liquid contents of a waste tank by modeling the liquid (slurry), the vapor space above it, the tank wall, and the cooling air outside of the tank. Results for a typical processing cycle of several months' duration can be obtained in 2-4 minutes CPU time on a VAX computer. This paper discusses the code's mathematical models, presents model results for a typical HLW process schedule, and compares the code predictions with operations data.

MODEL DEVELOPMENT

A computer code was developed to provide rapid analysis of transient thermal conditions in a HLW tank as it undergoes the mass transfers, heating, and cooling associated with its processing schedule. The analysis is based on solution of unsteady lumped mass and energy equations for the liquid phase (slurry), the vapor phase above the liquid, the tank wall, and the cooling air which circulates around the tank. Material transfers are made both to the slurry phase and to the vapor phase; a purge flow through the latter is adjusted to set a nominal tank pressure of one atmosphere. Since no spatial variation in temperature or properties is modeled, the code is not intended for predicting local effects (e.g., hot spots), but for rapidly predicting averaged conditions, with the degree of expected local variation being quantified via a separate analysis (e.g., by finite element).

A detailed derivation of the code's equation set has been documented[1]. The unsteady mass equation is:[2]

$$\frac{d}{dt}\int_V \rho dV + \int_{A_e} \rho\vec{v} \bullet \vec{n} dA = 0 \tag{1}$$

which, for a control volume with mass fluxes becomes

$$\left.\frac{dm}{dt}\right)_{c.v.} = \sum_{in} \dot{m}_i - \sum_{out} \dot{m}_j \tag{2}$$

where the sign convention is handled by explicitly summing positively-signed streams for each direction of flow. Conservation of energy gives:[2]

$$\frac{d}{dt}\int_{c.v.} \rho u dV + \int_{A_e} \rho\left(u + \frac{v^2}{2} + gz\right)\vec{v} \bullet \vec{n} dA_e + \int_A \vec{q} \bullet \vec{n} dA - \int_A \vec{\tau} \bullet \vec{v} dA = 0 \tag{3}$$

which can be rewritten as:

$$\left[\sum_i \dot{m}_i c_{p,i}\left(T_i - T_{ref}\right) + \sum_j \dot{Q}_j - \left[\dot{m} c_v \left(T - T_{ref}\right)\right]_{c.v.}\right] \bullet \frac{1}{\left(mc_v\right)_{c.v.}} = \frac{dT}{dt} \tag{4}$$

where heats of vaporization and the sensible heat in the vapor are treated as heat flow terms in the liquid equation. For the tank wall, (4) reduces to:

$$\frac{dT}{dt} = \frac{\sum_j \dot{Q}_j}{(mc)_{c.v.}} \tag{5}$$

A set of equations of the forms (1), (4), and (5) describes the evolution in time of the mass and energy of the four components. It is also necessary to solve equation (2) for each separate material stream of the liquid phase, in order to keep track of the material properties of the mixture. This set of ordinary differential equations is then solved numerically. Given that the mass of each species component is computed as a function of time, mixture properties are calculated at any point in time as:

$$\rho_{mix} = \frac{\sum_j m_j}{V} \tag{6}$$

$$c_{p,mix} = \frac{\sum_j m_j c_{p,j}}{\sum_j m_j} \tag{7}$$

where the summations in equations (6) and (7) include the original tank contents.

To implement the equation set, the following energy transfer mechanisms are considered:

- Internal heat generation due to radiolytic decay in the liquid phase,
- Addition of energy to liquid due to mixing pump operation,
- Sensible heat transfer with incoming and outgoing mass fluxes in the liquid and vapor,
- Heat of condensation of steam influxes to the liquid,
- Sensible and latent heat transfer between liquid and vapor,
- Heat transfer from liquid and vapor to the cooling coils in the tank, and
- Heat transfer from liquid, vapor, and cooling air to the tank wall.

The computation of the vapor mass flux is complicated by several factors. Since the total tank volume is constant, as is the pressure in the vapor space, the nominally specified purge flow must adjust to accomodate the changing tank level governed by the liquid phase. From thermodynamics,

$$\frac{dm_i}{dt} = \left.\frac{\partial m_i}{\partial V}\right)_T \frac{dV}{dt} + \left.\frac{\partial m_i}{\partial T}\right)_V \frac{dT}{dt} \tag{8}$$

which can be written as

$$\frac{dm_i}{dt} = \rho_i \frac{dV}{dt} + \frac{V}{T}\frac{dT}{dt}\left[-\rho_i + \frac{1}{\mathrm{R}_i}\frac{dP_i}{dT}\right] \tag{9}$$

where the change in vapor pressure with temperature can be expressed empirically by, e.g., Antoine's equation. Equation (9) expresses the component derivative in terms of other derivatives. In particular, the mass and temperature derivatives are strongly coupled. Moreover, solution of equation (9) for the mass derivative is not sufficient to specify the mass flowrate of water vaporized from the liquid phase; values for the input and output vapor streams are needed, not just their difference.

A rigorous solution to equation (9) and specification of the required flowrates requires a more complex model than developed here, one which includes dynamic effects by incorporating the momentum equation into the model. In lieu of this, an approximate scheme which was found to work well in practice was used. In this scheme, the vapor phase is considered to have two components: water vapor and the purge gas (a pure gas or a known mixture). For the purge gas, a simplified form of equation (9) is used, i.e.,

$$\frac{dm_i}{dt} = \rho_i \frac{dV}{dt} \tag{10}$$

where

$$\left.\frac{dV}{dt}\right)_v = -\left.\frac{dV}{dt}\right)_l \tag{11}$$

since the total volume inside the tank is constant, and the rate of change of liquid volume is fixed by the mass flowrates of the (incompressible) liquid-phase streams. If the vapor volume increases, the incoming purge gas flowrate is increased over the nominal specification accordingly; if it decreases, the outgoing purge gas flowrate is increased over the nominal flowrate. Knowing $\frac{dm_i}{dt}$ and either the incoming or outgoing flowrate, the other can be calculated straightforwardly.

With the purge flowrates thus fixed, and the incoming and outgoing humidities specified by input, the vaporization rate from the liquid phase can be calculated. The mass of water vapor, per mass of purge gas at saturated conditions, is calculated as:[3]

$$Y_s' = \frac{P_w}{P - P_w}\frac{\overline{M}_w}{\overline{M}_g} \tag{12}$$

where P is constant at one atmosphere. The vaporization rate is the mass flowrate of water required to bring the purge gas influx from its initial fraction of saturation to the outgoing saturation fraction, i.e.,

$$\dot{m}_{vap} = \dot{m}_{g,in} Y_s'(\phi_o - \phi_i) \tag{13}$$

which is the mass flowrate of water into the vapor phase. The mass flowrate of water out of the vapor phase is simply

$$\dot{m}_{w,o} = \dot{m}_{g,o} Y_s' \phi_o \tag{14}$$

The basic scheme for the liquid and vapor heat transfer coefficients is to assume natural convection in the absence of agitation, and forced convection otherwise. Heat transfer will therefore be enhanced when agitation by the pumps occurs. When the agitation pumps are operated, an average forced convective heat transfer coefficient is computed for the region influenced by the pump (defined by a "radius of influence" which is an input parameter). The single, averaged heat transfer coefficient required by the lumped component formulation is then obtained as an area-weighted average of the forced and natural convection heat transfer coefficients. That is,

$$h = h_{fc}\frac{n\pi R_i^2}{A_b} + h_{nc}\frac{\left(A_b - n\pi R_i^2\right)}{A_b} \tag{15}$$

where n is the number of agitation pumps, and $n\pi R_i^2$ is less than or equal to the total surface area A_b.

The forced-convective component of equation (15) is determined as follows. It is assumed that standard heat transfer correlations for Newtonian flow are applicable, since the slurries of interest are considered Bingham plastics which behave roughly as Newtonian fluids above their yield stress.[4] The agitation pumps work by jet action; the jet centerline velocity (a function of radial distance) is assumed to be the appropriate velocity for use in the correlations. Finally, it is assumed that the criterion for turbulence is based on consideration of the conditions as the jet emerges from the nozzle.[5]

For the emergent jets of the HLW tanks' agitation pumps, the flow is turbulent and the Colburn equation[6] is used with radial distance as the relevant dimension. The jet centerline velocity as a function of radial distance can be modeled as:[5]

$$U_{cj} = 1.41 U_o \,\mathrm{Re}_o^{0.135}\frac{D_j}{r} \tag{16}$$

where U_o is the emergent velocity. Substituting into the Colburn equation gives:

$$h_{fc} = 0.0769\frac{k}{R_i}\mathrm{Re}_o^{0.908}\,\mathrm{Pr}^{1/3} \tag{17}$$

Convection to the cooling coils is modeled as flow across staggered tube bundles.[7] The relation is:

$$Nu_x = 0.35\left(\frac{X_t^*}{X_l^*}\right)^{0.2}\mathrm{Re}^{0.6}\,\mathrm{Pr}^{0.36}\left(\frac{\mathrm{Pr}}{\mathrm{Pr}_w}\right)^{0.25} \tag{18}$$

which includes a dependence on $\left(X_t^* / X_l^*\right)$, the ratio of the transverse and lateral distances between tubes, as well as a dependence on Prantdl numbers in the bulk and at the wall.

The orientation of the jet changes with respect to the coils as the jet rotates. The jet rotation means that the positions "lateral" and "transverse" change during the rotation; for the geometry of Tank 48, the factor $\left(X_t^* / X_l^*\right)^{0.2}$ varies between 0.87 and 1.15. For simplicity, then, this factor is set to unity. Given the lack of knowledge of liquid properties and of the tube wall temperature, and the weak dependence on the latter, the factor $\left(\mathrm{Pr}/\mathrm{Pr}_w\right)^{0.25}$ is likewise set to unity. With the above simplifications, equation (18) becomes:

$$Nu_x = 0.35\,\mathrm{Re}^{0.6}\,\mathrm{Pr}^{0.36} \tag{19}$$

for the forced convective heat transfer term. The average heat transfer coefficient is then weighted in accordance with equation (15).

For heat transfer between the liquid and vapor, some credit for enhanced heat transfer due to the vapor is taken when the agitation pumps are operating in the liquid. The heat transfer coefficient inside of the cooling coils is given by standard correlations: Seider-Tate for laminar flow and Dittus-Boelter for turbulent.[6] The air heat transfer coefficient in the cooling annulus includes radiative and natural convective contributions.[8,9]

A number of the surface areas which appear in the equations developed above are a function of the height of the liquid phase. This height is straightforwardly calculated at any point in time, since the total mass of the liquid is a solution variable, and the mixture density is likewise tracked. For the cooling coils, however, the surface area is not a linear function of height; the coils do not reach to the bottom or top of the tank, and additional area is associated with the coil bends; an empirical coil surface area function is implemented.

The method of solution for the equation set is a fourth-order Runge-Kutta solver with variable step size.[10] The implementation of the stepsize control logic achieves fifth-order accuracy using the fourth-order solver. The waste tank processes of interest involve step changes in heat addition and convective heat transfer coefficients. This presents numerical difficulties in that the size of an acceptable timestep changes drastically (i.e., by two or three orders of magnitude) as soon as the step occurs. To avoid these problems, the step changes are smoothed using a cubic polynomial function which satisfies the values and first derivatives at the ends of the smoothing interval.[11]

The most serious limitation in applying the model to a HLW tank is the lack of spatial variation. In particular, the liquid phase is expected to be non-uniform in temperature, as the non-Newtonian fluid is stirred at four locations by the agitation pumps, and non-uniform in composition, as the liquid phase separates into distinct layers when mixing ceases. The code is intended only to provide average temperatures for rapid design calculations; more detailed modeling is necessary to ensure that temperature criteria are satisfied locally. An improved formulation would also include an energy equation for the cooling water in the system of equations to be solved. The magnitude of the liquid temperature error in neglecting this effect was estimated as less than 10% for the process modeled in Figure 1. The relative error would increase as the temperature difference between the slurry and the cooling water decreases.

RESULTS AND DISCUSSION

Typical results for three batches of a HLW tank undergoing a 150 day processing cycle are shown in Figure 1. The temperature variations in the slurry reflect the various mass transfers in and out of the tank and the periods of enhanced heat transfer due to agitation. The three sharp peaks in the slurry temperature mark the end of each of three batch processing periods; the transfer pump energy constitutes a significant heat input at the end of each batch period. The heights of these peaks progressively decrease, since residual material from each batch accumulates in the tank. Within each batch period, the significant temperature differences between liquid and vapor during periods of quiescence are reduced when the mixing pumps are activated and enhanced heat transfer occurs. The washing period which follows the three batch operations, when the tank is near-full but the transfer pumps are operating, shows a steady temperature increase.

The model was developed for a fairly homogeneous HLW slurry, and one in which the difference between the cooling coil water temperature and the slurry temperature is significant. Figure 2 shows data from one of the HLW sludge tanks, for which operations data were available to compare to model predictions. Because the difference between the sludge and cooling water temperatures is low, the constant cooling water temperature assumption leads to greater relative error. When the model cooling water temperature was allowed to vary in accordance with the experimental data, however, the comparison between operating data and model prediction was within 2 °C. This is very good agreement, given the thermocouple error and especially considering that this tank contained a sludge-rich, inhomogeneous slurry.

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NOMENCLATURE

A_b	surface area of the bottom of the tank; this is also equal to interfacial area between liquid and vapor
c_p	heat capacity at constant pressure
c_v	heat capacity at constant volume
D_j	jet diameter (equal to nozzle diameter)
h	enthalpy
k	thermal conductivity
$\overline{M}$	molecular weight
m	mass
$\dot{m}$	mass flowrate
$\dot{m}_{c.v.}$	time rate of change of mass in control volume
Nu_x	local Nusselt number
P	pressure
P_i	pressure of incoming or outgoing stream; vapor pressure
Pr	Prandtl number
$\vec{q}$	heat-flux vector
$\dot{Q}$	rate of heat transfer
R_i	radius of influence for a jet
R_i	gas constant for species i
Re	Reynolds number
T	temperature
T_{ref}	reference temperature for definition of energy and enthalpy
t	time
$\vec{t}$	stress vector at a point on the control surface
U_{cj}	centerline jet velocity
V	volume
$v, \vec{v}$	magnitude of velocity; velocity vector
Y_s'	mass fraction of water vapor at saturated conditions

Greek

ρ	density
ϕ	saturation fraction

Subscripts

fc	forced convection
l	liquid
nc	natural convection
w	wall
vap	vapor

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Figure 1. Predicted Temperatures for 150-Day Processing Schedule

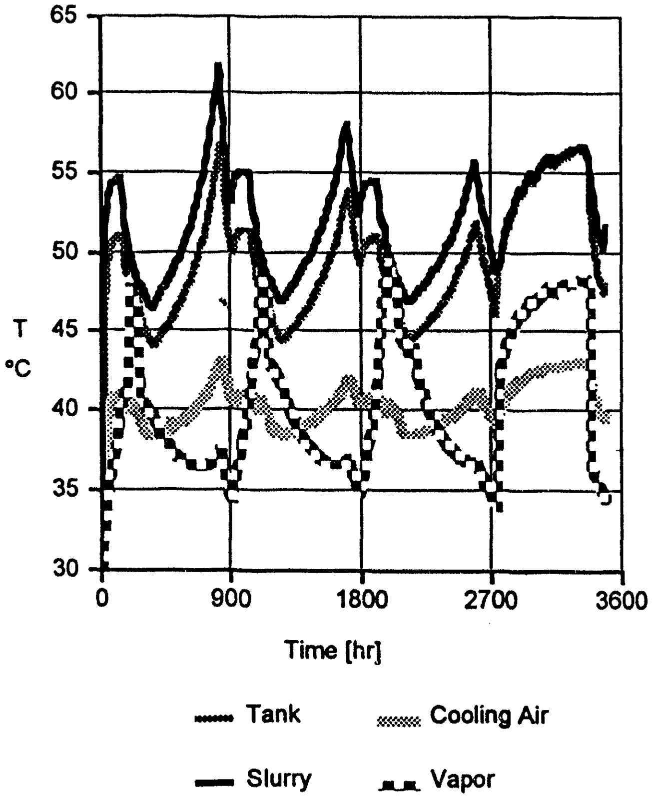
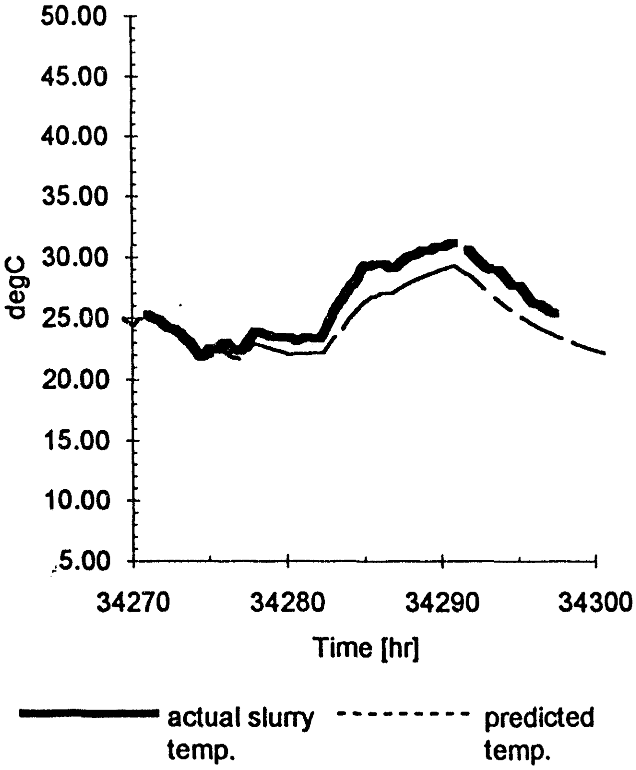


Figure 2. Predicted Slurry Temperature Compared to Operations Data from Inhomogeneous Sludge Tank



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