WPO 42834

Brinckerhoff

CALCULATION SHEET

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Calculation No. A141-GE-05

Project Title WIPP Seals (LSST)

Made by Marc C. Loken

Contract No. 4060/A141

Date 1/11/94

Subject SMC Thermal Calculations

Checked by LOS

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1 OBJECTIVE

The purpose of this calculation is to determine the expected temperatures within (and surrounding) a Salado Mass Concrete (SMC) emplacement due to its heat of hydration. The effects of seal length, room thermal properties, initial cooling of the SMC3, and heat transfer to the host salt are to be examined.

2 DESIGN BASES

2.1 Temperature Constraints

Large temperature gradients may cause thermal cracking upon cooling of concrete. A temperature difference of 36°F (20°C) between the interior of the concrete and its surrounding medium is known from both practical experience and laboratory experiments to be sufficient to cause thermal cracking [Freiesleben Hansen and Pedersen, 1982]. Strength loss caused by high internal temperatures within the concrete mass may also occur. ACI Guide 305 [1986] recommends that the concrete temperature be maintained below 100°F (38°C). A temperature increase of less than 25°F (14°C) during the first 4 hours after mixing (working time) has been recommended by Wakeley et al. [1993] to prevent rapid slump loss before hardening.

2.2 Design Assumptions

- The initial temperatures of the test facility and any concrete components stored in the facility are 27°C.
- The composition of three mixes of SMC3 is shown in Table 2-1. The density of SMC3 is 3,840 lb/yd^3 (2,280 kg/m^3). The cementitious material (cement + fly ash + Chem-Comp III) is 16 percent by weight of the total mix.
- The stratigraphy of the test facility can be neglected in the thermal modeling and equivalent axisymmetric models can be used.
- The test room can be considered thermally isolated; i.e., modeled as a single room in an infinite domain.
- The thermal properties of concrete are neither age- nor temperature-dependent.

2.3 Input Parameters

The heat of hydration of SMC3 is illustrated in Figure 2-1 which shows heat generation (Btu/lb$_{cem}$) as a function of time (hr), where the subscript "cem" refers to the total weight of cementitious material. The curves marked 231SM3 and 161SM3 were digitized and fit to the functional form:

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$$Q(t) = Q_\infty \exp\left[-(\tau_e/t)^\alpha\right] \qquad (1)$$

suggested by the Strategic Highway Research Program [1992] for describing the heat of hydration for concrete pavements, where Q_∞, τ_e, and α are the model parameters and t is time (hr). These model parameters were determined using the statistical program BMDP/386 and are summarized below in Table 2-2.

Table 2-1. Large Design Mix for SMC3

Serial No.	Batch Volume yd³	W/C[(a)]	SSD Batch Weights, lb/yd³						
			Cement	Fly Ash	CCIII[(b)]	Fine[(c)] Aggr.	Coarse[(c)] Aggr.	Salt	Water
159SM3	0.5	0.42	278	207	134	1,306	1,592	88	260
161SM3	5.0	0.36	278	207	134	1,301	1,601	88	225
231SM3	5.0	0.36	278	207	134	1,303	1,605	88	225

(a) Water weight (lb/yd³) ÷ weight of cement, fly ash, and Chem-Comp III (lb/yd³).

(b) Chem-Comp III.

(c) Batch design weight for fine aggregate is 1,292 lb/yd³; coarse aggregate is 1,579 lb/yd³.

Table 2-2. SCM3 Heat of Hydration Model Parameters

Parameter	Units	231SM3	161SM3
Q_∞	$\mathrm{Btu/lb_{cem}}$ $(\mathrm{W\text{-}hr/m^3_{con}})$	173.7 (40,837)	89.9 (21,135)
τ_e	hr	89.8	26.5
α	—	0.264	0.630

The conversion of units from $\mathrm{Btu/lb_{cem}}$ to $\mathrm{W\text{-}hr/m^3_{con}}$, where $\mathrm{m^3_{con}}$ refers to cubic meters of concrete, is given as follows:

1 $\text{Btu/lb}_{\text{cem}}$

$= [1\ \text{Btu/lb}_{\text{cem}}]\ [1055\ \text{J/Btu}]\ [2.2\ \text{lb/kg}]\ [2280\ \text{kg/m}^3]\ [1\ \text{W-s/J}]\ [1\ \text{hr/3600 s}]\ [0.16\ \text{lb}_{\text{cem}}/\text{lb}_{\text{con}}]$

$= 235\ \text{W-hr/m}^3_{\text{con}}$.

The volumetric heat generation rate (dQ/dt) of the concrete is required in performing the thermal analyses. Differentiating Equation 1 with respect to time results in:

$$dQ(t)/dt = Q(t)\ (\tau_e/t)^{\alpha}\ (\alpha/t) \qquad (2)$$

The heat of hydration for 231SM3 was used in this calculation since it results in the highest expected temperatures.

2.4 Problem Geometry

The room is assumed to be 20 ft (6.10 m) in width (W) and 12 ft (3.66 m) in height (H). The radius of the equivalent axisymmetric room is calculated as $R = (WH/\pi)^{1/2} =$ ~~2.43~~ m.

2.66 m (wcc)
2-10-94

2.5 Material Properties

The thermal properties of the heat-generating SMC3, the room air, and the surrounding halite are summarized in Table 2-3.

Table 2-3. Material Properties

Material	Thermal Conductivity (W/m-K)	Specific Heat (J/kg-K)	Density (kg/m³)	Volumetric Heat Generation Rate (W/m³)
Halite	(Eq. 3)	860.	2,300.	0.
SMC3	2.145	971.	2,280.	(Eq. 2)
Air	24.	1,016.	1.3	0.

$$k(T) = k_{300}(300/T)^{\lambda} \tag{3}$$

where

$k(T)$ = Thermal conductivity of salt as a function of temperature

T = Temperature (K)

k_{300} = Thermal conductivity at reference temperature (T = 300 K)

= 5.0 W/m-K

λ = Exponent describing temperature dependence

= 1.14

The thermal properties of the WIPP salt are taken from Bailey et al. [1992]. The thermal properties of the SMC3 are assumed to be similar to those of SMC6 reported in Wakeley et al. [1993]. The enhanced thermal conductivity of the room air is a reasonable approximation of a ventilated room as found previously by Loken et al. [1987].

3 CONCLUSIONS

A number of conclusions can be made, based on the results of this calculation. Simply stated, these conclusions are given below.

1. Unless some type of artificial cooling or chilling of the SMC is used, a peak temperature > 52°C and a maximum temperature difference between the concrete and the host medium > 13°C are likely to occur in mass emplacements of SMC.
2. Although the thickness of emplacements (length of seal) of SMC affects the peak temperature, the peak temperatures for thicknesses greater than 20 ft can be estimated using an infinite seal length. Additional analyses would be required to find the relationships among emplaced thickness, time of emplacement after mixing, and peak temperature.
3. While the salt is a good heat sink for conducting heat away from the concrete in the long term, its short-term influence on the peak temperature in the concrete mass is negligible.
4. The adiabatic temperature rise of SMC3 measured in Waterways Experiment Station (WES) lab testing was reproduced using the numerical modeling capabilities of SPECTROM-41.

5. The influence of possible age- and temperature-dependent thermal properties for green and hardened concrete need to be measured, or at least tested in additional numerical studies, to ascertain if such dependency causes larger peak temperatures.

6. When large-scale emplacements are to be made underground at the WIPP, consideration should be given to using heat flux meters to measure the radiative and convective heat loss rates from the form face. Such information would allow a better representation of the cooling than that provided by modeling air as a "high conductivity" material.

7. The thermomechanical aspects of cracking need to be analyzed because of the expected temperature gradients across the concrete/salt interface and the large difference between the thermal expansion of these two materials.

4 MODELING CONSIDERATIONS

An axisymmetric representation of the room, the seal, and the surrounding halite is shown in Figure 4-1. The left vertical boundary is the axis of rotation along the length of the room. The lower horizontal boundary is a plane of symmetry located at the midlength of the seal. The upper horizontal and right vertical boundaries are beyond the thermal influence of the heat-generating SMC3 throughout the simulation period (1 yr). The temperatures were calculated using the finite element program **SPECTROM-41** [Svalstad, 1989]. The maximum temperature at the midpoint of the SMC3 (Point A, Figure 4-1) is the primary output of this analysis. Six calculations were performed, as described in Table 4-1.

Table 4-1. Summary of Cases

CASE I.D.	DESCRIPTION	INPUT FILE (*.INP)	MESH FILE (*.GEN)	FASTQ INPUT (*.FQI)
A	Baseline Case Length = 20 ft Room = Air T_0 = 27°C	SS_TEMP20	NEW20	SS_SEAL20
B	Length = 6 ft	SS_TEMP6	NEW6	SS_SEAL6
C	Length = ∞	SS_TEMP_INF	NEW_INF	SS_SEAL_INF
D	Room = 10 ft SMC3	SS_TEMP	NEW	SS_SEAL
E	T_0 = 17°C	SS_TEMP20_COOL	NEW20	SS_SEAL20
F	Adiabatic	SS_TEMP1	none	none

The baseline case (A) considers a seal length of 20 ft, room thermal properties characteristic of a ventilated room, and an initial SMC3 temperature of 27°C. Case B is the same as A with the exception that the seal length is 6 ft. A seal of infinite length is examined in Case C. In Case D, a 10-ft plug of hardened (nonheat-generating) SMC3 occupies the room adjacent to the heat-generating SMC3. The SMC3 is chilled by 10°C before emplacement in Case E. Case F simulates the adiabatic conditions in the WES laboratory experiment and examines the effectiveness of the surrounding halite at dissipating the heat of hydration of the SMC3. All computer programs used in this analysis are listed in Table 4-2.

Table 4-2. Computer Programs Used

Computer Program	Version
FASTQ	3.0
SPECTROM-41	2.00
BLOT	1.01.1
BMDP/386	1990
XTRAC	1.08
GRAPH III	10.23

5 CALCULATIONS

5.1 Baseline Case

The results of the baseline case (A) are shown in Figure 5-1. From an initial temperature of 27°C, the temperature of the SMC3 increases to a maximum of 52.5°C at 0.02 yr (175 hr). Subsequently, the temperatures decrease asymptotically to the in situ temperature. Figure 5-2 shows the isotherms within and surrounding the SMC3 at the time of peak temperature (0.02 yr). As can be seen, the 38°C isotherm (one of the temperature constraints) encompasses almost the entire mass of the SMC3. The temperature difference between the SMC3 and the host salt is also shown in Figure 5-1. The maximum temperature difference is 14.0°C and occurs at 0.02 yr after placement.

5.2 Effect of Seal Length

The effects of seal length on the expected SMC3 temperature are shown in Figure 5-3. This figure shows the SMC3 midpoint temperature as a function of time for seal lengths of 20 ft (Case A), 6 ft (Case B), and ∞ (Case C). The maximum temperature of a 6-ft seal is 45.2°C and occurs at 0.008 yr after placement. Thus, reducing the seal length has the effect of reducing the maximum SMC3 temperature and the time to peak temperature. In this case, the temperature rise in the seal is reduced by 29 percent when the volume (length) of the concrete seal is reduced by 70 percent. On the other hand, seal lengths greater than 20 ft result in the same peak temperatures as the baseline case, although cooling is slower because there is no heat loss due to ventilation of the room.

5.3 Effect of Room Properties

The effects of the thermal properties of the room are shown in Figure 5-4. As can be seen in this figure, reducing the thermal diffusivity of the room four orders of magnitude from 0.018 (Case A) to $9.7(10^{-7})$ m^2/s (Case D) does not affect the peak midpoint temperatures at all. It affects the long-term (postpeak) transient behavior slightly because of the insulating behavior of the 10-ft plug.

5.4 Effect of Initial Cooling

In Case E, the SMC3 was cooled to 17°C prior to placement (e.g., by mixing with ice instead of water). The effect of this initial cooling is shown in Figure 5-5, where the peak SMC3 temperature is reduced by 8.3°C. Thus, this cooling is a very effective method of reducing the SMC3 temperature. In this case the peak temperature rise is reduced by 70 percent, in comparison to Case A.

5.5 Effect of Heat Transfer to Salt

In Case F, the ability of the halite to dissipate the heat of hydration is examined. The early-time simulation of Case F (less than 192 hr) basically reproduces the WES laboratory experiment, in which no heat was lost to the surrounding environment. Figure 5-6 shows that the surrounding halite does not significantly affect the SMC3 midpoint temperatures before 0.02 yr, at which time the baseline midpoint temperature peaks.

6 REFERENCES

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Project Title WIPP Seals (LSST)
Contract No. 4060/A141
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RSI-213-93-031

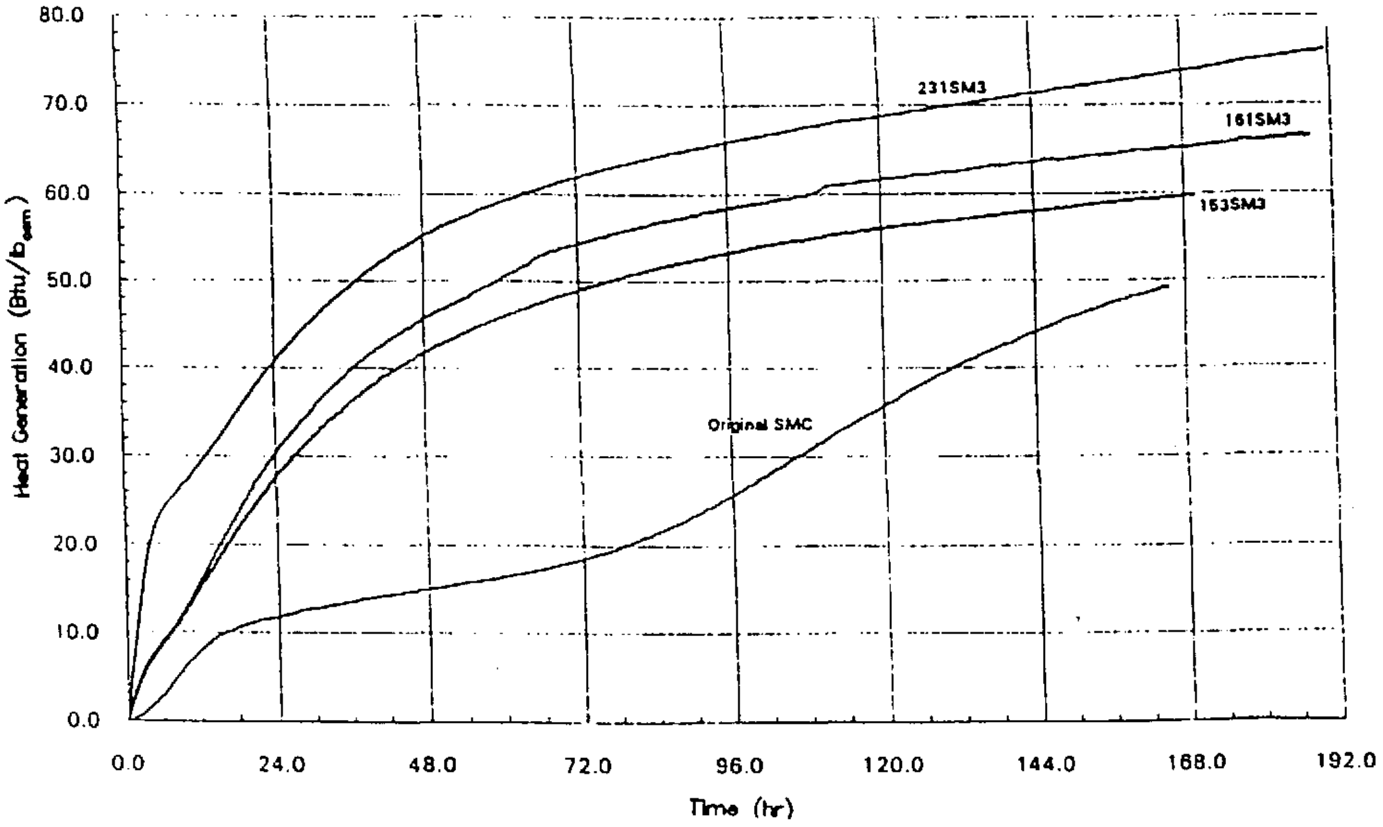

Figure 2-1. Heat Generation of Salado Mass Concrete Mixtures.

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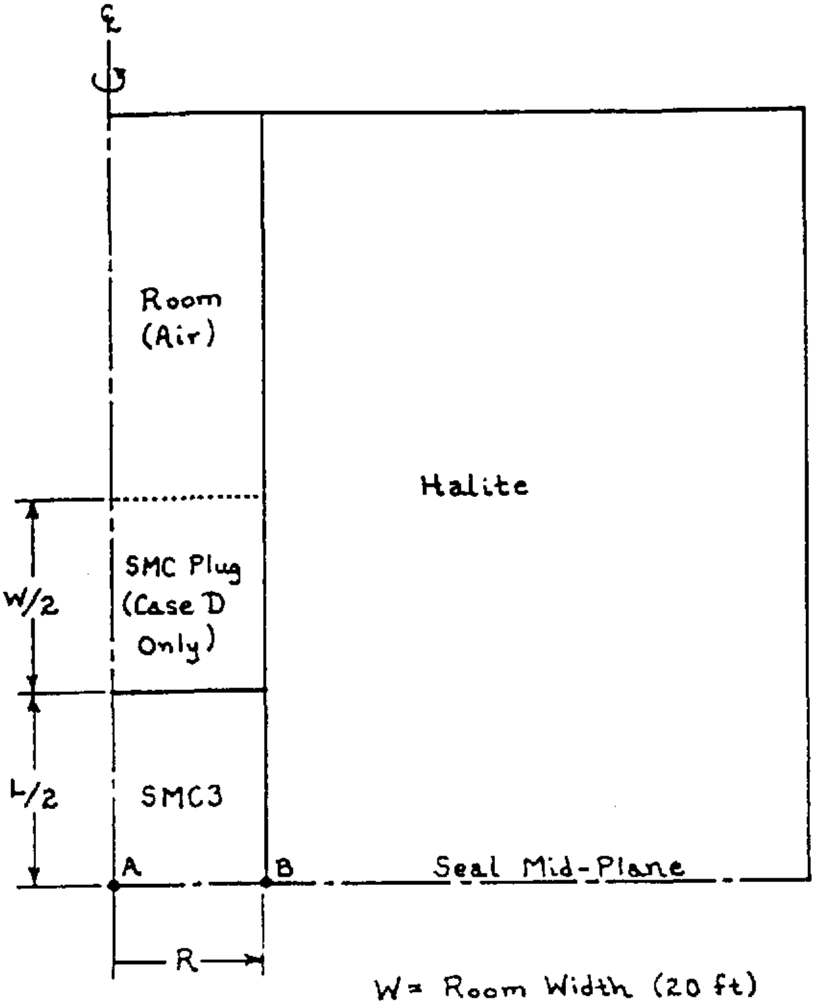

W = Room Width (20 ft)

Point A = SMC3 Midpoint

L = Seal Length (6 ft - Case B
∞ - Case C
20 ft - Other Cases)

Point B = SMC3/Salt Interface

R = Equivalent Radius = 2.43 m
2.66m (mcc)
2-10-94

Figure 4-1. Axisymmetric Model.

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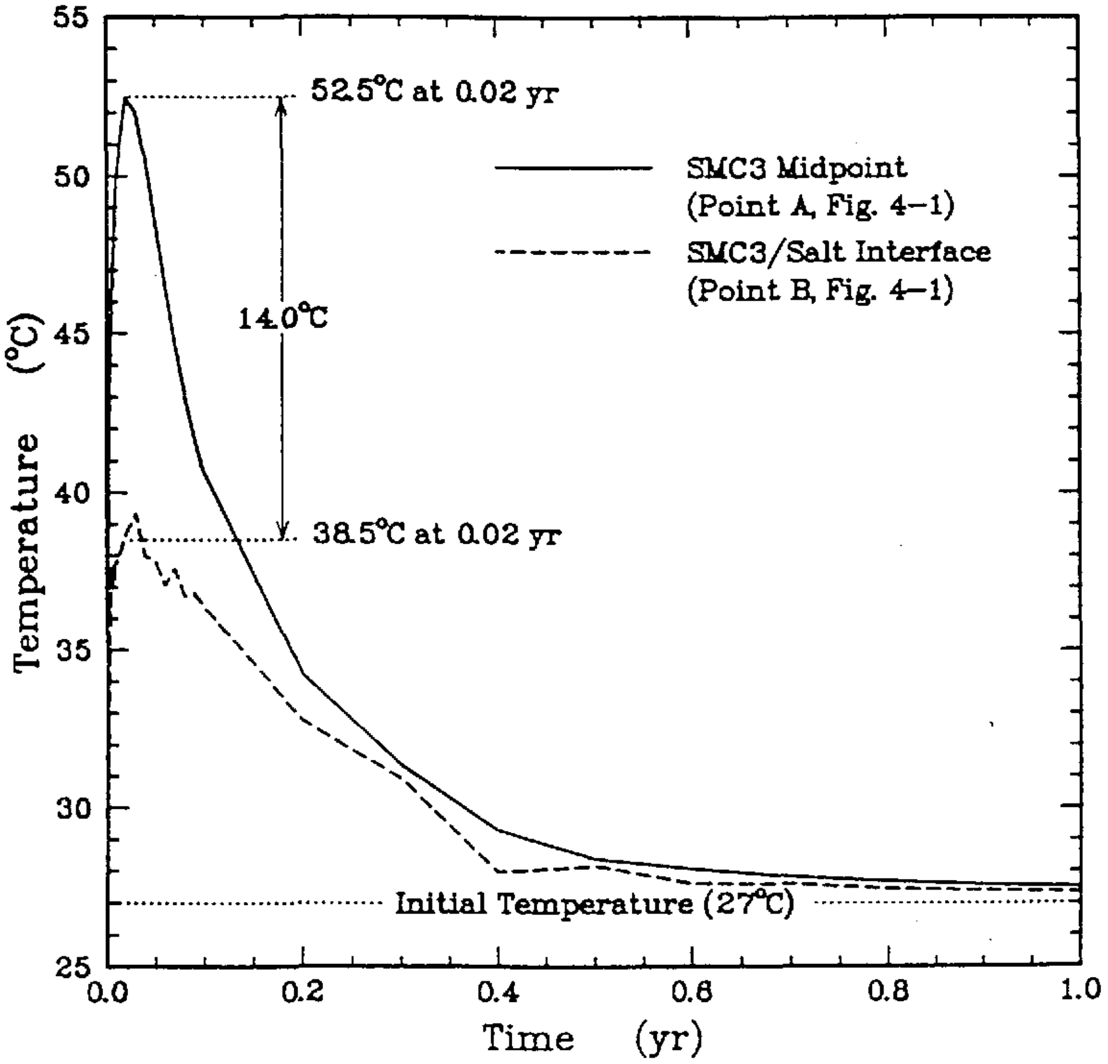

Figure 5-1. Temperature Historical for Baseline Case A.

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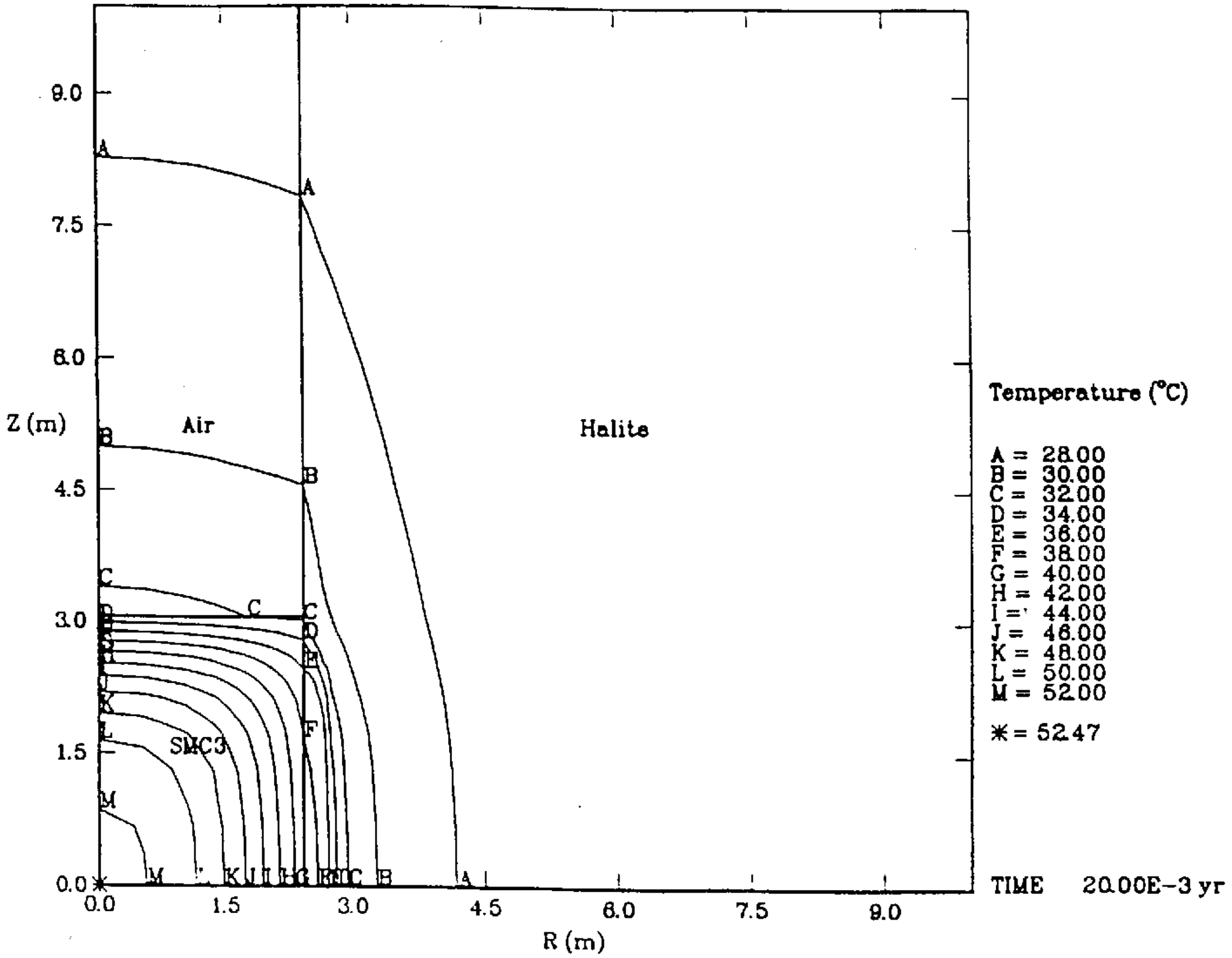

Figure 5-2. Isotherms at 0.02 Years for Baseline Case A.

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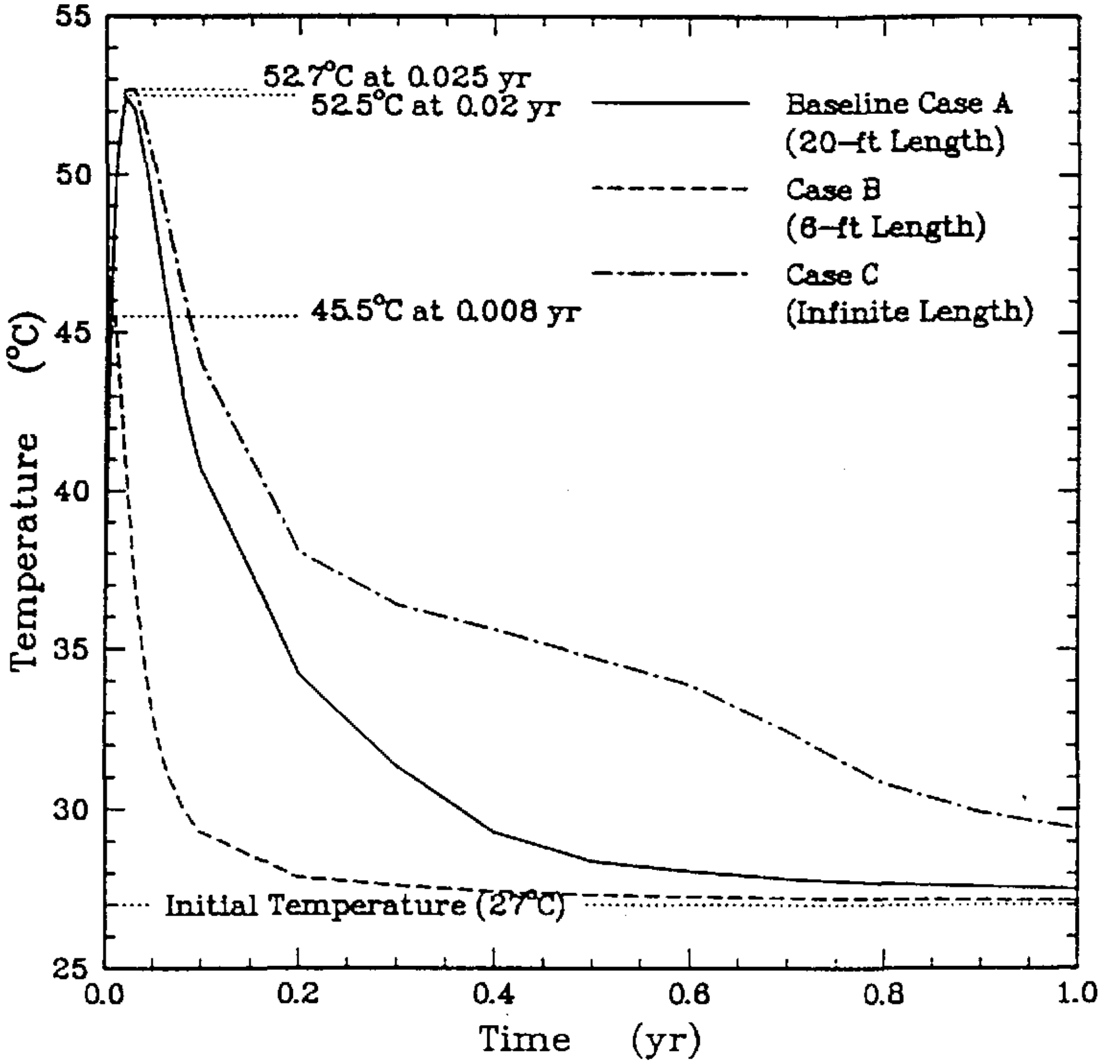

Figure 5-3. Effect of Seal Length — SMC3 Midpoint Temperatures for Cases B and C.

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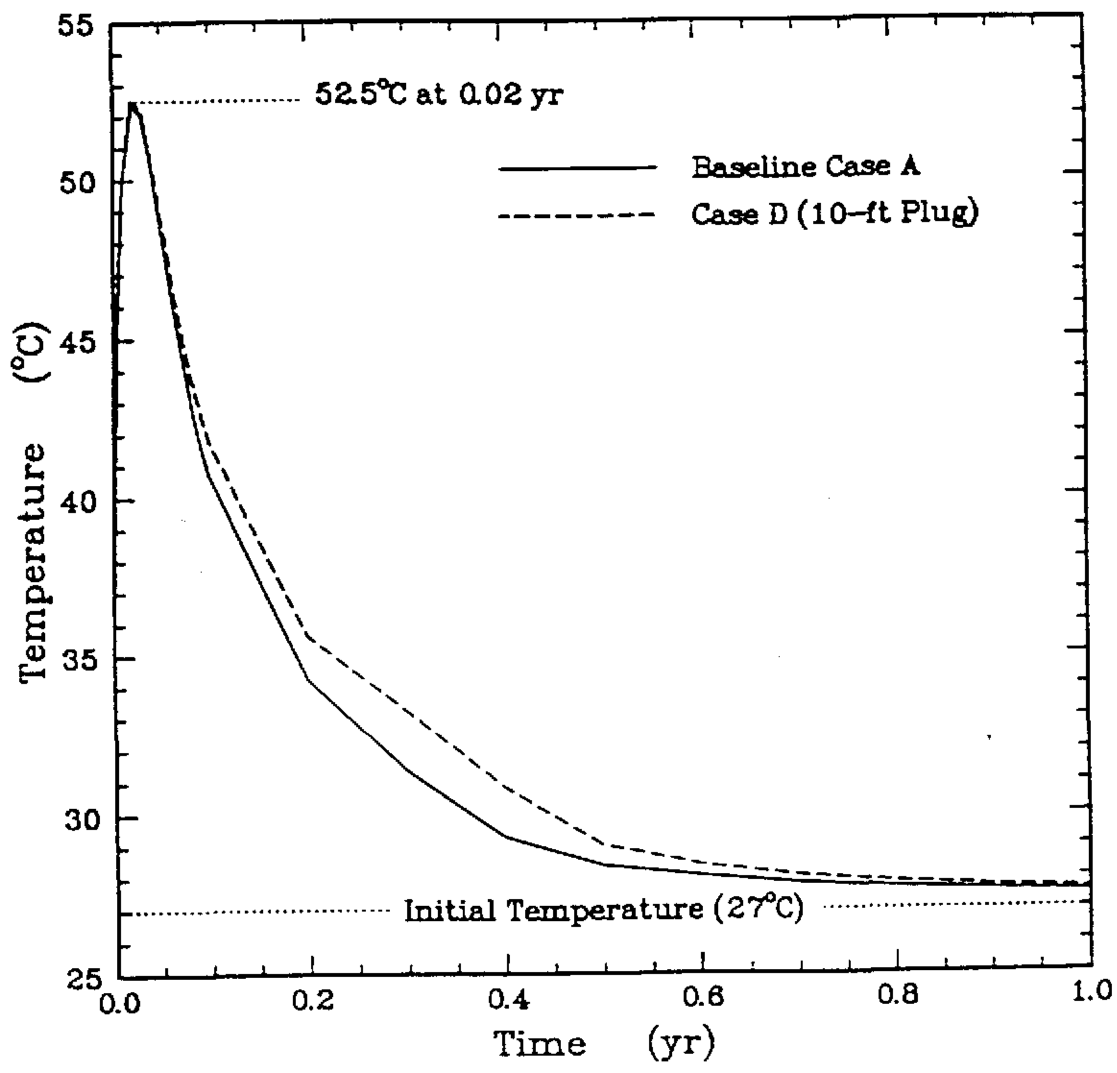

Figure 5-4. Effect of Room Properties — SMC3 Midpoint Temperatures for Case D.

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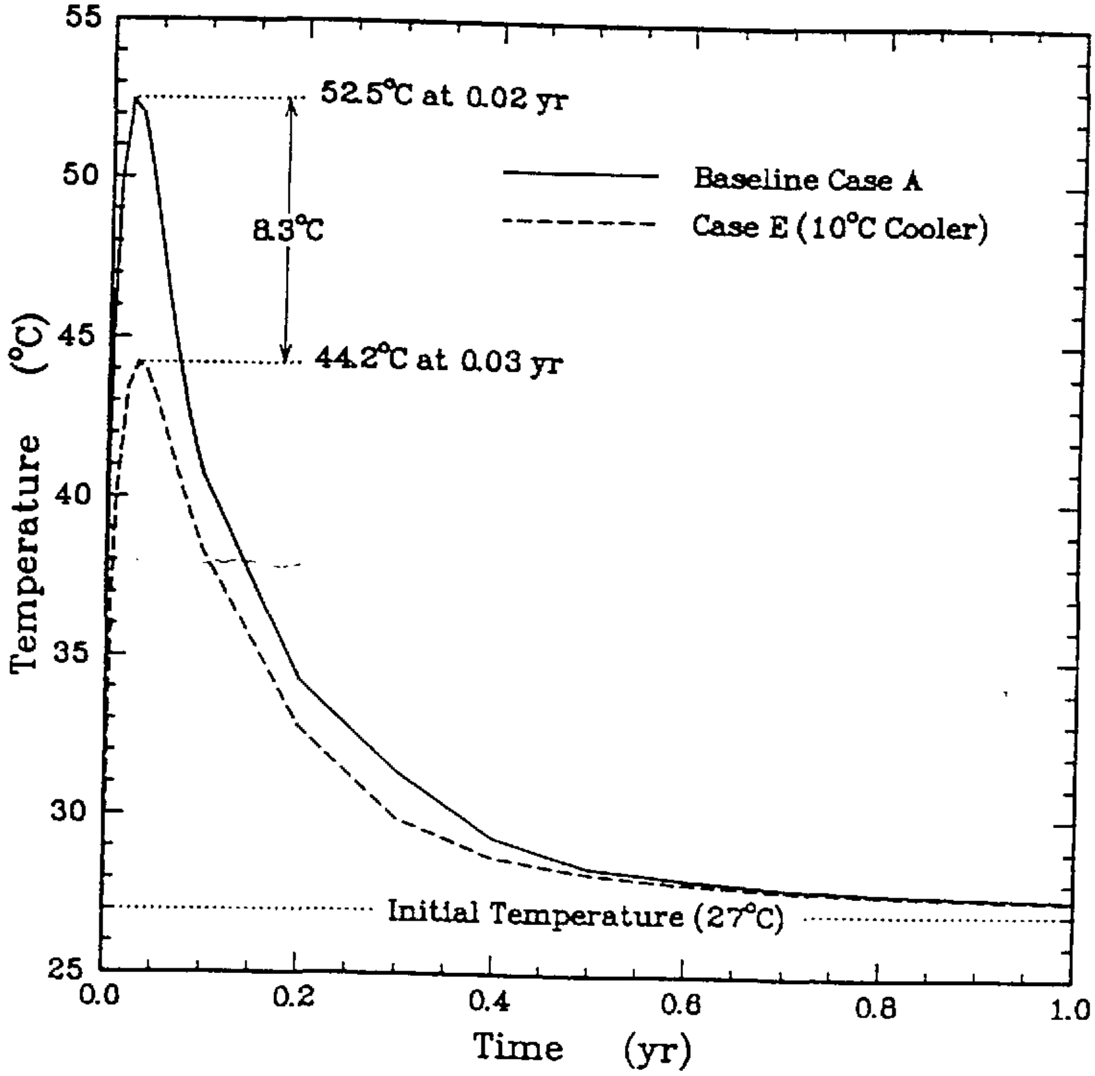

Figure 5-5. Effect of Initial Cooling — SMC3 Midpoint Temperatures for Case E.

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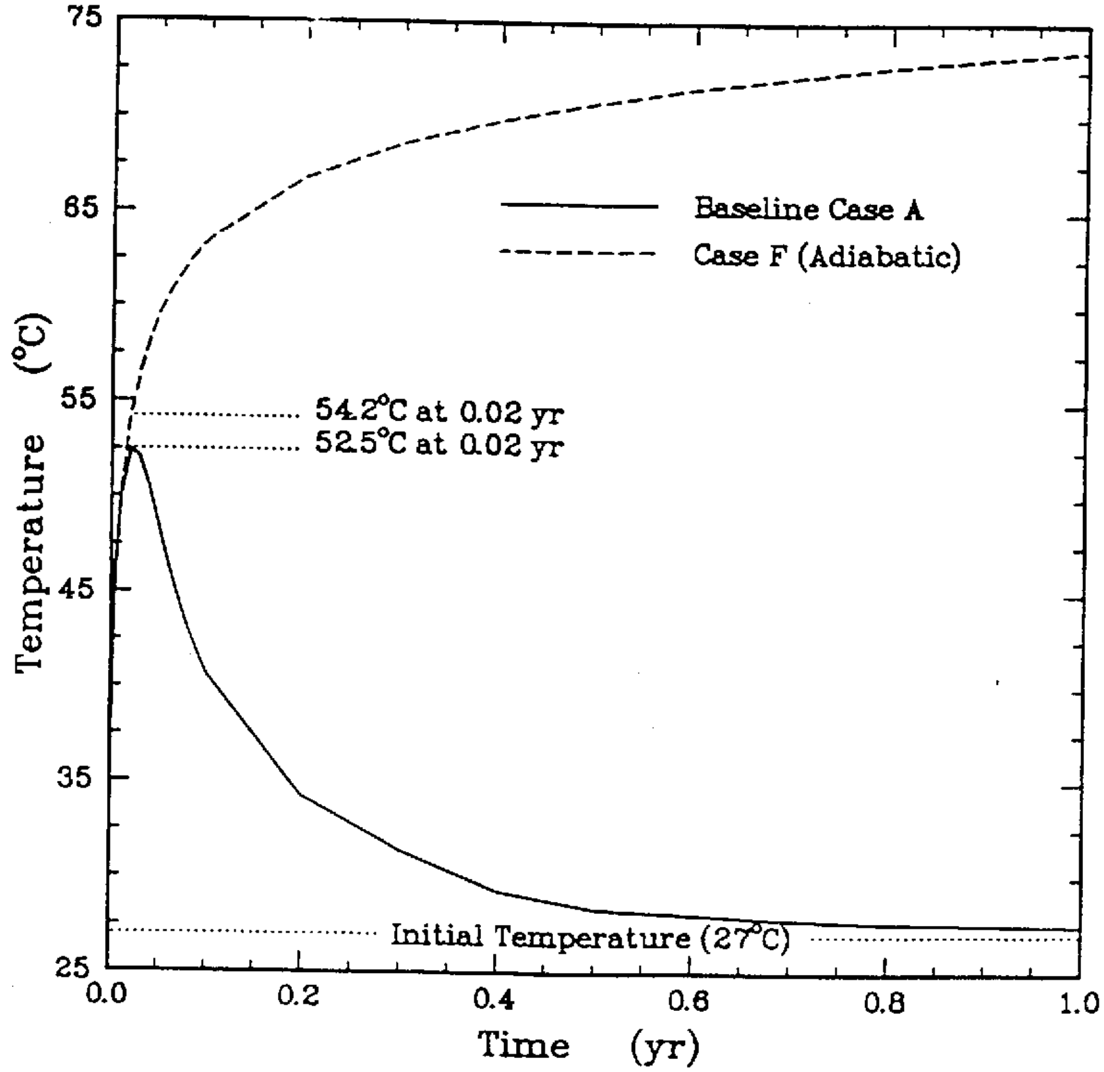

Figure 5-6. Effect of Heat Transfer to Salt — SMC3 Midpoint Temperatures for Case F.