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Thermal Analysis of the ISCO 1680 Portable Wastewater Sampler

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THERMAL ANALYSIS OF THE ISCO 1680 PORTABLE WASTEWATER SAMPLER

by

Philip C. L. Lin
Instrumentation Development Branch
Environmental Monitoring and Support Laboratory
Cincinnati, Ohio 45268

DISCLAIMER

FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory - Cincinnati conducts research to:

Develop and evaluate techniques to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments, and solid waste.

Investigate methods for the concentration, recovery, and identification of viruses, bacteria, and other microbiological organisms in water. Conducts studies to determine the responses of aquatic organisms to water quality.

Conduct an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.

The Instrumentation Development Branch of the Environmental Monitoring and Support Laboratory provides functional designs relating to water quality instrumentation systems. This report, on an investigation of the heat transfer characteristics of an automatic wastewater sampler, provides a mathematical model with which manufacturers can design a portable sampler capable of preserving samples by icing under certain extreme environmental conditions.

Dwight G. Ballinger
Director
Environmental Monitoring and Support Laboratory
Cincinnati

ABSTRACT

A mathematical model was developed to simulate the operation of the ISCO 1680 automatic wastewater sampler. This study was similar to the one carried out earlier with the Manning S-4000 sampler. The objective was to determine the feasibility of developing an automatic sampler with an adequate ice compartment for sample preservation. The model was used to confirm the validity of sample cooling predictions under variable conditions. Experimental measurements on the sample cooling process were also conducted.

Data obtained during operation of the ISCO sampler cooling system under varying conditions indicated that the accuracy of the mathematical model was within ±2^{o}C. Also, the theoretical sample temperature history was in phase with that of the corresponding test sample. Good agreement between theoretical and experimental results was obtained.

The sampler has a cooling space equivalent to 10 kg of ice which can keep 24 500-ml samples at an equilibrium temperature of 0^{o}C from an initial sample temperature of 66.2^{o}C if no heat is absorbed from the surroundings. However, only half of the cooling space can be packed with cube ice unless the container is filled with water and placed in a freezer. Furthermore, a large amount of heat transfer from the environment to the sampler was found in the tests. About 70 to 80 percent of the cooling capacity of the sampler was lost to the surroundings. After an exposure of 24 hours at an ambient temperature ranging from 30 to 35^{o}C, the final lowest temperature of the sample was in a range of 13-19^{o}C for an initial sample temperature of 20-30^{o}C. Also, it took 6 to 8 hours for a sample to reach its lowest temperature. It is therefore concluded that the sampler insulation is insufficient, and the sample cooling rate is slow.

Based upon the mathematical model, two prototype redesigns of the ISCO 1680 sampler cooling system are proposed in this report. The first new design would require 13.6 kg of ice to lower the temperature of 24 500-ml samples to about 4^{o}C at a cycle time of 1 hour and with a temperature of 30^{o}C for both the environment and the initial sample during a 24-hour period. The second design would require 9.6 kg of ice to keep the same amount of sample to about 4^{o}C under similar conditions to those above with the exception that the temperature for both the environment and the initial sample was 35^{o}C.

This project verified the feasibility of using mathematical models for the development of specifications for a sampler cooling system.

CONTENTS

FIGURES

SYMBOLS

A	Contact area between the inner coolant and the sampler bottom, 538 cm^2 (0.58 ft^2).
$A_{f,i}$	Contact area between bottle i (odd number) and the inner coolant, 93 cm^2 (0.1 ft^2).
$A_{k,i}$	Contact area between bottles i and k, 59 cm^2 (0.065 ft^2).
A_{oi}	Contact area between bottle i (even number) and the sampler wall, 133 cm^2 (0.143 ft^2).
A_{or}	Contact area between outer coolant i and the sampler wall, 75 cm^2 (0.08 ft^2).
$A_{r,i}$	Contact area between bottle i (odd number) and outer coolant i, 84 cm^2 (0.09 ft^2).
$A_{rl,i-1}$	Contact area between outer coolant i-1 and bottle i (even number), 84 cm^2 (0.09 ft^2).
$A_{rr,i+1}$	Contact area between outer coolant i+1 and bottle i (even number), 84 cm^2 (0.09 ft^2).
$C_{f,i}$	Thermal conductance between sample i (odd number) and the inner water coolant, cal/hr-cm^2-^oC.
$C_{k,i}$	Thermal conductance between samples i and k, cal/hr-cm^2-^oC.
C_p	Specific heat of water, 1 cal/gm-^oC.
$C_{r,i}$	Thermal conductance between sample i (odd number) and outer coolant i, cal/hr-cm^2-^oC.
$C_{rl,i-1}$	Thermal conductance between sample i (even number) and outer coolant i-1, cal/hr-cm^2-^oC.
$C_{rr,i+1}$	Thermal conductance between sample i (even number) and outer coolant i+1, cal/hr-cm^2-^oC.
dx	Thickness of the bottle, 1.0 mm.
g	Gravitational acceleration, 980 cm/sec^2.
h	Surface film coefficient, cal/hr-cm^2-^oC.

h_{bi}	Surface film coefficient between sample i (even number) and the sampler wall, cal/hr-cm^2-^oC.
$h_{f,i}$	Surface film coefficient between sample i (odd number) and the inner water coolant, cal/hr-cm^2-^oC.
h_{ice}	Surface film coefficient between the ice and the inner water coolant, cal/hr-cm^2-^oC.
$h_{k,i}$	Surface film coefficient between bottles k and i, cal/hr-cm^2-^oC.
h_o	Surface film coefficient between the environment and the sampler wall, cal/hr-cm^2-^oC.
$h_{r,i}$	Surface film coefficient between sample i (odd number) and outer coolant i, cal/hr-cm^2-^oC.
j	j th iteration.
j+i	j+i th iteration.
K	Thermal conductivity of the sampler wall, 1.49 cal/hr-cm-^oC (0.1 Btu/hr-ft-^oF).
K_a	Thermal conductivity of air, 0.22 cal/hr-cm-^oC (0.015 Btu/hr-ft-^oF).
K_b	Thermal conductivity of the bottle, 3.72 cal/hr-cm-^oC (0.25 Btu/hr-ft-^oF).
kk	Number of bottles filled with sample.
K_w	Thermal conductivity of water, 5.21 cal/hr-cm-^oC (0.35 Btu/hr-ft-^oF).
l	Bottle height, 17.78 cm (7 in.)
m	Sample mass, gm.
M	Mass of the inner water coolant, gm.
m_r	Mass of outer coolant i, gm.
n	n time steps.
Q_{ice}	Heat gain (negative) through the ice to the inner water coolant, cal/hr.
Q_{oi}	Heat gain through the sampler wall to sample i (even number), cal/hr.
Q_{or}	Heat gain through the sampler wall to outer coolant i, cal/hr.
R_{ice}	Radius of the ice (assume that the ice is a cylindrical body with a height of bottle length), cm.

t	Time, hr.
T_f	Water temperature in the inner coolant in ^oC.
T_{fo}	Ice temperature, 0^oC.
T_i	Temperature in sample i in ^oC.
T_k	Temperature in sample k in ^oC.
T_m	Mean surface temperature, ^oC.
T_o	*Ambient temperature*, ^oC.
$T_{r,i}$	Temperature in outer coolant i in ^oC.
w	Relaxation factor, 1.5.
Δx	Thickness of the sampler bottom, 3.18 cm (1.25 in.).
Δt	Time increment, 1/60 hr.
Δx_{oi}	Average thickness of the sampler wall at the location of sample i (even number), 3.18 cm (1.25 in.).
Δx_{wi}	Average air gap between bottle i (even number) and the sampler wall, 5 mm.
Δx_{or}	Average thickness of the sampler wall at the location of outer coolant i, 4.76 cm (1.87 in.).
ΔT	Half of temperature difference between two fluids, ^oC.
N_{nu}	Nusselt number.
N_{pr}	Prandtl number, μ Cp/Kw, or 13.37-0.2556 Tm for water.
N_{gr}	Grashof number, $l^3 \rho^2 g\beta\Delta T/\mu^2$.
μ	Viscosity, 64.35-0.57 Tm gm/cm-hr, for water.
ρ	Water density, 1 gm/cm^3.
β	Thermal expansion coefficient, (8.379 Tm+54) $x10^{-6}/^oC$ for water.
C, a	Constants.

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SECTION 1

INTRODUCTION

As a result of a thermal analysis of the Manning[1] sampler, now being prepared for publication, a mathematical model was developed for predicting the sample cooling process. In that study, it was found that the Manning sampler was not capable of preserving the samples at 4°C under normal conditions and that the sample cooling rate in the sampler was slow. However, the mathematical model developed for the Manning sampler cooling system did predict the sample cooling process well. A modification of that sampler cooling system was therefore proposed based on the mathematical model. According to the model, the redesign of the sampler cooling system could preserve the samples at 4°C at a temperature of 35°C for both the environment and the initial sample over a 24-hour period. Since the model showed promise for the development of the automatic sampler cooling system, a further study to substantiate the validity of the mathematical model was developed for the sample cooling process in the ISCO 1680 sampler. The same numerical technique, the Crank-Nicolson Implicit, was utilized. A laboratory test to confirm the accuracy of the model was also conducted.

SECTION 2

CONCLUSIONS

The laboratory tests indicate that the sample cooling rate in the ISCO 1680 sampler is slow. Also, the sampler cooling capacity is inadequate for sample preservation under normal operating conditions. Conclusions from the test include:

- The contact area between the coolant and the sample bottles is not enough.

- The ice capacity is insufficient. It is not possible to fill the coolant compartment with the designed capacity of ice unless it is filled with water and placed in a freezer.

- The sampler insulation is insufficient to reduce the heat transfer from outside the sampler.

Accuracy of the mathematical model verified by experimental measurements of sample temperatures indicates that the following conclusions can be drawn from the simulation model:

- The maximum temperature difference for any sample between experimental and predicted results at any given time is within 2°C.

- The corresponding temperature histories for each sample are in phase with respect to time.

- Both results show the same trend of temperature-time histories for all samples.

In general, they are in good agreement. The computer simulation model developed for the sampler cooling system is generalized. The applications of the model, which are also included in Reference 1, are:

- The mathematical model can provide a design guideline for the sampler cooling system and minimize experimental work and manpower in evaluating the sampler cooling capability.

- The computer program can be applied to different combinations of sampler material, bottle thickness, number of bottles, number of samples, ice mass, sample mass, cycle time, duration time, etc. provided the sampler geometry is similar.

- Temperature-time histories of samples can be calculated and plotted directly from the program.

- Experimental data of sample temperatures can be fed into the program for plotting.

SECTION 3

RECOMMENDATIONS

The ISCO 1680 sampler cooling system is not acceptable under normal operating conditions. Several recommendations which are suggested in the study of the Manning[1] sampler are also applicable to the ISCO sampler. They are:

- Improve the sampler insulation.
- Increase the cooling space.
- Increase the contact area between the coolant and the bottle.
- Increase the ice capacity by placing the container in a freezer.

Two prototype designs of the cooling system are proposed based on the above. The first redesign of the container is based on the following modifications in the design specifications:

- The sampler bottom thickness is increased to 7.62 cm (3 in.).
- The capacity of the coolant is increased to 13.6 kg of ice.
- The contact area is increased by 32 cm^2 (0.034 ft^2).
- The thermal conductivity of the sampler bottom with loose polyurethane foam inside is less than 0.744 cal/hr-cm-^{o}C (0.05 Btu/hr-ft-^{o}F).

In the second design, the bottle radius is reduced from 3.18 cm (1.25 in.) to 2.79 cm (1.1 in.), and the bottle length is increased from 17.78 cm (7 in.) to 20.83 cm (8.2 in.). The contact area is therefore increased by 14 percent. The container wall thickness is increased by 3 cm (1.2 in.) and that of the sampler bottom is 7.62 cm (3 in.). It is assumed that the thermal conductivity of the container wall with polyurethane foam inside is less than 0.744 cal/hr-cm-^{o}C (0.05 Btu/hr-ft-^{o}F) and that the ice capacity is about 9.6 kg. Both designs can reduce the temperature of a sample from 30^{o}C to about 4^{o}C in 3 hours and hold it at 4^{o}C during a 24-hour period under testing conditions.

SECTION 4

DESCRIPTION OF SAMPLER

The ISCO 1680 sampler as shown in Figure 1 is equipped with a peristaltic pump with a pumping rate of 1400 ml/min for a typical pump and 5000 ml/min for a superspeed pump. The controls and electronics are housed in a watertight stainless steel container. The power source is either a line source of 117 volts AC or a 12-volt battery.

The sampler casing is constructed of double-walled plastic separated with polyurethane foam insulation. The sample bottles have a capacity of 500 ml and are made of high density polyethylene.

The sampler is designed to collect up to 28 separate sequential samples of a predetermined volume. Also, it is possible to fill 4 consecutive bottles during each sampling period and allow each discrete bottle to be composed of 1 to 4 samples for the optional multiplexing controls. Samples are collected from either a time mode or a flow mode. In the time mode, samples are taken at intervals from 1 to 999 minutes; or in the flow mode, they are collected at intervals of 1 to 999 flow pulses. The interval between samples is displayed with a light emitting diode (LED) either in minutes or pulses.

Ice can be stored in the central section of the sampler for sample preservation. The cooling space has an approximate capacity of 10 kg of solid ice.

The sequence of operation of the sampler is described as follows:

1. The sampling interval is set for either minutes or flow pulses.

2. The peristaltic pump runs in the reverse direction to purge the intake line.

3. The pump then runs in the forward direction to deliver the preset volume. This is measured with the revolution of the pump and the lift of the sample from the source. This sample is then channeled to the sample bottle through the funnel spout onto the distributor plate.

4. The pump direction again changes to purge the intake line, and then the pump shuts off.

5. The distributor funnel moves to the next bottle to be filled.

6. This completes a cycle. This process continues until the 28th bottle is filled, at which time the sampler automatically shuts off.

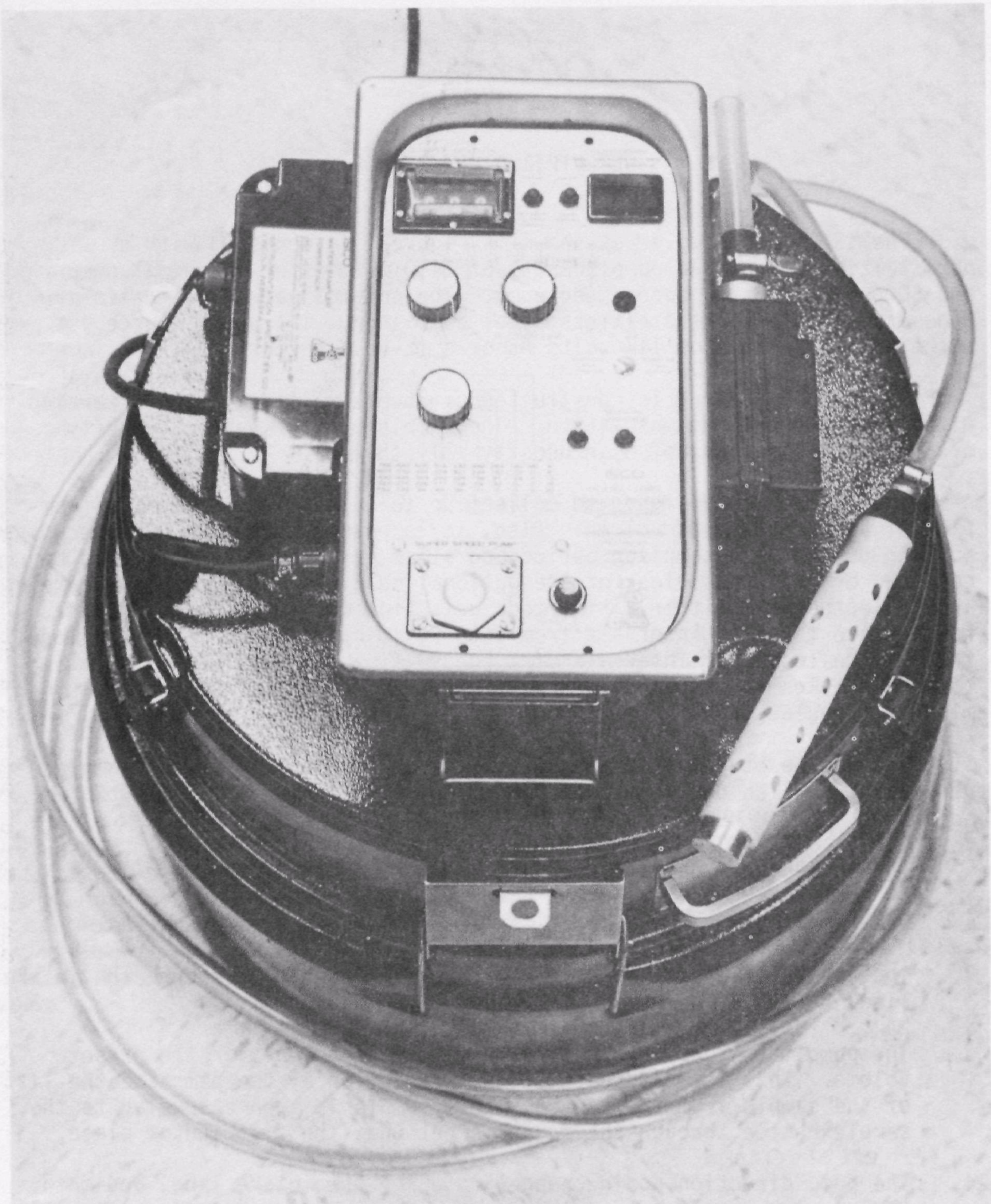

Figure 1. Photograph of sampler.

SECTION 5

THERMAL ANALYSIS OF SAMPLER COOLING SYSTEM

The ISCO 1680 sampler has an ice compartment in its central section and has 28 cylindrical bottles arranged as shown in Figure 2. The unusual arrangement of the bottles presents a thermal problem which cannot be solved in as straightforward a manner as in the Manning sampler. To facilitate the thermal analysis of the sampler, sample bottles are labelled from 1 to 28 as shown in Figure 3. The outer bottles are even-numbered and the inner ones are odd-numbered. The sampling sequence of the sampler is the same as the number sequence in Figure 3. The number of outer coolant (not shown in Figure 3) is also labelled corresponding to that of the inner bottles.

In this study, three phases of heat transfer, i.e., radiation, conduction, and convection, are investigated.

HEAT TRANSFER BY CONVECTION AND CONDUCTION IN THE SAMPLER

In addition to the assumption of transient response of the sample with negligible internal resistance to the heat, the following hypotheses also proposed in the Manning[1] study are made:

- Heat transfer in the sample occurs only in the r- and θ- directions.
- No heat transfer exists for bottles without samples.
- Heat transfer to the coolant comes from the samples in the r-direction and from the top and bottom of the sampler in the axial direction.

Four heat transfer equations were then derived, each of which is as follows:

i. Heat Transfer Equation for (Odd Numbered) Samples in Inner Bottles

$$mC_p \frac{dT_i}{dt} = C_{f,i} A_{f,i}(T_f - T_i) + C_{r,i} A_{r,i}(T_{r,i} - T_i) + \sum_{\substack{k=i-2 \\ k \neq i}}^{k=i+2} C_{k,i} A_{k,i}(T_k - T_i) \tag{5-1}$$

where

i = sample number, 1, 3, 5,.....27.

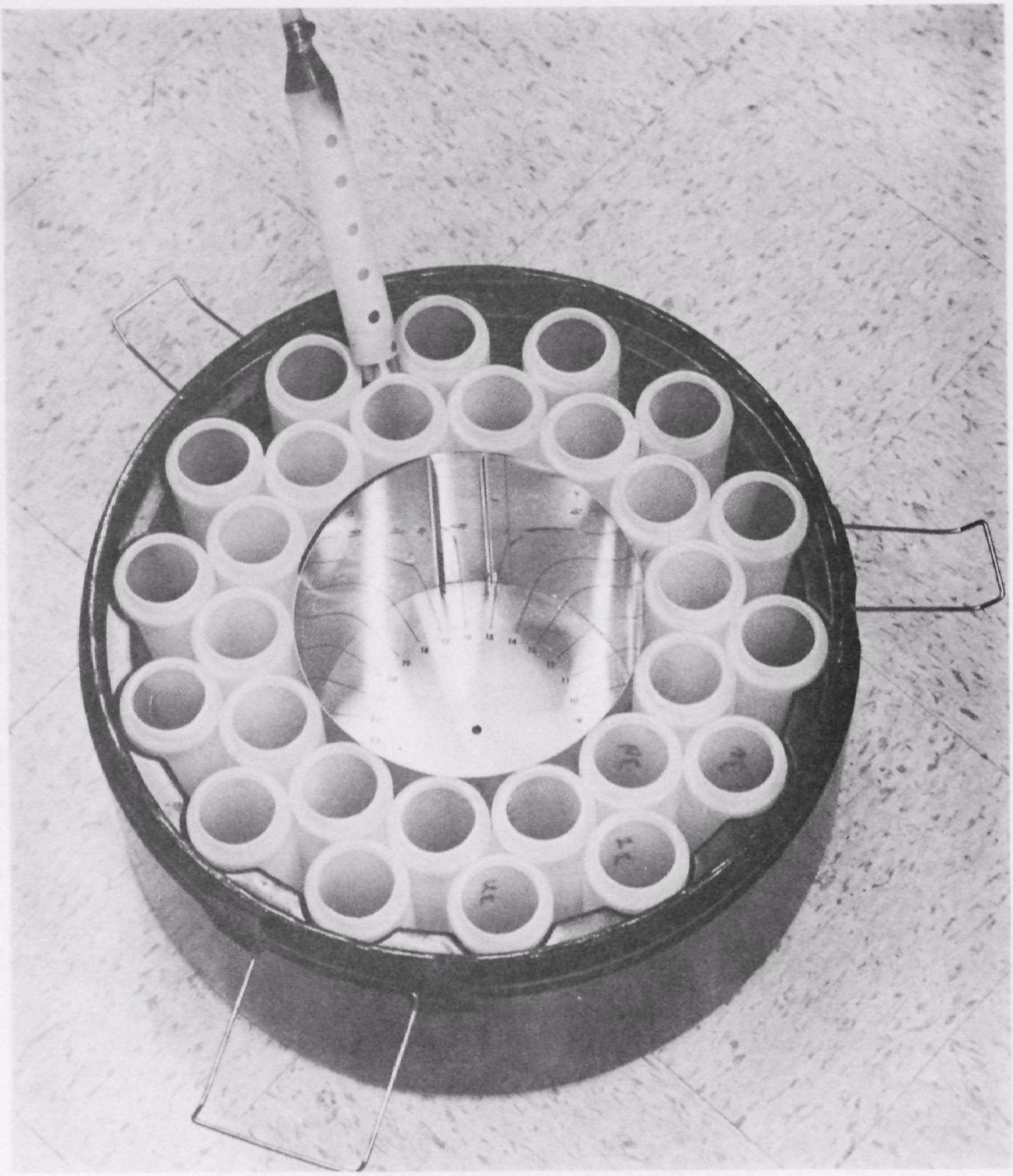

Figure 2. Sample container.

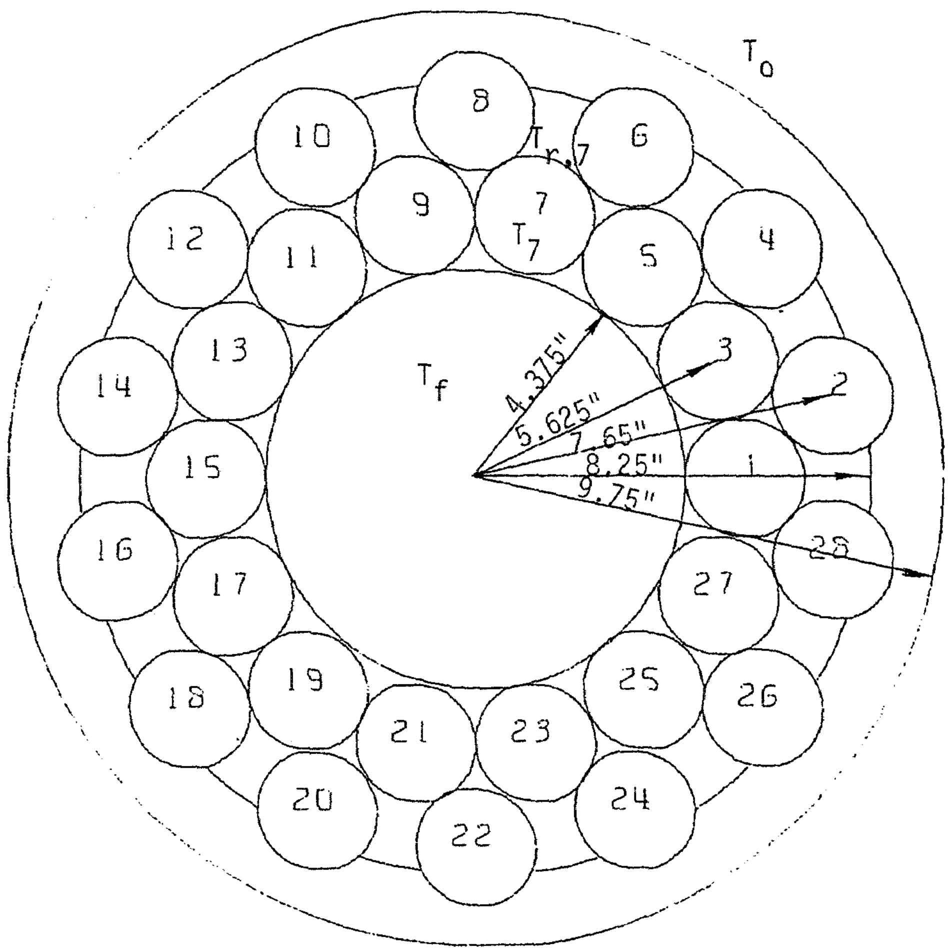

Figure 3. Top view of sample container.

In this equation, the first term is the transient temperature response of sample i. The second, third, and fourth terms represent heat gain of sample i through the inner water coolant, outer coolant i, and the neighboring samples, respectively. Symbols in equation (5-1) and following subsequent equations are explained in the "SYMBOLS" section for convenience.

By introducing:

$$\tau_{f,i} = \frac{C_{f,i}\ A_{f,i}}{mC_p}$$

$$\tau_{r,i} = \frac{C_{r,i}\ A_{r,i}}{mC_p}$$

$$\tau_{k,i} = \frac{C_{k,i}\ A_{k,i}}{mC_p} \tag{5-2}$$

The transformed equation becomes:

$$\frac{dT_i}{dt} = \tau_{f,i}(T_f - T_i) + \tau_{r,i}(T_{r,i} - T_i) + \sum_{\substack{k=i-2 \\ k\neq i}}^{k=i+2} \tau_{k,i}(T_k - T_i) \tag{5-3}$$

ii. Heat Transfer Equation for (Even Numbered) Samples in Outer Bottles

$$mC_p \frac{dT_i}{dt} = C_{rl,i-1}\ A_{rl,i-1}(T_{r,i-1} - T_i) + C_{rr,i+1}\ A_{rr,i+1} (T_{r,i+1} - T_i) + \sum_{\substack{k=i-1 \\ k\neq i}}^{k=i+1} C_{k,i}\ A_{k,i}\ (T_k - T_i) + Q_{oi} \tag{5-4}$$

where

i = sample number 2, 4, 6,....,28.

On the right hand side of equation (5-4), the first and second terms are heat gain from outer coolants i-1 and i+1 to sample i, respectively. The third term is the total heat contribution from the neighboring samples and the last term is the heat gain from outside the sampler to sample i. By similar transformations introduced in equation (5-2), equation (5-4) becomes:

$$\frac{dT_i}{dt} = \tau_{rl,i-1} (T_{r,i-1} - T_i) + \tau_{rr,i+1} (T_{r,i+1} - T_i) +$$

$$\sum_{\substack{k=i-1 \\ k \neq i}}^{k=i+1} \tau_{k,i}(T_k - T_i) + \frac{Q_{oi}}{mC_p} \tag{5-5}$$

<u>iii. Heat Transfer Equation for the (Odd Numbered) Outer Water Coolants</u>

$$m_r C_p \frac{dT_{r,i}}{dt} = C_{r,i} A_{r,i}(T_i - T_{r,i}) + C_{rl,i} A_{rl,i}(T_{i+1} - T_{r,i})$$

$$+ C_{rr,i} A_{rr,i}(T_{i-1} - T_{r,i}) + Q_{or} \tag{5-6}$$

where

i = outer coolant number, 1, 3, 5, ...,27.

The total heat contribution to the outer coolant i is from four sources. The first three terms on the right hand side of equation (5-6) represent heat exchange from the three neighboring samples and outer coolant i. The last term is heat gain from outside the sampler. By using the same transformations as in i, equation (5-6) becomes:

$$\frac{dT_{r,i}}{dt} = \tau_{r,i}(T_i - T_{r,i}) \frac{m}{m_r} + \tau_{rl,i}(T_{i+1} - T_{r,i}) \frac{m}{m_r} +$$

$$\tau_{rr,i}(T_{i-1} - T_{r,i}) \frac{m}{m_r} + \frac{Q_{or}}{m_r C_p} \tag{5-7}$$

<u>iv. Heat Transfer Equation for the Inner Water Coolant</u>

$$MC_p \frac{dT_f}{dt} = \sum_{i=1,3}^{kk} C_{f,i} A_{f,i}(T_i - T_f) + \frac{2A}{\frac{\Delta x}{K} + \frac{1}{h_o}} (T_o - T_f)$$

$$+ Q_{ice} \tag{5-8}$$

In this equation, the first term on the right hand side is the total heat transfer between the inner samples and the inner water coolant. The second and third terms are heat gain from the sampler bottom and top, and the ice, respectively. The total heat, obtained from the right hand side of the equation, leads to the temperature response of the inner water coolant. By the similar transformations as in i, equation (5-8) becomes:

$$\frac{dT_f}{dt} = \sum_{i=1,3}^{kk} \tau_{f,i}(T_i - T_f)\frac{m}{M} + \frac{2A}{(\frac{\Delta x}{K}+\frac{1}{h_o})MC_p}(T_o - T_f)$$

$$+ \frac{Q_{ice}}{MC_p} \qquad (5\text{-}9)$$

Equations (5-3), (5-5), (5-7), and (5-9) may be solved simultaneously for T_i, $T_{r,i}$, and T_f in terms of time t, if the boundary and initial conditions are provided.

SOLAR IRRADIATION ON A SAMPLER

A surface used as a heat rejection surface in the solar environment should have a low value of solar absorptivity and a high value of infrared emissivity, since the surface radiates mainly in the infrared band. Reference 1 presents a detailed discussion of this subject.

SECTION 6

NUMERICAL ANALYSIS OF MATHEMATICAL MODEL

NUMERICAL TECHNIQUE

Numerical solutions were obtained by transforming the mathematical expressions as shown in the previous section through a numerical technique, the Crank-Nicolson Implicit,[2] into finite difference forms.

Four corresponding finite difference equations are:

$$T_i^{j+1} = T_i^j + w\,[a_2^n\,(\tau_{f,i}^n\, T_f^j + \tau_{r,i}^n\, T_{r,i}^j + \sum_{\substack{k=i-2\\ k\neq i}}^{k=i+2} \tau_{k,i}^n\, T_k^j + a_1^n) - T_i^j] \tag{6-1}$$

where

$$a_1 = \frac{2}{\Delta t}\, T_i + \tau_{f,i}(T_f - T_i) + \tau_{r,i}(T_{r,i} - T_i) + \sum_{\substack{k=i-2\\ k\neq i}}^{k=i+2} \tau_{k,i}(T_k - T_i)$$

$$a_2 = \frac{\Delta t}{2} \Big/ [1 + \frac{\Delta t}{2}\,(\tau_{f,i} + \tau_{r,i} + \sum_{\substack{k=i-2\\ k\neq i}}^{k=i+2} \tau_{k,i})]$$

$$T_i^{j+1} = T_i^j + w\,[b_2^n(\tau_{rl,i-1}^n\, T_{r,i-1}^j + \tau_{rr,i+1}^n\, T_{r,i+1}^j + \sum_{\substack{k=i-1\\ k\neq i}}^{k=i+1} \tau_{k,i}^n\, T_k^j + b_i^n) - T_i^j] \tag{6-2}$$

where

$$b_1 = \frac{\tau_{rl,i-1}}{2} (T_{r,i-1} - T_i) + \frac{\tau_{rr,i+1}}{2} (T_{r,i+1} - T_i) +$$

$$\sum_{\substack{k=i-1 \\ k \neq i}}^{k=i+1} \tau_{k,i}(T_k - T_i) + \frac{2}{\Delta t} T_i + \frac{2\ Q_{oi}}{mC_p}$$

$$b_2 = \frac{\Delta t}{2} / [1 + \frac{\Delta t}{2} (\tau_{rl,i-1} + \tau_{rr,i+1} + \sum_{\substack{k=i+1 \\ k \neq i}}^{k=i+1} \tau_{k,i})]$$

$$T_{r,i}^{j+1} = T_{r,i}^{j} + w[c_2^{n}(\tau_{r,i}^{n} T_i^{j} + \tau_{rl,i}^{n} T_{i+1}^{j} + \tau_{rr,i}^{n} T_{i-1}^{j}) \frac{m}{m_r} +$$

$$c_1^{n} c_2^{n} - T_{r,i}^{j}] \qquad (6\text{-}3)$$

where

$$c_1 = \frac{m}{m_r} [\tau_{r,i}(T_i - T_{r,i}) + \tau_{rl,i}(T_{i+1} - T_{r,i}) +$$

$$\tau_{rr,i}(T_{i-1} - T_{r,i})] + \frac{2}{\Delta t} T_{r,i} + \frac{2\ Q_{or}}{m_r C_p}$$

$$c_2 = \frac{\Delta t}{2} / [1 + \frac{m \Delta t}{2 m_r} (\tau_{rl,i} + \tau_{r,i} + \tau_{rr,i})]$$

$$T_f^{j+1} = T_f^{j} + w[d_2^{n}(\frac{m}{M} \sum_{i=1,3}^{kk} \tau_{f,i}^{n} T_i^{j} + d_1^{n}) - T_f^{j}] \qquad (6\text{-}4)$$

where

$$d_1 = \frac{m}{M} \sum_{i=1,3}^{kk} \tau_{f,i} (T_i - T_f) + \frac{2A}{(\frac{\Delta x}{K} + \frac{1}{h_o}) MC_p} (2T_o - T_f) +$$

$$\frac{2\ Q_{ice}}{MC_p} + \frac{2\ T_f}{\Delta t}$$

$$d_2 = \frac{\Delta t}{2} / [1 + \frac{\Delta t}{2} (\frac{m}{M} \sum_{i=1,3}^{kk} \tau_{f,i} + \frac{2A}{(\frac{\Delta x}{K} + \frac{1}{h_o}) MC_p})]$$

Equations (6-1) to (6-4) were solved simultaneously for T_i, $T_{r,i}$, and T_f for the n+1 th time step by a successive overrelaxation technique.[2] The same procedure was repeated for solutions of the successive time steps until all bottles were filled with sample or until the specified duration time was reached. Equations (6-1) to (6-4) cannot, however, be solved without the boundary and initial conditions provided.

BOUNDARY AND INITIAL CONDITIONS

Boundary conditions for equations (6-1) to (6-4) are partially given in Figure 3. The following are also required for equations (6-1) to (6-4). Heat transfer, Q_{oi}, through the sampler wall to an (even numbered) outer sample is:

$$Q_{oi} = \frac{A_{oi} (T_o - T_i)}{(\frac{\Delta x_{oi}}{K} + \frac{\Delta x_{wi}}{K_a} + \frac{1}{h_o} + \frac{1}{h_{bi}} + \frac{dx}{K_b}) mC_p} \tag{6-5}$$

Heat transfer, Q_{or}, through the sampler wall to outer coolant is:

$$Q_{or} = \frac{A_{or} (T_o - T_{r,i})}{(\frac{\Delta x_{or}}{K} + \frac{1}{h_o} + \frac{1}{h_{r,i}})} \tag{6-6}$$

Heat transfer, Q_{ice}, from the solid ice to the inner water coolant is:

$$Q_{ice} = 2\ p_i\ R_{ice}\ l\ h_{ice}\ (T_{fo} - T_f) \qquad (6\text{-}7)$$

Coefficients such as $\tau_{r,i}$, $\tau_{f,i}$, and $\tau_{rr,i}$ in equations (6-1) to (6-4) have to be determined for the n th time-step before equations can be solved for the n+1 th time-step. These coefficients were defined in equation (5-2) in the previous section, and $C_{f,i}$, $C_{r,i}$, and $C_{k,i}$ are defined as:

$$C_{f,i} = \frac{1}{\frac{2}{h_{f,i}} + \frac{dx}{K_b}}$$

$$C_{r,i} = \frac{1}{\frac{2}{h_{r,i}} + \frac{dx}{K_b}} \qquad (6\text{-}8)$$

$$C_{k,i} = \frac{1}{\frac{2}{h_{k,i}} + \frac{2\ d_x}{K_b}}$$

All parameters in equations (6-1) to (6-8) are specified except surface film coefficients. By introducing a dimensionless heat transfer coefficient:

$$N_{nu} = \frac{h_l}{K_w} \qquad (6\text{-}9)$$

in which

N_{nu} = Nusselt number

The Nusselt number was found to obey the following relationship:

$$N_{nu} = C(N_{pr}\ N_{gr})^a \qquad (6\text{-}10)$$

in which

C, a = constants

N_{pr} = Prandtl number

N_{gr} = Grashof number

The Nusselt number for a vertical sample bottle was approximated by that of a vertical plate. Values for a and C for a vertical plate free convection were listed by Chapman.[3] According to Chapman, the following approximations can be used for a vertical plate:

$$10^{-1} < N_{gr}\,N_{pr} <= 10^{4} \quad : \text{use Figure 4}$$

$$10^{4} < N_{gr}\,N_{pr} <= 10^{9} \quad : C = 0.59,\ a = \frac{1}{4}$$

$$10^{9} < N_{gr}\,N_{pr} <= 10^{12} \quad : C = 0.129,\ a = \frac{1}{3} \qquad (6\text{-}11)$$

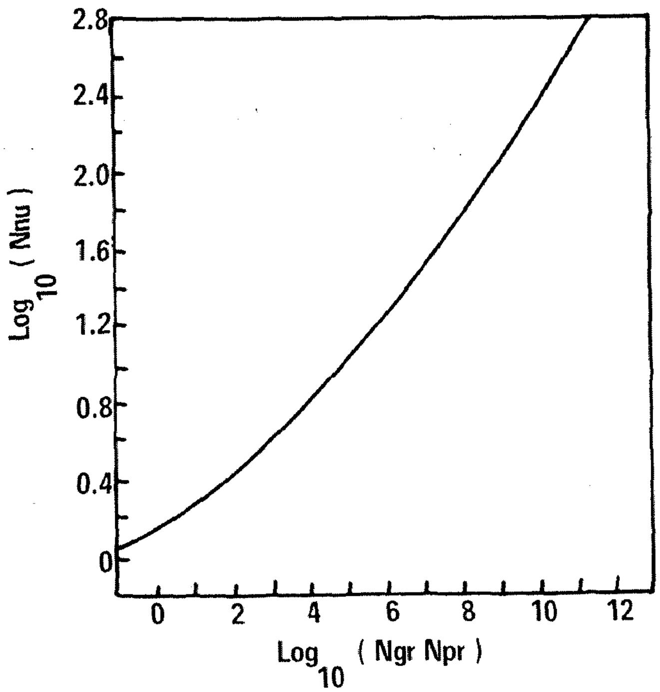

Figure 4. Recommended correlation for free convection around vertical plane surfaces.

SECTION 7

LABORATORY SETUP AND TEST PROCEDURES

The mathematical model on the ISCO sampler cooling system was experimentally verified in three separate laboratory tests. The laboratory facilities used in this study included:

- Environmental chamber, Zero-Temp Inc.
- Electronik 16 recorder, Honeywell Industrial Division
- Bath & circulator, Forma Scientific, Inc.
- Matheson thermometer, -1 to 51°C, 1/10 division.

A thermocouple was placed centrally in each of the 28 bottles in the sampler and the wires were firmly taped to the sampler casing. The sampler was then placed in the environmental chamber. The leads from the thermocouples were passed through a hole of the chamber and connected to the Honeywell Electronik 16 recorder. However, the recorder would record only 24 discrete temperature readings at intervals of 6 seconds at a recording speed of from 1 to 8 in./hr. It was found that to distinguish 24 discrete temperature readings was difficult even at a maximum recording speed of 8 in./hr. Therefore, only about 12 randomly chosen thermocouples were hooked to the recorder for each run. The accuracy of the recorder was about ±0.5°C in the testing range of 0 to 40°C. A temperature-controlled water bath filled with sample was also placed in the chamber, completing the setup of the laboratory test.

Test procedures for each run were as follows:

1. The bath and circulator were turned on and the temperature controller was set to the desired temperature of the water sample to be taken.

2. The environmental chamber was turned on and its dry-bulb temperature was set to the desired ambient temperature.

3. A Matheson thermometer was used to check the reading of the temperature controller after the bath and circulator reached a steady state.

4. After the chamber reached a steady state, weighted ice and water were placed in the sampler ice compartment. The initial water temperature was measured.

5. The recorder was turned on.

6. The sampler cycle time was set and the sampler began to collect the first sample from the bath and circulator.

7. The run was stopped after the duration time was reached or the total number of samples was taken.

SECTION 8

RESULTS AND DISCUSSION

The thermal properties of the sampler were estimated in this study. According to Brandrup and Immergut,[4] the thermal conductivity of polyethylene (high and low density) is 2.88 cal/hr-cm-^{o}C (0.1935 Btu/hr-ft-^{o}F), but is 3.57 and 4.76 cal/hr-cm-^{o}C (0.24 and 0.32 Btu/hr-ft-^{o}F), respectively for a density of 0.945 and 0.976 gram/cm^3 as listed in Macromolecules, Volume 1 edited by Elias.[5] In this study, the thermal conductivity of the sample bottle, which is made of high density polyethylene, was assumed to be 3.72 cal/hr-cm-^{o}C (0.25 Btu/hr-ft-^{o}F); that of the sampler wall, made of double-walled plastic separated with compressed polyurethane foam, was assumed to be 1.49 cal/hr-cm-^{o}C (0.1 Btu/hr-ft-^{o}F). Loose polyurethane foam has a value of thermal conductivity ranging from 0.2-0.37 cal/hr-cm-^{o}C (0.015-0.025 Btu/hr-ft-^{o}F).

COMPARISONS BETWEEN EXPERIMENTAL AND THEORETICAL RESULTS

Accuracy of the computer simulation model was tested again as described in Reference 1. An energy-balanced sample equilibrium temperature in the sampler, without heat gain from surroundings, was compared with those obtained by solving equations (6-1) to (6-4) using the assumptions as in Reference 1, i.e., the thermal conductivity of the wall approached zero and the bottle surface film coefficient was equal to 2976 cal/hr-cm^2-^{o}C (200 Btu/hr-ft^2-^{o}F).

Results shown in Figure 5 indicated that it took about 1 hour for the temperature of sample 1 to drop from 30 to 0.03^{o}C, and the final temperature of all samples was about 3.72^{o}C after 24 hours. By comparing the energy-balanced equilibrium temperature of 3.43^{o}C with 3.72^{o}C, this program was considered sufficiently accurate for the present purpose.

The experimental results and theoretical calculations are compared in plots 6 to 8. Dashed lines on all plots represent results from experiments; solid lines represent those theoretically predicted. For the reader's convenience, detailed testing conditions on the 1680 sampler are summarized in Table 1.

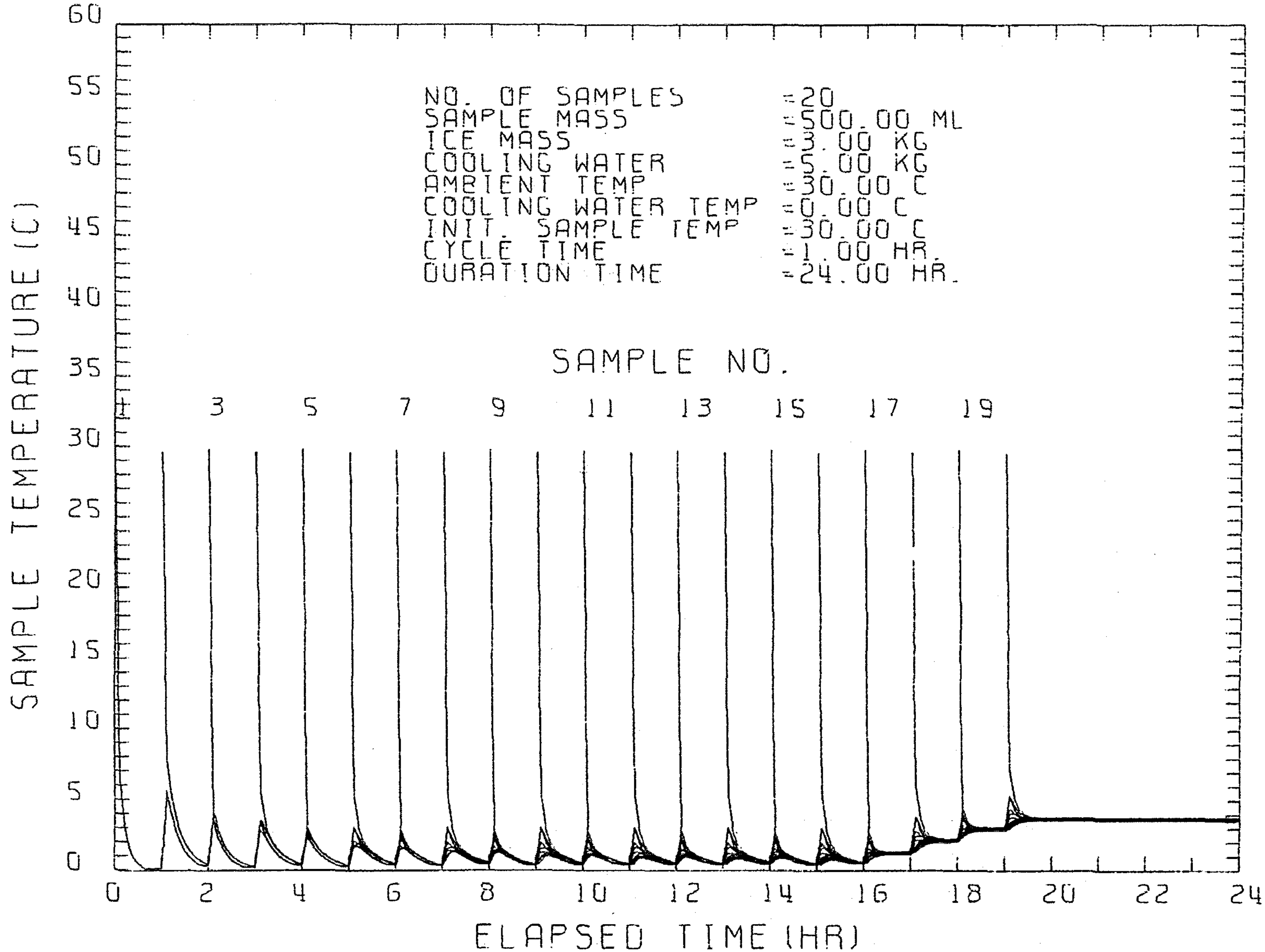

Figure 5. Accuracy test of sample temperature predicted by mathematical model.

TABLE 1. TESTING DATA ON ISCO 1680 SAMPLER

Test number	1	2	3
Number of samples	24	24	24
Sample volume, ml	500	500	430
Ice Mass, kg	4.57	4.65	4.43
Cooling water, kg	5.00	5.00	5.00
Ambient temp., ^oC	35.00	30.00	30.00
Initial sample temp., ^oC	25.00	30.00	20.00
Cooling water temp., ^oC	11.00	13.00	10.00
Cycle time, hr	1.00	1.00	1.00
Duration time, hr	24.00	24.00	24.00
Bottle height, cm	17.78	17.78	17.78
Bottle thickness, mm	1.00	1.00	1.00
Thermal conductivity of bottle, cal/hr-cm-^oC	3.72	3.72	3.72
Thermal conductitity of sampler wall, cal/hr-cm-^oC	1.49	1.49	1.49

Test 1

In this test, crushed ice was packed into the ice compartment, and cooling water was poured over the ice to increase the contact area between the coolant and bottles. Results obtained from the test and the program are shown in Figure 6. The experimental measurements shown in dashed lines indicated that a minimum temperature of 6.5^oC (first sample) was reached at an elapsed time of 5 to 6 hours and persisted for about 2 to 3 hours. The cooling rate for each sample was rapid at the beginning of the sampling period. For example, the temperature in sample 1 dropped 18^oC within 1 hour. The cooling rate then decreased rapidly after the next sample was taken. This is due to heat transfer from the latter sample to the former one. Furthermore, the equilibrium temperature should theoretically be 0^oC if no heat transfer from the surroundings is assumed. However, the final temperature of the first sample at 19.5^oC after 24 hours indicated that heat gain from surroundings to the sampler was extremely high. About 427 kcal (1697 Btu) were absorbed by the coolant from outside the sampler and 66 kcal (261 Btu) were extracted from the samples. Therefore, approximately 81 percent of the cooling capacity of the sampler was lost to surroundings.

Comparisons between the experimental results and the values predicted by the model indicated the following:

- The temperature-time histories for each corresponding sample are closely in phase.

- A maximum temperature difference of 2^oC is observed.

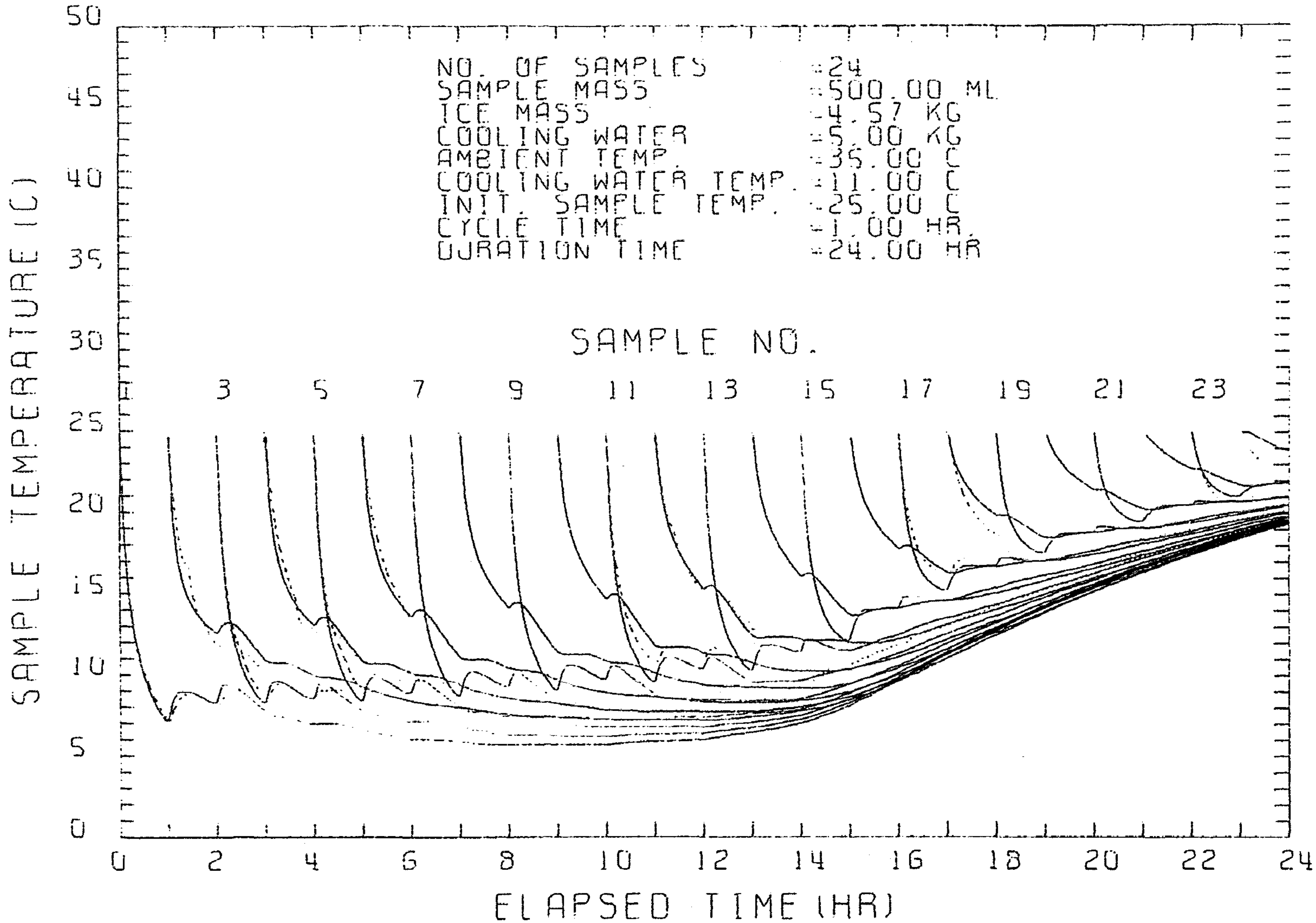

Figure 6. Comparison of predicted and observed sample temperatures, Test No. 1.

- The difference between these values at the lowest temperature for the first sample is 1-2°C.

- The predicted final temperatures are in a range of 20-24°C.

Test 2

Figure 7, which shows the results of Test 2 and the mathematical model, indicates that a minimum temperature of 6.1°C was reached at an elapsed time of 7 to 8 hours.

The final temperature of the first sample after 24 hours was 17.7°C, which was 12.3°C below its initial temperature. Theoretically, the equilibrium temperature for all samples should be 2.57°C in an adiabatic condition. However, during the 24-hour period, about 327 kcal (1298 Btu) of heat were transferred to the coolant from outside the sampler and 147 kcal (585 Btu) were transferred from the samples.

A temporary sharp increase in temperature for sample i was obtained while sample i+1 or i+2 was being taken. This is due to a large temperature difference between samples i and i+1 or i+2. In general, the sample cooling rate was similar to that of Test 1.

Comparisons between the values obtained in the test and the predicted values indicate similar temperature-time histories for each corresponding sample. The maximum temperature difference is about 2°C.

Test 3

Test 3 is similar to Tests 1 and 2. Results from both the model and the test are plotted in Figure 8.

It took about 7 hours for the first sample to reach its lowest temperature (4.6°C) and 24 hours to reach the final temperature (13.1°C), which would be 0°C in the perfectly insulated sampler. The heat transfer to the coolant from outside the sampler and the samples was estimated at about 342 kcal (1358 Btu) and 83 kcal (328 Btu), respectively for 24 hours.

The model indicates that the minimum temperature occurs in about 8 hours and that the final temperature of the first sample is 1°C higher than the observed result. The maximum temperature difference between the observed and the predicted results is about 2°C.

In summary, the results indicate that the cooling rate of a sample in the 1680 sampler is rapid within a cycle time and then decreases rapidly even though the cooling rate of the inner samples is generally faster than that of the outer ones. In general, it takes about 6 to 8 hours for a sample to reach its minimum temperature. Also, the results show that the sampler cooling capacity is inadequate and the sampler needs additional insulation.

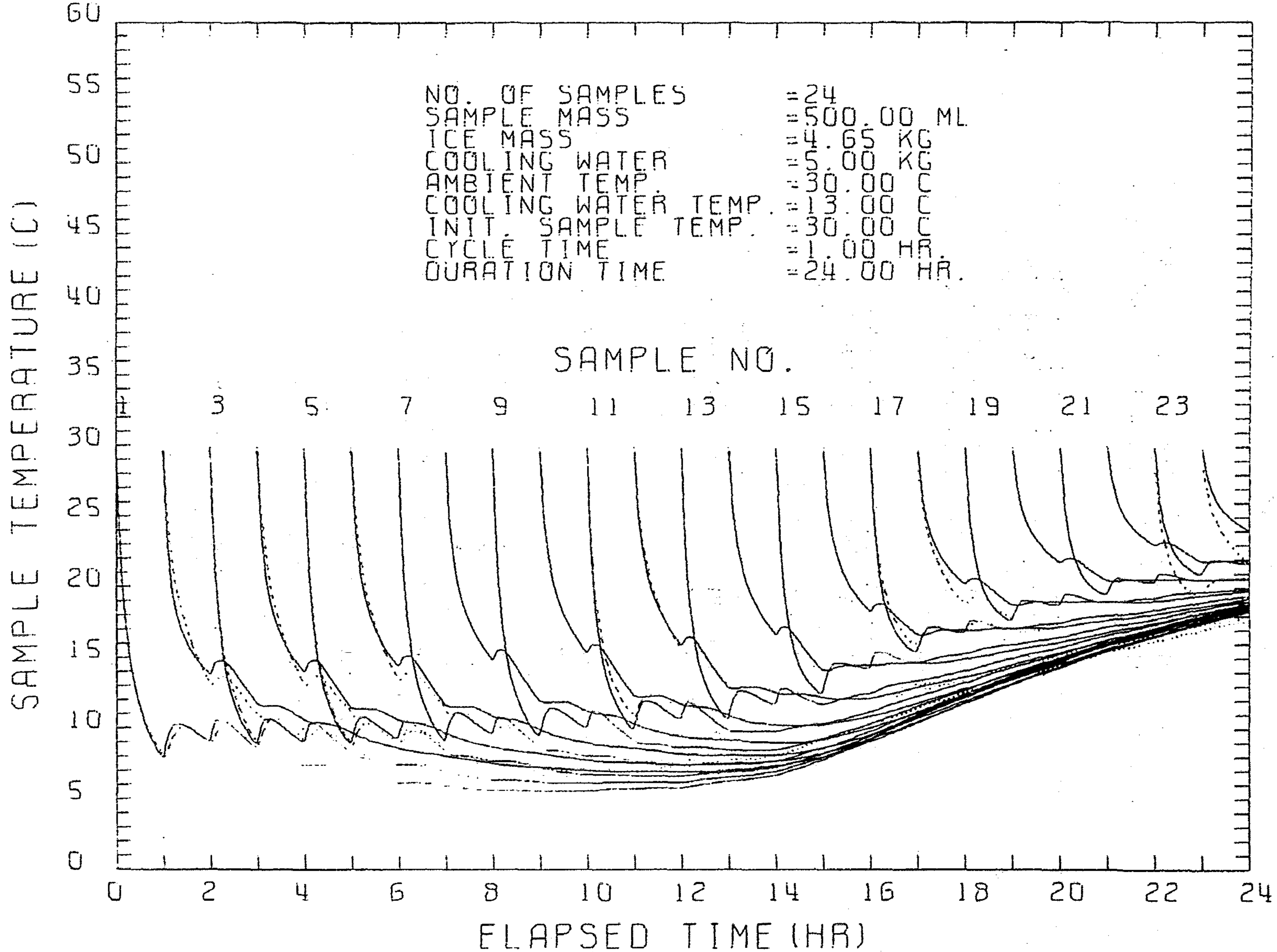

Figure 7. Comparison of predicted and observed sample temperatures, Test No. 2.

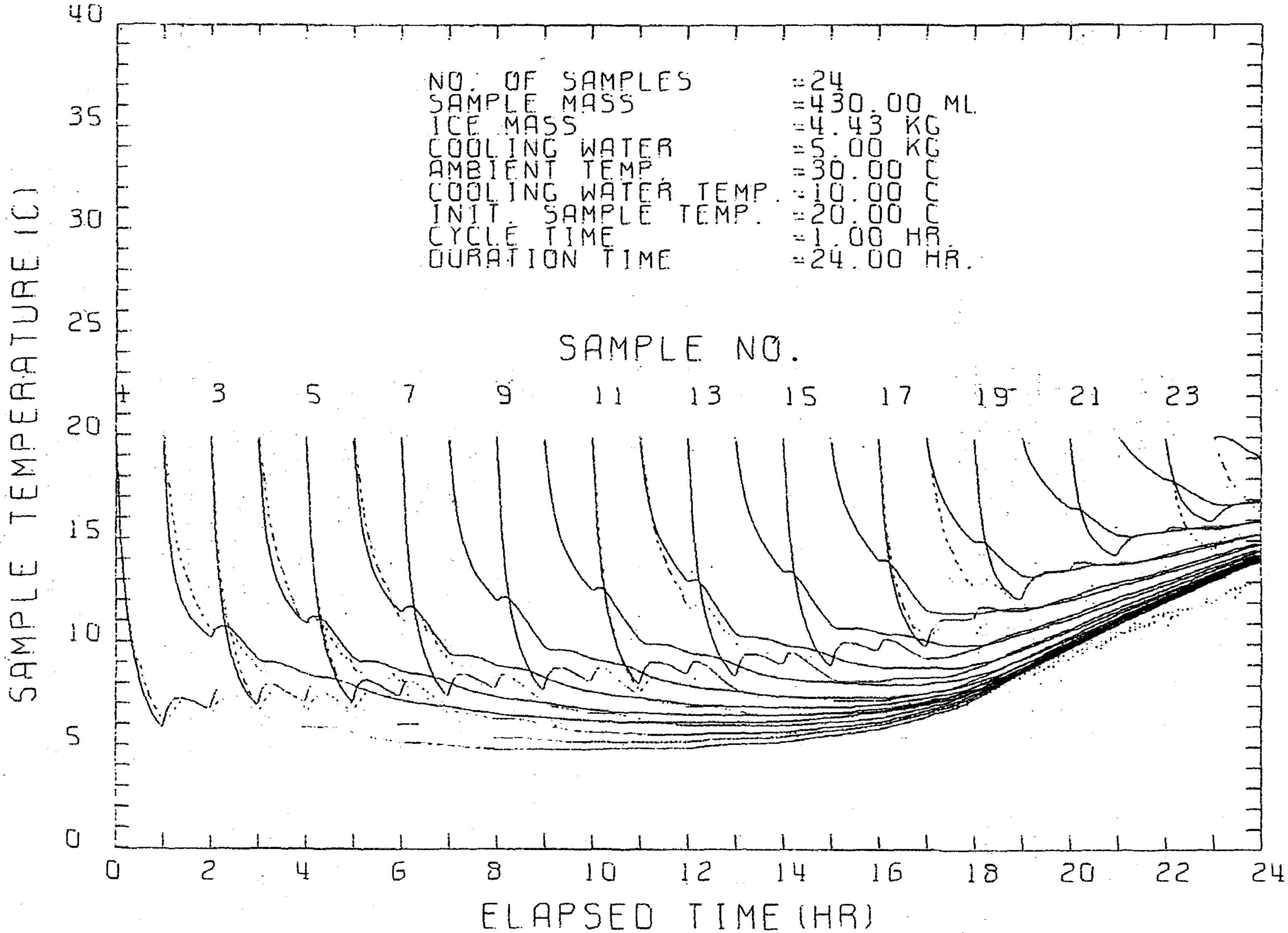

Figure 8. Comparison of predicted and observed sample temperatures, Test No. 3.

Comparisons between the tests and the calculations indicate that both results show a similar trend of sample cooling process for all samples. Accuracy of the model, in general, is within 0-2^{o}C.

MODIFICATION STUDY OF SAMPLER COOLING SYSTEM

The 1680 sampler cooling system can technically hold up to 10 kg of ice if it is filled with water and placed in a freezer for a period of time. It can hold about 7 and 3 kg of ice respectively in the central and outer portions of the container. Since this is rarely done, the cooling capacity is generally less than the designed maximum. In this study, no experimental test was conducted under such conditions; however, two theoretical results under the maximum cooling capacity were obtained to determine the necessity of the modification of the sampler cooling system. The results shown in Figures 9 and 10 were obtained under the following conditions:

- Ambient temperature = 30^{o}C.
- Initial sample temperature = 20 and 30^{o}C.
- Ice in the central portion of the container = 6.9 kg.
- Initial water in the central portion of the container = 0.2 kg.
- Ice in the outer portion of the container = 2.7 kg.
- Initial water in the outer portion of the container = 0.2 kg.
- Cycle time = 1 hour.

Figure 9 indicates that the first sample temperature drops rapidly to 3^{o}C in 1 hour and then rises sharply to about 4.5^{o}C. This is due to the fillings of bottle 2. Temperature then drops again to 3^{o}C within the next hour. While sample 3 is being taken, the temperature in sample 1 rises again to 4^{o}C and then drops to 3^{o}C at the third hour. The mutual effect among samples 1, 2, and 3 is very obvious. The temperature in sample 1 reaches a minimum of about 2^{o}C at the sixth hour and then rises to 4^{o}C after 24 hours. The same phenomena occur for all other samples.

Two kg of ice remain and the final temperature of all samples is in the range of 4-5^{o}C after 24 hours which indicates that the cooling rate is better than achieved in the experimental tests. At the same time, it also shows that cooling capacity is sufficient under these conditions. The cooling rate of outer samples is still slightly lower than that of the inner ones (the initial sample temperature is assumed to be 20^{o}C and the ambient temperature is 30^{o}C).

Figure 10 shows similar results to those shown in Figure 9. Final temperatures of all samples are in the range of 5-6^{o}C and 1 kg of ice remains after 24 hours. One can therefore conclude that the cooling capacity of the sampler is barely enough under these conditions (30^{o}C for

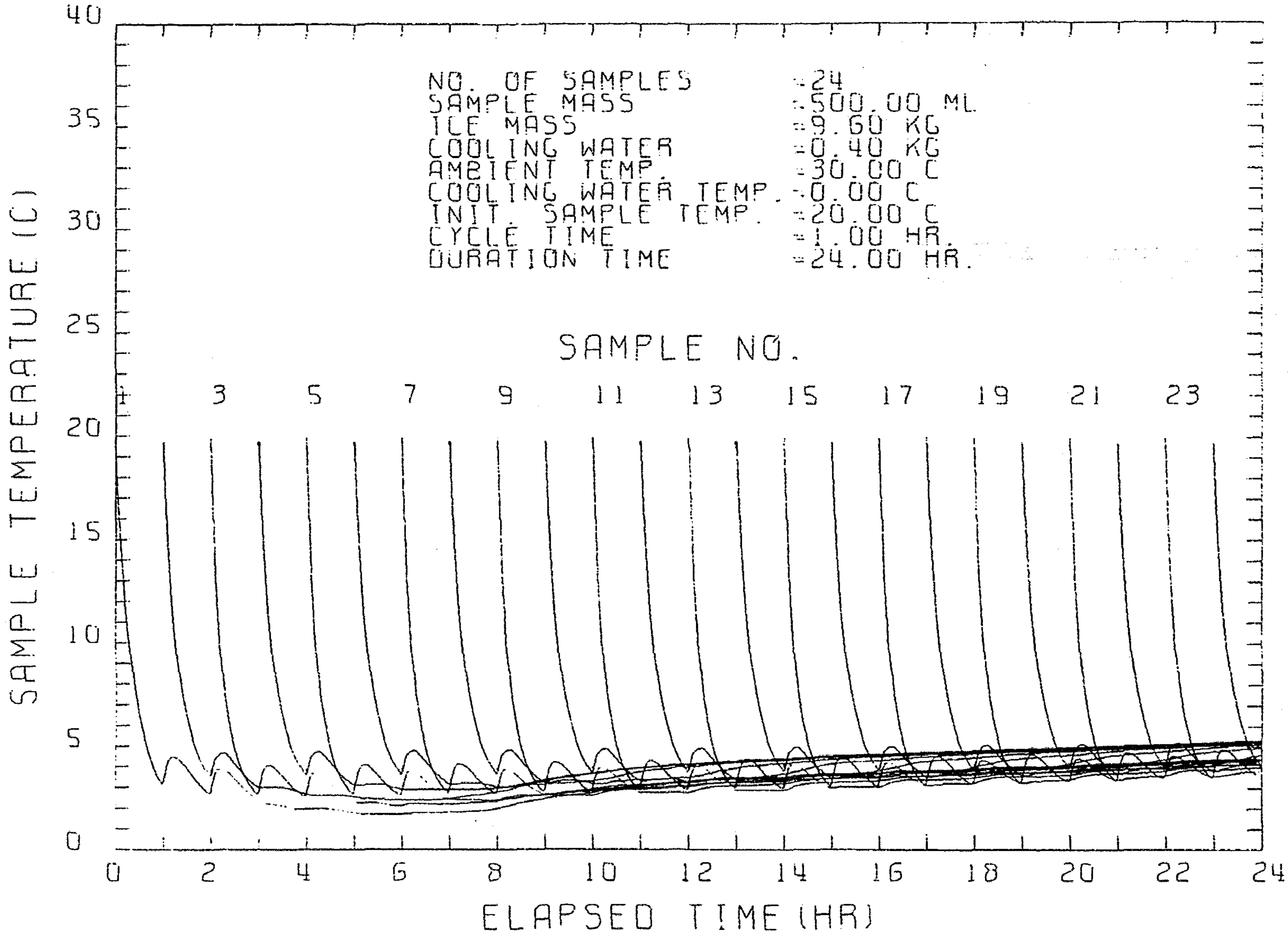

Figure 9. Predicted sample temperatures using the original sample container charged with 9.6 kg of ice (20°C for initial sample).

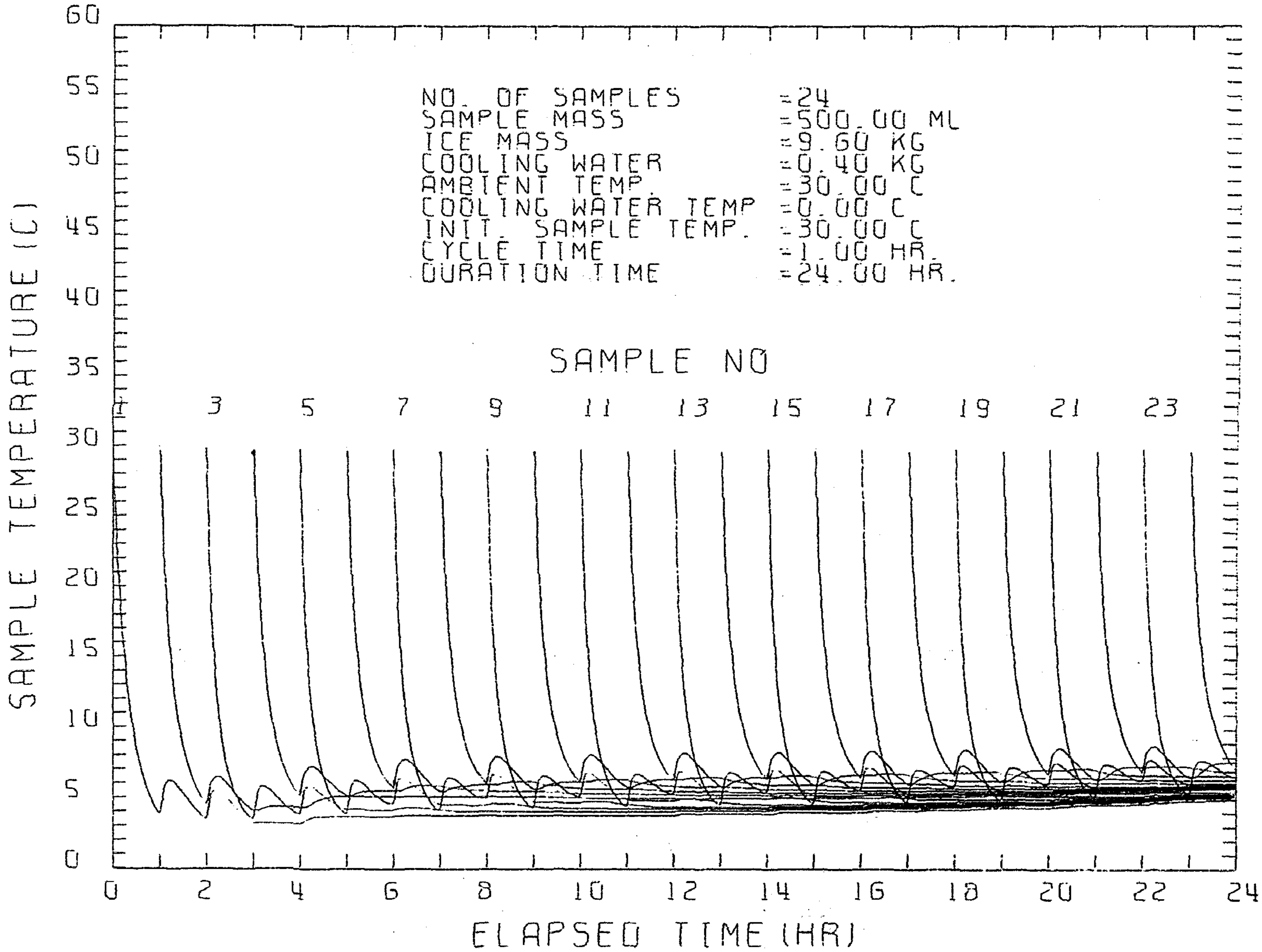

Figure 10. Predicted sample temperatures using the original sample container charged with 9.6 kg of ice (30^0 for initial sample).

both the ambient and the initial sample); that the contact area between the outer bottles and the coolant is not sufficient; and that the heat transfer from outside the sampler to the outer samples is somewhat high.

The above results indicate that a redesign of the sample container is necessary. Based on the mathematical model, a new bottle container is suggested as shown in Figure 11. This new container has a bottom thickness of 7.62 cm (3 in.) instead of the original 3.175 cm (1.25 in.). Polyurethane foam is then inserted between the double-walled plastic. Its thermal conductivity is assumed to be 0.744 cal/hr-cm-^{o}C (0.05 Btu/hr-ft-^{o}F). The ice capacity is increased to about 13.6 kg, but the other parameters remain the same as in the original sampler.

Figure 12 shows the results from the computer program under an average temperature of 30^{o}C for both the surroundings and the initial sample for the new container. The first sample temperature drops quickly below 4^{o}C within 1 hour and increases sharply to about 6^{o}C. It then drops again to 3^{o}C in the next hour. While sample 3 is being taken, temperature in sample 1 again rises rapidly to 6^{o}C and then decreases below 4^{o}C at the third hour. The final temperature after 24 hours is below 4^{o}C. This process repeats again for all other inner samples. The same phenomena are observed as in the inner samples for the outer ones, although their cooling rates are slower. In general, it takes about 3 hours for the outer samples to reach below 5^{o}C.

At the end of 24 hours, about 2.56 kg of ice remain. It is therefore clear that the cooling capacity is adequate under these conditions. However, the contact area between the outer bottles and the coolant should be increased if the sampler is to be used at a higher environmental temperature. At the same time, the wall thickness of the sampler should also be increased to reduce heat gain from the outside to the outer samples.

To further increase the contact area and the sampler wall thickness, a further modification is suggested. If the bottle radius is reduced from 3.18 cm (1.25 in.) to 2.79 cm (1.1 in.) and the bottle length is increased from 17.78 cm (7 in.) to 20.83 cm (8.2 in.), the contact area will be increased by 14 percent. In this design, the bottle volume is not changed, but the sampler wall thickness is increased by 3 cm (1.2 in.) It is assumed that the thermal conductivity of the wall and the bottom filled with loose polyurethane foam would be less than 0.744 cal/hr-cm-^{o}C (0.05 Btu/hr-ft-^{o}F). The ice capacity would be 9.6 kg, which is similar to that of the original container.

Figure 13 shows the predicted sample temperatures obtained with this design using a temperature of 35^{o}C for both the surroundings and the initial sample. Similar results as in Figure 12 are obtained. It takes about 3 hours for an inner sample to drop and stay below 4^{o}C and 5 to 6 hours for an outer one to remain below 5^{o}C. At the end of 24 hours, about 2.5 kg of ice is not melted. Hence, the cooling capacity is sufficient for the sample to stay at 4-5^{o}C, although the cooling rates of the outer samples are still slightly low.

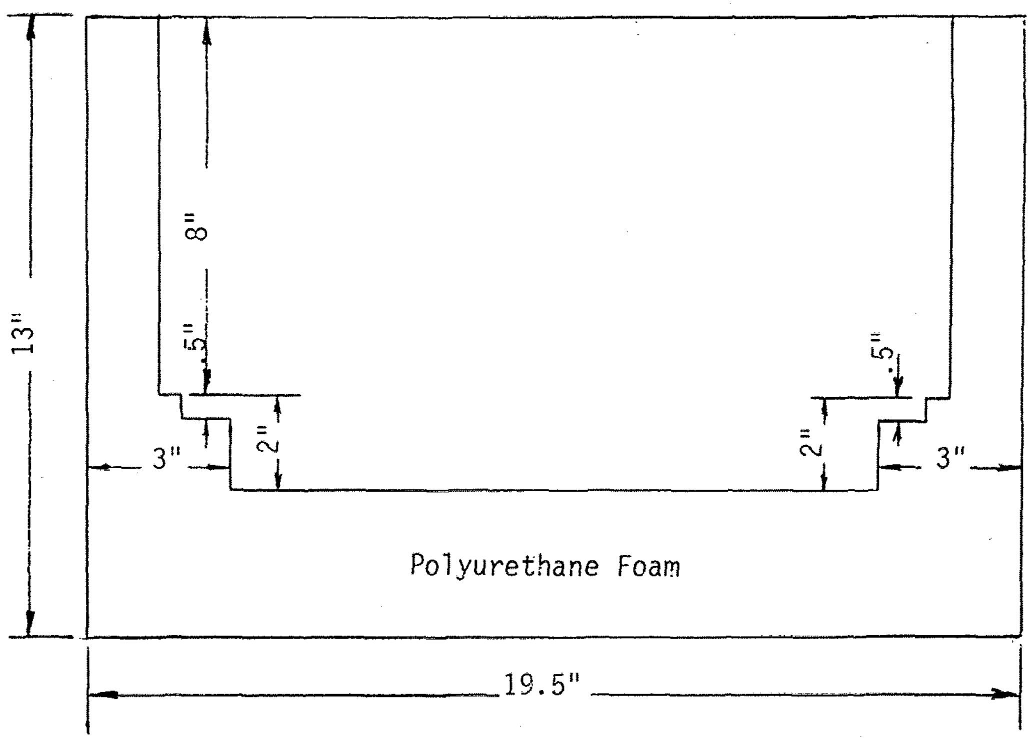

Figure 11. Modified design of sample container (modification 1).

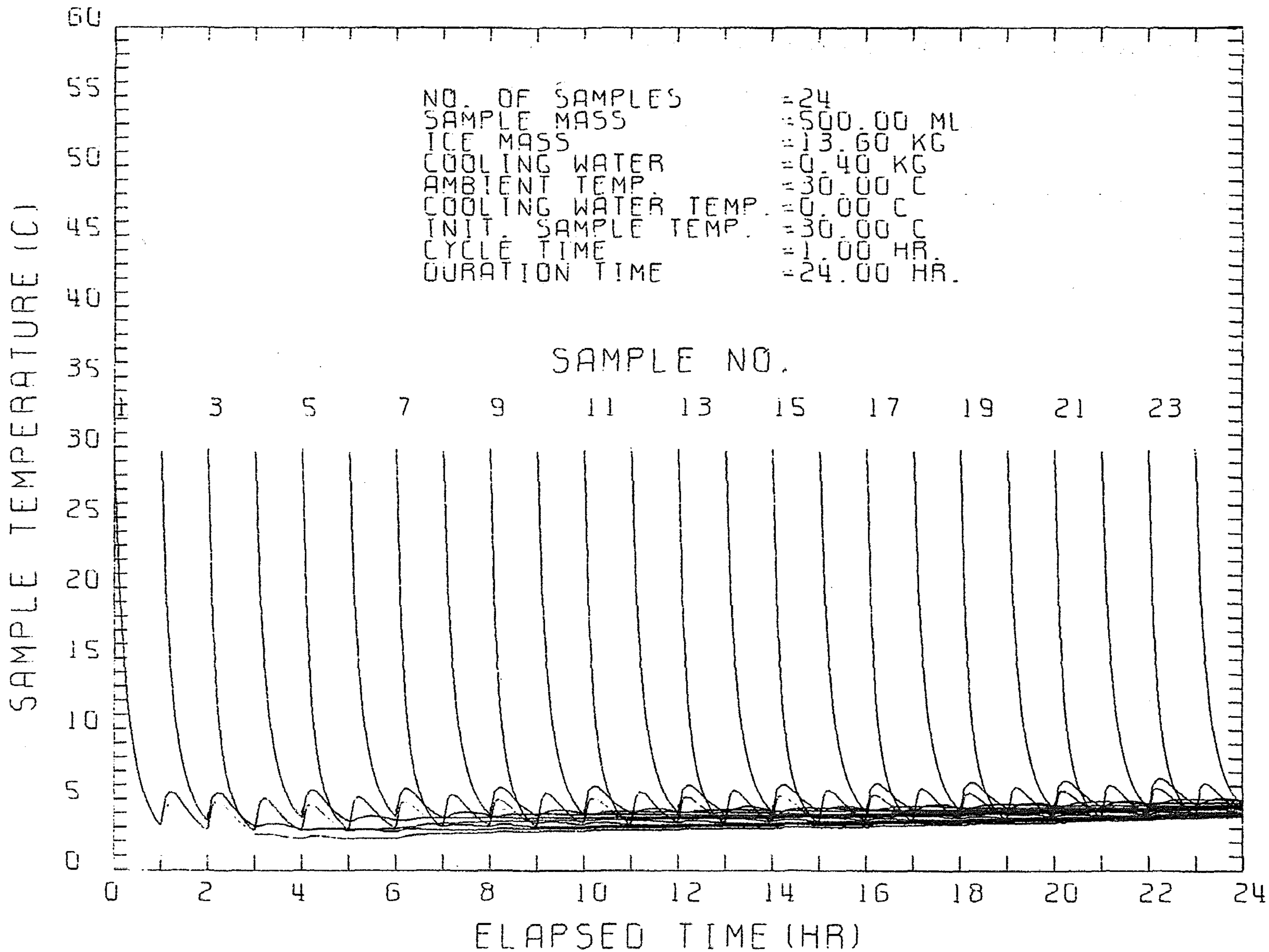

Figure 12. Predicted sample temperatures in the redesigned sampler (modification 1).

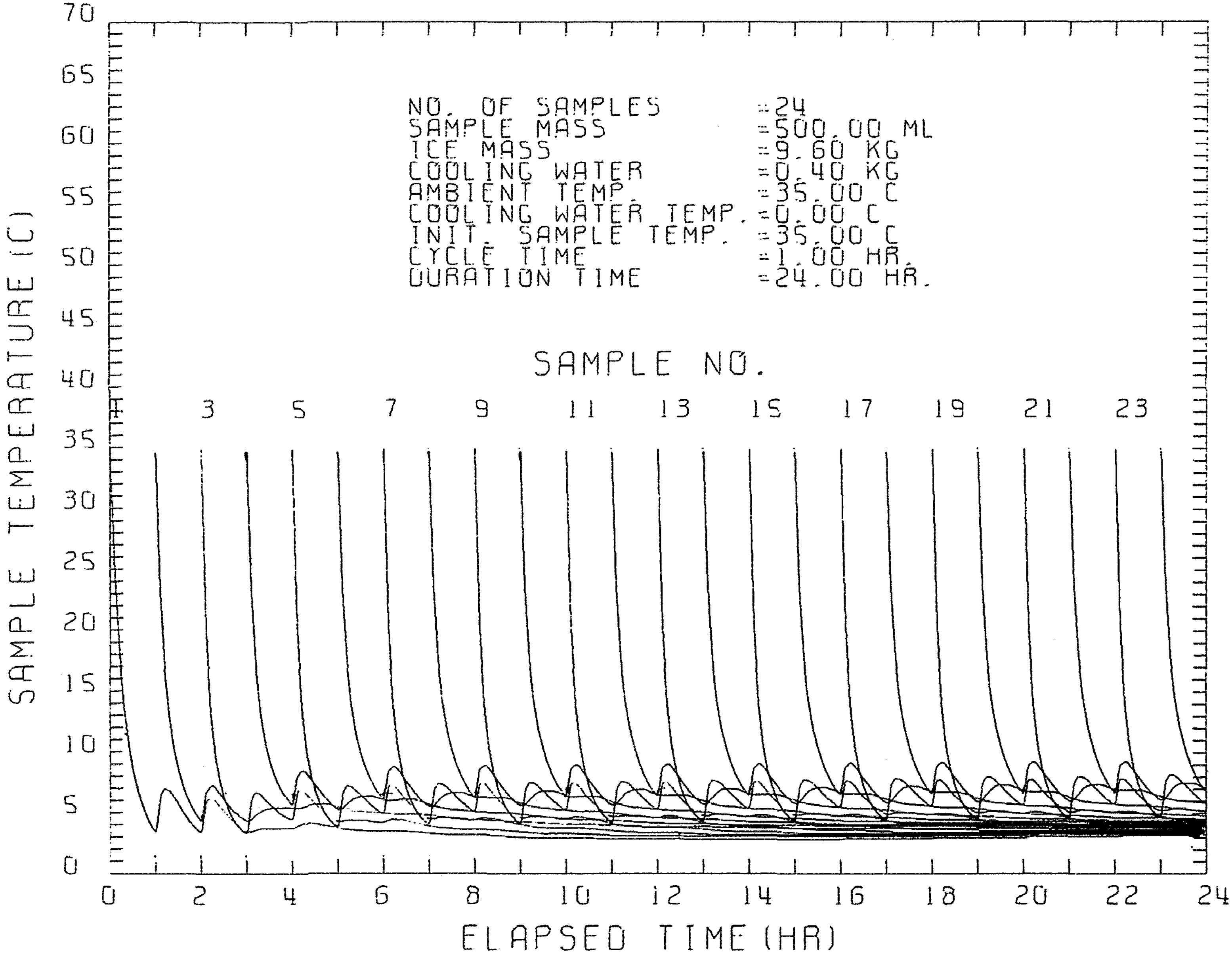

Figure 13. Predicted sample temperatures in the modified sampler (modification 2).

This study concludes that by icing it is possible to lower 24 samples of 500 ml each to about 4°C during a 24-hour period under conditions mentioned above.

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

A mathematical model was developed to simulate the operation of the ISCO 1680 automatic wastewater sampler. This study was similar to the one carried out earlier with the Manning S-4000 sampler. The objective was to determine the feasibility of developing an automatic sampler with adequate ice compartment for sample preservation. The model was used to confirm the validity of sample cooling predictions under variable conditions. Experimental measurements on the sample cooling process were also conducted.

Data obtained during operation of the ISCO sampler cooling system under varying conditions indicated that the accuracy of the mathematical model was within ±2°C. Also, the theoretical sample temperature history was in phase with that of the corresponding test sample. Good agreement between theoretical and experimental results was obtained.

This project verified the feasibility of using mathematical models for the development of specifications for a sampler cooling system.

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