

Dynamic Modeling of Thermal and Gas Toxicity in Fires

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Abstract: A physiochemical model is presented which predicts the air temperature and gas concentration changes expected to occur in a compartment of an aerospace vehicle as a result of an unwanted fire. The change in compartment air temperature can be predicted from the heat release rates of the burning materials and the net heat loss from the compartment. The changes in gas concentration within the compartment are predicted from the temperature-dependent chemical kinetics of the material pyrolysis and the net mass loss from the compartment. Exposure to gases and elevated temperatures generated by the fire produces life-threatening ill effects in humans. Parameters used to measure thermal effects were the time to reach and the duration of an average skin temperature of 45° C and a body enthalpy of 100-252 kcal representing a pain and metabolic threshold. The parameters used to measure toxic gas effects were the time to reach and the duration of time exposed to harmful levels of gas concentration. Synergistic effects of gas mixtures or of exposure to combined thermal effects and toxic gas and smoke are not considered in the analysis. The analysis was applied to the case of a small fire in the electronics area of an aerospace vehicle. In this case a polyvinyl chloride electrical insulation decomposes generating HCl gas which is released into the compartment. A parametric study is made of skin temperature and body enthalpy as a function of heat release, ventilation rates, and physical stress levels. The results of the analysis showed that ventilation at relatively low rates could effectively reduce thermal and toxic gas effects while stress could increase and prolong

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thermal effects. Survival times were still affected, even when thermal effects were minimized by ventilation, because the test gas, HCl, is toxic at very low levels of concentration. The analysis also emphasized the need to determine the heat and mass transfer characteristics of the specific compartment in which the fire occurs as well as determining the fire properties. The compartment properties can be as important as the fire properties in determining the threat level of the fire.

An occupant in an area in which a fire occurs either attempts to escape or remains subject to the local fire conditions. The threats to human survival can be assigned to multiple factors, among them are the effects of heat, toxic gas, and smoke due to the combustion processes. The relative quantities and generation rates of each also depend on the chemical nature of the fuel, and the geometry, atmosphere, and mass and heat-transfer characteristics of the fire area.

Heat produced can cause tissue destruction, metabolic disturbances, and pain; toxic gases generated also affect survival; chemical toxicants are inhaled or react with the eyes and skin; smoke also can be toxic chemically and, in addition, decreases light transmission, visibility, and recognition of appropriate escape routes. All of these effects result in deterioration of mental and physical abilities and a decrease in the ability to escape and survive.

Often an assessment of the importance of these threats is not available, especially with regard to a dynamic fire scenario. Evidence may be obliterated as part of the casualty or extrapolation of standard fire test data or behavioral and biological data obtained from simulated tests on animals is not obvious. Therefore, it would be helpful to develop a model of a compartment environment describing the fire dynamics which are pertinent to their effects on the human system. This model might be used to estimate or identify critical or limiting parameters and their relation to the time scale of escape and survival. The purpose of this study has been to develop such a model.

It must be realized that the human system is immensely complicated to model; the complex fire environment compounds the modeling problem. Rather than beginning with as complete a model as possible, we have used a simple model which can be expanded as the need arises. For example, the present model does not predict fire chemistry but uses, as a starting point, hypothetical or

laboratory data for fire properties, such as heat release calorimetry. Thus, the model developed is more a method of extrapolating existing laboratory data for constant conditions to that of time-dependent conditions in another environment, and also defines and selects parameters which affect and are an estimate of survival times.

Model Development and Application

The core of the model was developed by the Lockheed Corp. and NASA, Manned Spacecraft Center, Houston, to study thermal effects on the crew of spacecraft during operation or extravehicular activity. A brief description of the model follows and how it was modified for its application to fire scenarios in an aerospace vehicle. A more detailed description of the spacecraft model can be found in References 1 and 2. A list of the necessary input variables for the model can be found in Table I.

Time Scale of the Fire Threat. In the model it is assumed that the fire victims are enclosed in a volume in which the fire occurs or a volume which is heated by an external fire with no intrusion of flames (see Figure 1). It is also assumed that the victims will not have physical contact with open flames and that their proximity to the fire will not result in immediate exposures to a large radiant energy source. This type of fire history is typical of the initial stages of a large fire or the total history of a relatively small fire. Thus, survival times may be on the order of minutes compared to negligible survival times for the case of contact with flames or close proximity to a major fire radiation source.

Transfer Mechanisms and Enclosure Description. In the model the victim is enclosed within a ventilated space in which heat can transfer through walls and vents by forced or natural convection. Heat transfer within the enclosure,

Table

Fig. 1

between the victim and the internal atmosphere and walls, occurs by convection and radiation. Mass transfer can occur between the victim and the atmosphere and walls because of the excessive heat. The victim is covered by a garment, except for the victim's head and hands, and heat is conducted to the atmosphere through the garment. Perspiration is assumed rapidly absorbed by the garment and evaporates from the garment surface to cool the victim if the atmosphere is not saturated.

The enclosure atmosphere is assumed perfectly mixed. (This assumption will be relaxed at a later date in favor of a mamillary diffusion and perfectly mixed matrix for the space.) Heat, gases, and smoke can be generated within the volume and can be transferred out. Thermal effects are considered by computing the skin temperature and noting which skin areas reach 45° C, a pain threshold. The internal temperatures of portions of the body, as well as the total body enthalpy, are also monitored. When the internal body temperatures reach those representative of body deterioration, associated with functional impairment and death, the enthalpy is in the range of 100-252 kcal, respectively. Predicted atmospheric gas concentrations are computed and compared to constant and single species concentration symptomology available in various literature. Conservative toxic effects are noted for periods of time for which the concentration exceeds a specific constant concentration value. No smoke or aerosol effects are included in the model to date.

A summary of typical mass and energy balances can be found in the Appendix.

Fire Scenarios. In the model, materials within the enclosure either burn or pyrolyze due to the increased temperature generated by the fire. The model presently requires that the fire heat release rate or material temperature history be input, i.e., their time dependence must be defined. Two options for time functional forms are included in the model: ramp functions and the

Beta distribution function common to statistics. Thus, the temperature or heat release rate can follow these histories. Typical forms are shown in Figure 2.

Fig. 2

Pyrolyzing materials are assumed to decompose according to chemical kinetic rate equations dependent on either a computed temperature based on a heat balance or an arbitrary wall or atmospheric temperature history. This temperature history may be generated by or be independent of the fire history. The material temperature is assumed uniform, i.e., there is no temperature gradient within the pyrolyzing material.

Parametric Studies. The model was applied to a candidate fire scenario to study the effects of thermal and toxic gas on fire victims. A study was made to determine the effect of varying specific fire parameters. The parameters investigated were: variable stress levels, ventilation rates, and heat release rates. Only one victim was assumed present in a confined area of the vehicle. The characteristics of the vehicle and the victim used in the model are given in Table I. The fire scenario assumed was a small fire in an electronics area which burned for a total of 10 min. The fire generated a heat release rate curve according to a Beta (3, 11) or a Beta (3, 3) curve shown in Figure 2. The temperature history of pyrolyzing electrical insulation, the only source of toxic gas considered in the scenario, was also assumed to follow a Beta (3, 11) or a Beta (3, 3) curve as shown in Figure 3. The electrical insulation was assumed to be polyvinyl chloride (PVC) which can form HCl on pyrolysis. Only the concentration of HCl was predicted and its toxic effects studied. No further reaction of the HCl with spacecraft materials or settling of its aerosols was considered, and the possible effects of other gases were not studied.

Fig. 3

Results

The computed compartment temperatures for the variable heat release rates specified and various ventilation rates are shown in Figure 4. The ventilation rates are low and equivalent to zero to four changes of volume per minute. In all cases a maximum in compartment temperature occurs due to cooling phenomena such as ventilation, and the variable heat release rate due to the fire. Generally, with the ventilation rates chosen and with the higher heat release rate, the net heating effect and temperature rise occur over a 5-min period while the maximum temperature occurs at about 2 min.

Figures 5 and 6 show the effect of the ventilation rate on thermal toxicity. The average skin temperature versus time for varying ventilation rates is plotted in Figure 5. A maximum in average skin temperature is apparent. This maximum in skin temperature lags the maximum in compartment temperature by about 1 min, a time lag due to the required time for heat transfer to the skin to occur and due to the cooling effect of the body's innate cooling process, sweating. In the assumed scenario, at the low ventilation rates, the average skin temperature exceeds the pain threshold of 45° C due to heat. At the higher ventilation rates, the compartment temperatures are lower, heat transfer is less, and the cooling effect of sweating is even greater because of increased mass transfer effects. These mass transfer effects are a result of the increased velocity of air which increases the sweat evaporation rate. In these cases the skin pain threshold is not reached.

Figure 6 shows the effect of variable ventilation rates on the body enthalpy. Again, a maximum occurs as a function of time. This maximum lags the maximum in compartment temperature by approximately 2 min. This time lag represents even longer times for heat transfer to occur within the body. Only at the low ventilation rates does the body enthalpy exceed a body function

impairment value, 100 kcal at about 4 min. Enthalpy values for a high-stress state, a metabolic activity level of 504 kcal/hr comparable to heavy physical strain, also appear in Figure 6. The effect of a stressed state is to both increase and prolong the increased body enthalpy levels. In the case of moderate ventilation rates, remaining in an unstressed state causes no thermal shock, while in a high-stress state, thermal shock does occur due to increased body enthalpy. This thermal shock is maintained for prolonged periods of time (see Figure 6) at a ventilation rate of 566 liters/min. This effect of stress is due to the additional heat generated by the body itself caused by increased metabolic activity associated with the stressed state.

Figure 7 shows the HCl concentration generated as a function of ventilation rate for the thermal histories specified. The quantity of PVC decomposed is 10 g. This is equivalent to decomposition of 30.48 cm of insulation in a bundle of insulated wire consisting of 20 wires. In all cases a maximum occurs for the HCl concentration as a function of time. The kinetics of decomposition are so rapid at these temperatures that almost all of the PVC is decomposed within the first minute. The toxic thresholds for HCl are also shown in Figure 7. A 10-min emergency limit is set at 0.0544 mg/l (30 ppm). Work is impossible at concentrations of 0.1815 mg/l (100 ppm). An immediate lethal concentration of HCl is 3.63 mg/l (2000 ppm). From these limits and the predicted HCl concentration history, human symptomology can be estimated for the scenario. Table II lists the length of time to reach each limit as well as the length of time the limit has been exceeded. It is obvious that the most serious consequences occur in the unventilated compartment, concentrations reaching and remaining at lethal levels for extended periods. At increasing ventilation rates, the period of danger due to toxicity of HCl decreases. In some cases the length of time over the limit is short enough that one can hold

Fig. 7

Table

his breath until the risk of inhaling a dangerous concentration of HCl has passed.

A comparison of both the thermal and toxic effects shows that for these particular scenarios, toxic effects can occur minutes before thermal shock. In some cases toxic effects remain even though ventilation has reduced thermal effects to the point where they are insignificant. In the case of PVC, this is due to the reaction kinetics being extremely rapid compared to convective flow rates; all the HCl is dumped rapidly into the system before convective flow can sweep it out. It is also because of the fact that gases such as HCl are toxic at extremely low concentration levels. To reduce concentrations below these levels, dangerously long exposure times may be required.

A comparison of the different heat release rate histories and PVC temperature histories was also made (Figures 2 and 3). The comparison was made between the Beta (3, 3) and Beta (3, 11) functions. Because the Beta functions are normalized, the areas under each of these curves are equal. Thus, a comparison of the heat release rate histories represents a comparison of the response of the system to equal total energies, but different heat release rates. A comparison of the material temperature histories represents a comparison of equivalent average temperatures. If one considers that the material is subjected to heating and that the material has a constant specific heat, then the material is also exposed to equivalent total energy histories but different heating rates. Figure 4 shows the computed compartment temperature for both heat release rate histories. Figure 8 shows the heat release rates and the heat losses through the compartment walls for each case. The net heating effect of the rapid fire history (B 3, 11) is nearly 50% greater than the slow fire history (B 3,3). Although not included here, an analogous treatment may be made for gas or aerosol effects. It is the net generation of HCl that is




Fig. 8

important. Thus, the loss of HCl in the enclosure by settling of aerosol or chemical reaction should also be included. It is obvious then that to define the fire threat due to heat release rate or toxic gas concentration, one must also define the heat and mass transfer characteristics of the environment in which the heat or gas is released to determine whether the net heat or mass release rate is a fire threat. Figures 9 and 10 show the HCl concentration and body enthalpy histories for the case of no ventilation. Here again, at the low heat release rate (Beta (3, 3)), HCl toxicity is even more significant than the thermal effect. For the slow heat release rate, the body enthalpy never exceeds a critical value but the HCl concentration reaches lethality in about 3 min.

Figs.
and 10

Conclusions

A simple model has been developed to collect and coordinate fire information in order to predict dynamic thermal and toxic effects of fires. Body enthalpy and average skin temperature can be predicted and used as a measure of thermal effects. Toxic gas concentrations can be predicted and used to estimate human symptomology.

The relative importance of thermal and toxic effects depends on multiple factors such as ventilation, stress, chemical kinetics, heat losses, heat generation rates, etc. In order to ascertain both the magnitude and relative importance of thermal and toxic effects, these factors must be adequately known for the fire environment. The model then can be used to predict their interaction with the victim of the fire; as a result, the time to reach and time in excess of the toxic and thermal thresholds can be estimated. In the application of the model to an example fire scenario involving PVC insulation, it was predicted that HCl toxicity could be a serious consequence even when

thermal effects are minimized. In addition, ventilation can effectively reduce thermal and toxic effects at relatively low ventilation rates while stress was found to increase the threat of thermal shock.

Appendix

A summary of the energy and mass balances used in the model follows:

1. Energy balance on the enclosure atmosphere

$$mC_p \frac{dT}{d\theta} = N(QS) + \dot{m}C_p T_E - Q_w + QCD - \dot{m}C_p T + QG$$

where:

θ = time

C_p = heat capacity

T = atmosphere temperature

T_E = environment temperature

N = number of occupants

QS = rate of heat transfer from occupants to atmosphere

Q_w = rate of heat transfer at wall

QCD = rate of heat transfer due to moisture condensing at wall

QG = rate of heat generated by chemical reaction

\dot{m} = rate of mass transfer due to ventilation, thermal effects, and chemical reaction³

2. Energy balance on man

The general equations for the core, muscle, fat, and skin compartments are as follows:

• Core

$$[\text{Mass} \cdot C_p]_{\text{core}} \frac{dT_{\text{core}}}{dt} = Q_{\text{MET}}_{\text{core}} - Q_{\text{COND}} - Q_{\text{CONV}} = Q_{\text{STOR}}_1$$

- Muscle

$$[\text{Mass} \cdot C_p]_{\text{muscle}} \frac{dT_{\text{muscle}}}{dt} = Q_{\text{MET}}_{\text{muscle}} + Q_{\text{COND}} - Q_{\text{COND}'} = Q_{\text{STOR}}_2 - Q_{\text{CONV}}'$$

- Fat

$$[\text{Mass} \cdot C_p]_{\text{fat}} \frac{dT_{\text{fat}}}{dt} = Q_{\text{MET}}_{\text{fat}} + Q_{\text{COND}'} - Q_{\text{COND}''} - Q_{\text{CONV}''} = Q_{\text{STOR}}_3$$

- Skin

$$[\text{Mass} \cdot C_p]_{\text{skin}} \frac{dT_{\text{skin}}}{dt} = Q_{\text{MET}}_{\text{skin}} + Q_{\text{COND}''} - Q_{\text{CONV}'''} = Q_{\text{STOR}}_4 - Q_{\text{RAD}} - Q_{\text{SEN}} - Q_{\text{LAT}}$$

where the simulation model divides the body into 10 elements: head, trunk, right and left arms, right and left hands, right and left legs, and right and left feet. Each consists of core, muscle, fat layer, and skin nodes. Considering the central blood as an element, there are 41 distinct compartments, and each compartment is assumed to be at a uniform temperature having a discrete temperature distribution. The general equation for each compartment is simply written in the form of a heat balance as

$$\text{heat stored} = \text{heat in} - \text{heat out}$$

The human body may be considered in the same manner as a heat engine. That is, heat is produced (QMET) by the oxidation of fuel (food) for energy, and heat is dissipated by conduction (QCOND), convection (QCONV), radiation (QRAD), and mass transfer at the skin surfaces (QSEN and QLAT). Heat produced in excess of that which can be dissipated will be stored in the tissues (ΣQ_{STOR}) with a resulting rise in body temperatures.

3. Mass balance on enclosure

$$\frac{dG_{\text{ASI}}}{dt} = G_{\text{ASIIIN}} + G_{\text{ASIGEN}} - G_{\text{ASIOUT}}$$

where:

G = time

G_{ASI} = mass of enclosure gas I

GASIN = gas I convected in
GASIOUT = gas I convected out³
GASIGEN = gas I generated or used by man, chemical reaction or fire

References

- (1) L. H. Kuznetz, "Control of Thermal Balance Liquid Circulating Garment Based on a Mathematical Representation of the Human Thermoregulatory System," NASA TM X-58,190, October 1976.
- (2) L. W. Morgan, G. Collett, and D. W. Cook, Jr., MSC Program J196, NASA Johnson Spacecraft Center, Houston, Texas.
- (3) The enclosure is assumed to be perfectly mixed and to have a constant volume and pressure. The ideal gas law is assumed to hold. Ventilation as well as changes in temperature or chemical reaction may cause a flow out of the volume. On cooling or chemical reaction it may also be possible to have a net mass flow into the volume without flow-out. In this case, the flow-in is assumed to be of a gas with the properties of the environment. The flow rates are calculated according to the differential form of the ideal gas law with respect to time.

Table I. Model Input Requirements

Model	Test case parameters	
Enclosure description		
Initial compartment temperature or subsequent history	16.7° C	(62° F)
Initial wall temperature or history	10.6° C	(51° F)
Compartment pressure	1 atm	(1 atm)
Gravity	1 G	(1 G)
Initial compartment dewpoint	10° C	(50° C)
Ventilation rates	0-2.24 m ³ /min	(0-80 ft ³ /min)
Air velocity in compartment	0-3.65 m/min	(0-12 ft/min)
Volume of compartment	0.56 m ³	(20 ft ³)
Surface area of compartment	4.6 m ²	(50 ft ²)
Dewpoint of ventilating air	1.67° C	(35° F)
Thermal and toxic factors		
Composition of decomposing material and pyrolysis gases	PVC, HCl	
Kinetic rate expression for decomposition	$\text{Rate HCl (wt)} = 1.09 \cdot \exp(-9143(^{\circ}\text{K})/\text{temp}(^{\circ}\text{K})) \cdot \text{HCl}(1 - \text{HCl}/\text{HCl}_{\text{max}})(\text{O}_2)^{1/2}$ $[\text{Rate HCl (wt)} = 1.09 \cdot \exp(-16457(^{\circ}\text{R})/\text{temp}(^{\circ}\text{R})) \cdot \text{HCl}(1 - \text{HCl}/\text{HCl}_{\text{max}})(\text{O}_2)^{1/2}]$	
Heat release rate history	$\text{Beta (3, 11)} \cdot 2.22 \text{ kcal/g}$ $[\text{Beta (3, 11)} \cdot 4000 \text{ (Btu)/wt(1b)}]$	

Table I. Concluded

Quantity of heat-generating material	454 gm (1 lb)
Quantity of toxic gas-generating material	10 g (0.022 lb)
Decomposing material history	Temp(°C) = 10.6°C + Beta (3, 11) · 251°C (Temp(°F) = 51°F + Beta (3, 11) · 484°F)
Human Factors	
State of stress of victim (metabolic rate)	75.6-504 kcal/hr (300-2000 Btu/hr)
Composition of garment	--- ---
Thickness of garment	0.85 cm (0.028 ft)
Conductivity of garment	4.84×10^{-4} W/cm °C (0.028 BTU/ft °F hr)
Emissivity of garment	0.97 (0.97)

Table II. HCl survival limits [Beta (3,11)]

Ventilation rate	Time to reach, min			Time over, min		
	30 ppm (0.0544 mg/liter)	100 ppm (0.1815 mg/liter)	2000 ppm (3.63 mg/liter)	30 ppm (0.0544 mg/liter)	100 ppm (0.1815 mg/liter)	2000 ppm (3.63 mg/liter)
0 m ³ /min (0 ft ³ /min)	~0.5	~0.5	~0.5	>15	>15	>15
0.56 m ³ /min (20 ft ³ /min)	↓	↓	↓	~4.5	~3.5	~1.0
1.12 m ³ /min (40 ft ³ /min)	↓	↓	↓	~2.5	~2.0	~0.7
2.24 m ³ /min (80 ft ³ /min)	↓	↓	↓	~1.0	~1.0	~0.7

Figure Captions

Figure 1. Transfer mechanisms.

Figure 2. Typical fire history functional forms; Beta and ramp functions.

Figure 3. Temperature history of PVC.

Figure 4. Effect of heating rates and ventilation on cabin temperature vs time.

Figure 5. Effect of ventilation on average skin temperature vs time.

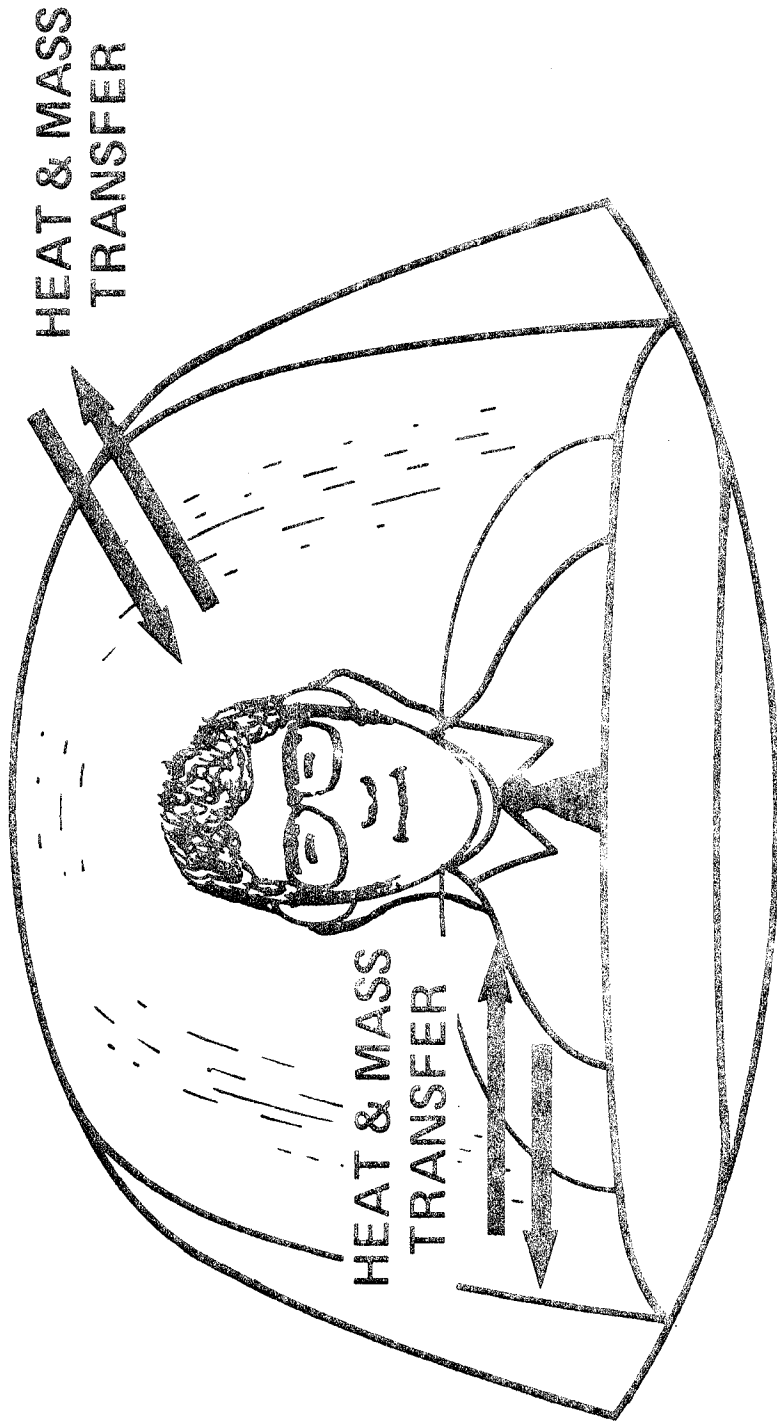
Figure 6. Effect of ventilation and stress on body enthalpy vs time.

Figure 7. Effect of ventilation rate on concentration of HCl vs time.

Figure 8. Comparison of heat rates vs time.

Figure 9. Effect of temperature and kinetics on concentration of HCl vs time
(no ventilation).

Figure 10. Effect of fire heat release rates on body enthalpy vs time
(no ventilation).



MAN & ENCLOSURE

- NATURAL CONVECTION
- FORCED CONVECTION
- EVAPORATION
- RADIATION

ENCLOSURE & ENVIRON

- NATURAL CONVECTION
- FORCED CONVECTION
- CHEMICAL REACTION

FIG. 1

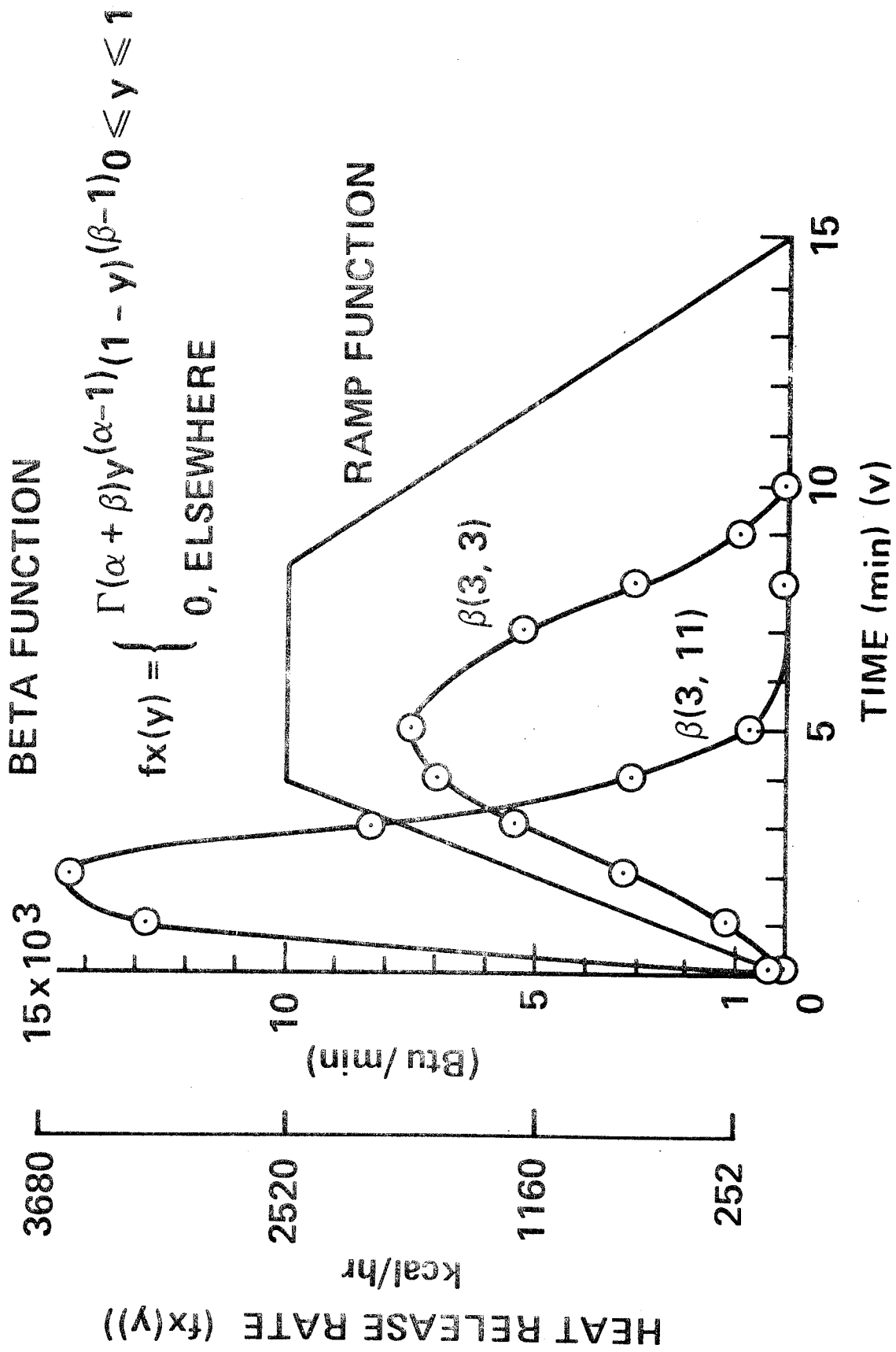


Fig. 2

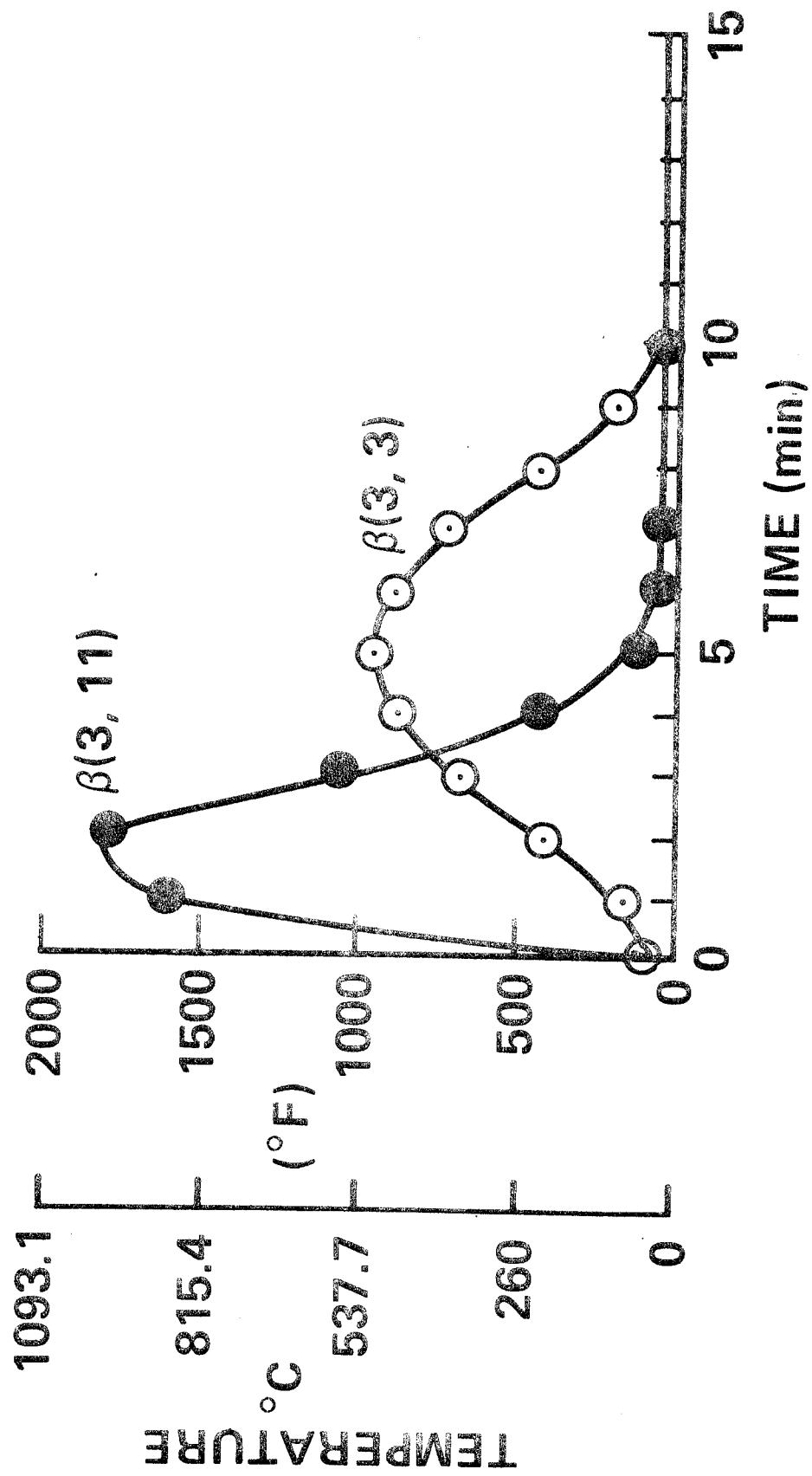


Fig. 3

METABOLIC RATE HEAT RATE VENT. RATE

	kcal/hr	(Btu/hr)	β	m^3/min	(ft^3/min)
○	75.6	(300)	(3, 11)	0	(0)
●				.56	(20)
□				1.12	(40)
△	75.6	(300)	(3, 3)	2.24	(80)
▽				0	0

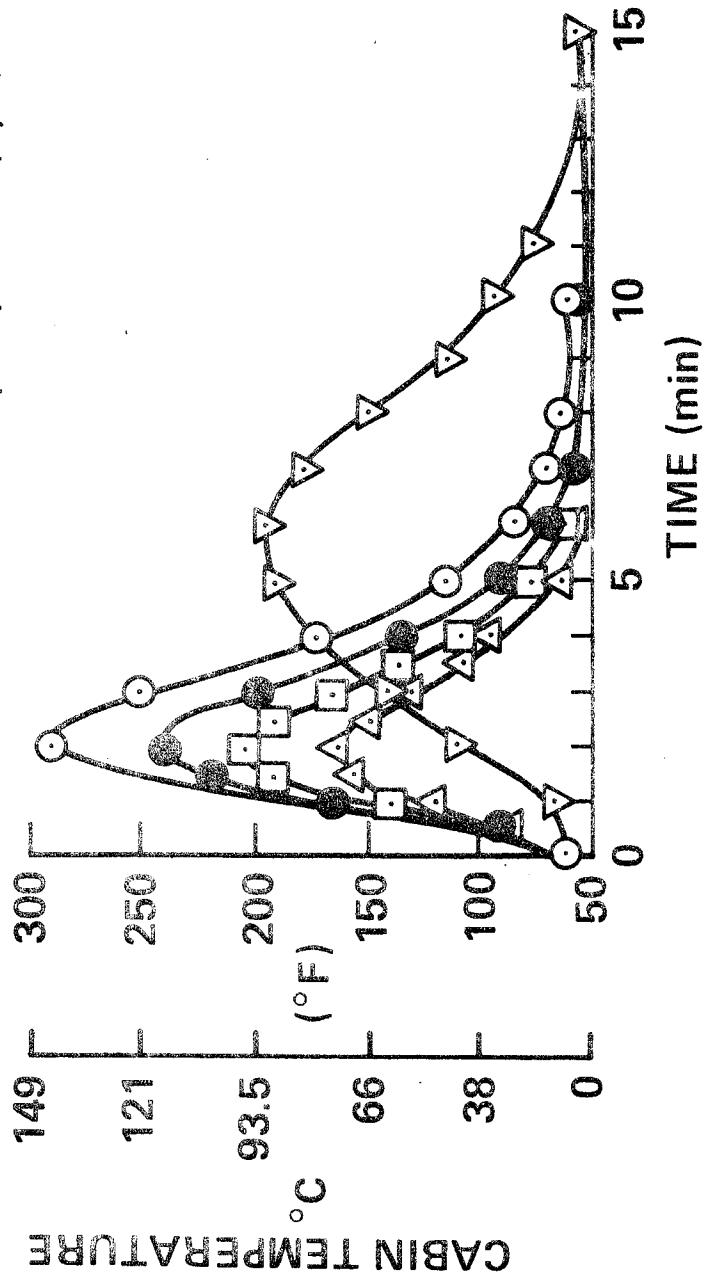


Fig. 4

TIME TO REACH 45°C (113°F)

- ~ 2 min
- ~ 3 min
- , Δ ∞

MINUTES OVER 45°C (113°F)

- ~ 3 min
- ~ 1 min
- , Δ 0

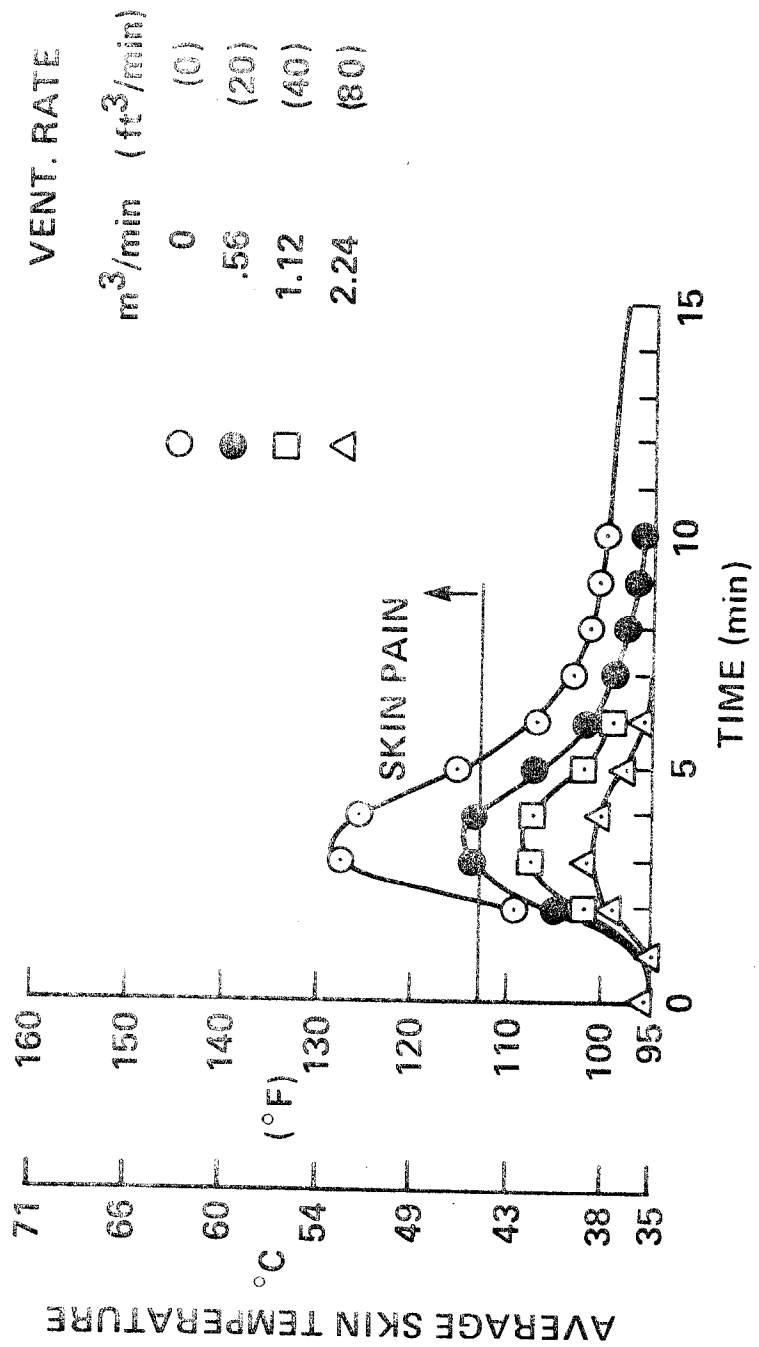


Fig. 5

METABOLIC RATE		HEAT RATE		VENT RATE	
kcal/hr (Btu/hr)		β	m^3/min	ft^3/min	
○	75.6 (300)	}	0	(0)	
●	75.6 (300)		.56	(20)	
□	75.6 (300)		1.12	(40)	
△	75.6 (300)		2.24	(80)	
▽	504 (2000)		0	(0)	
◇	504 (2000)		.56	(20)	

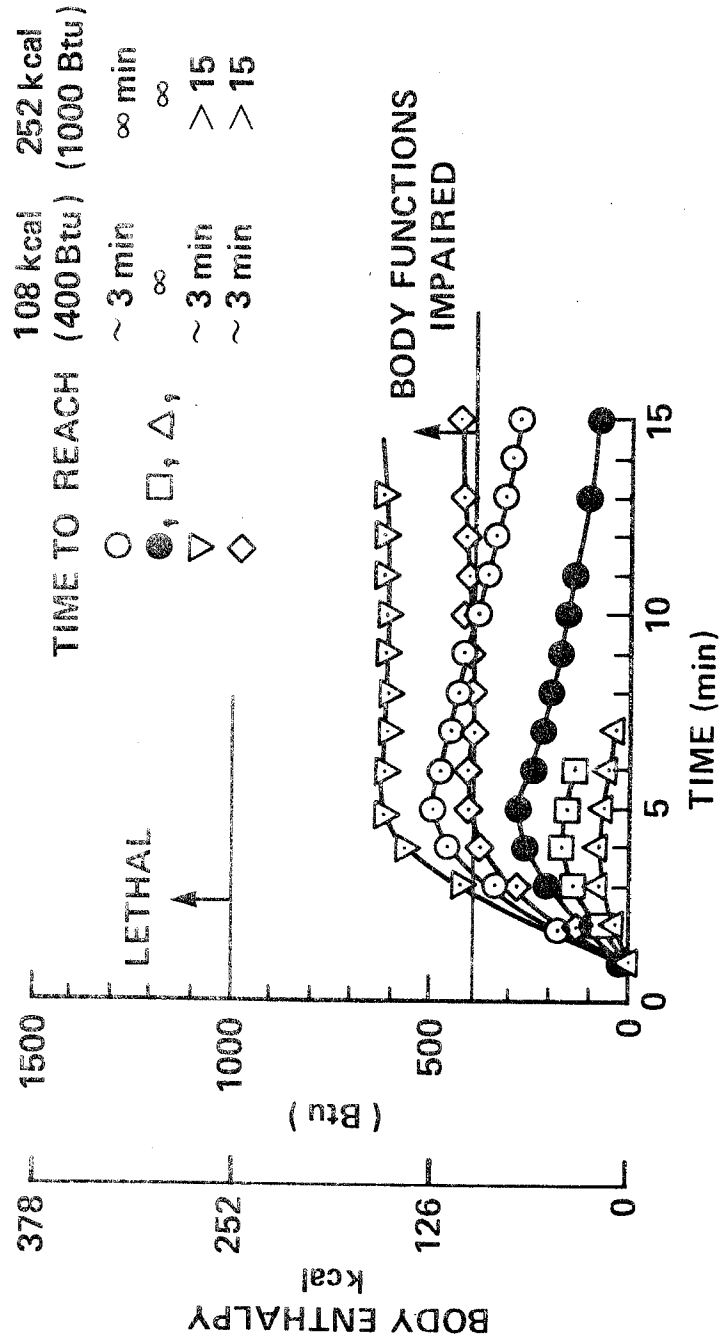


Fig. 6

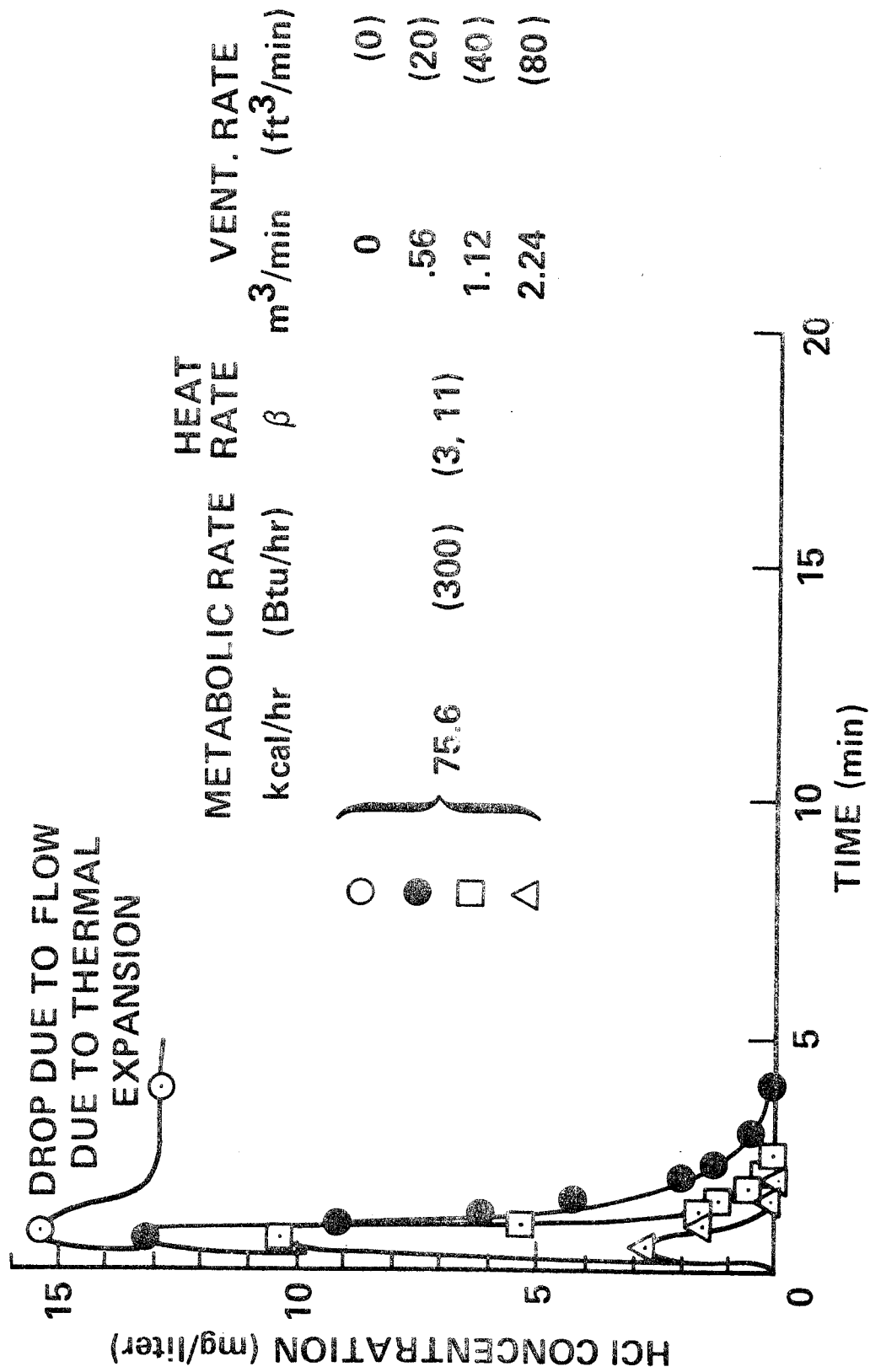


FIG. 7

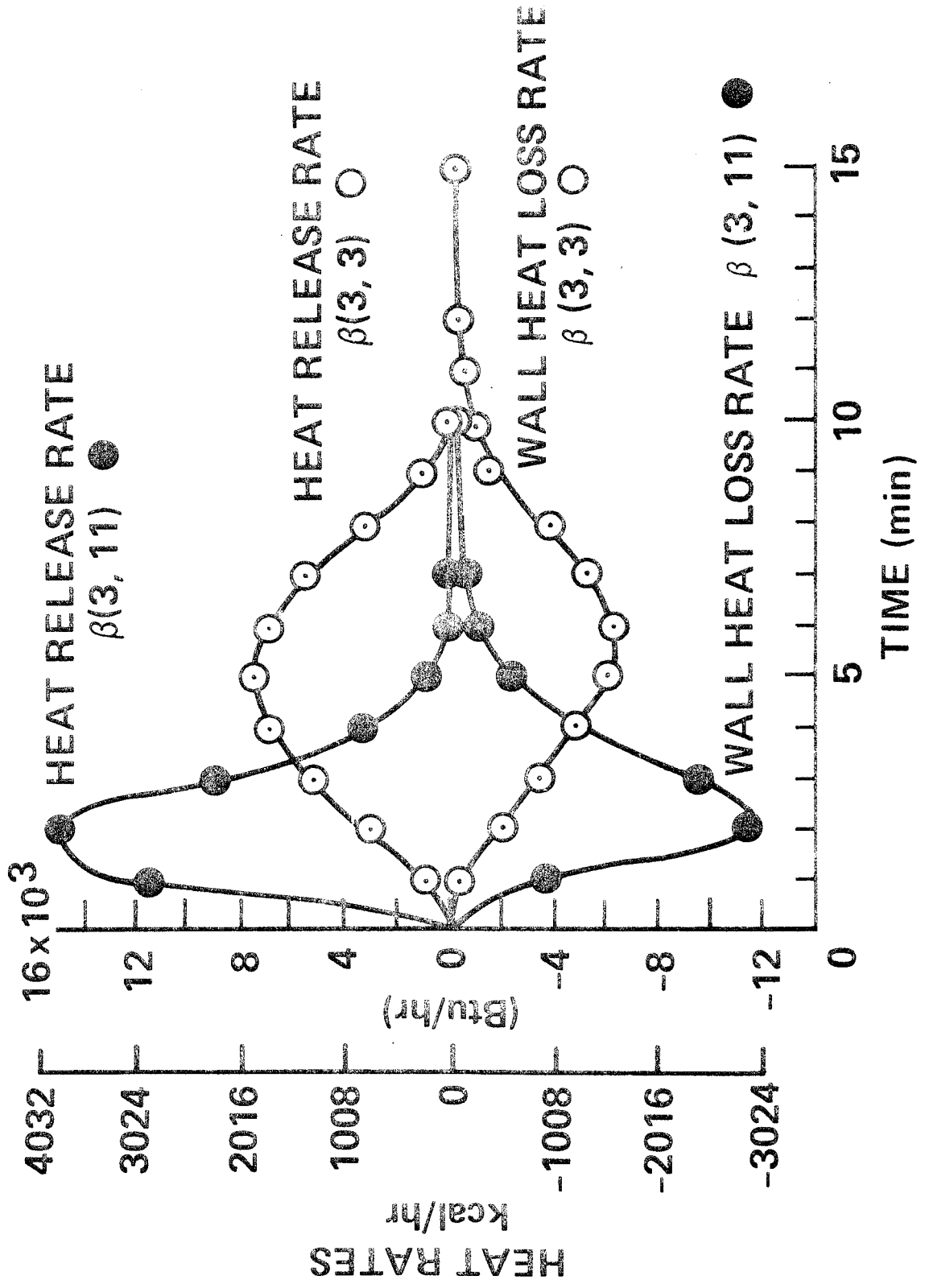


Fig. 8

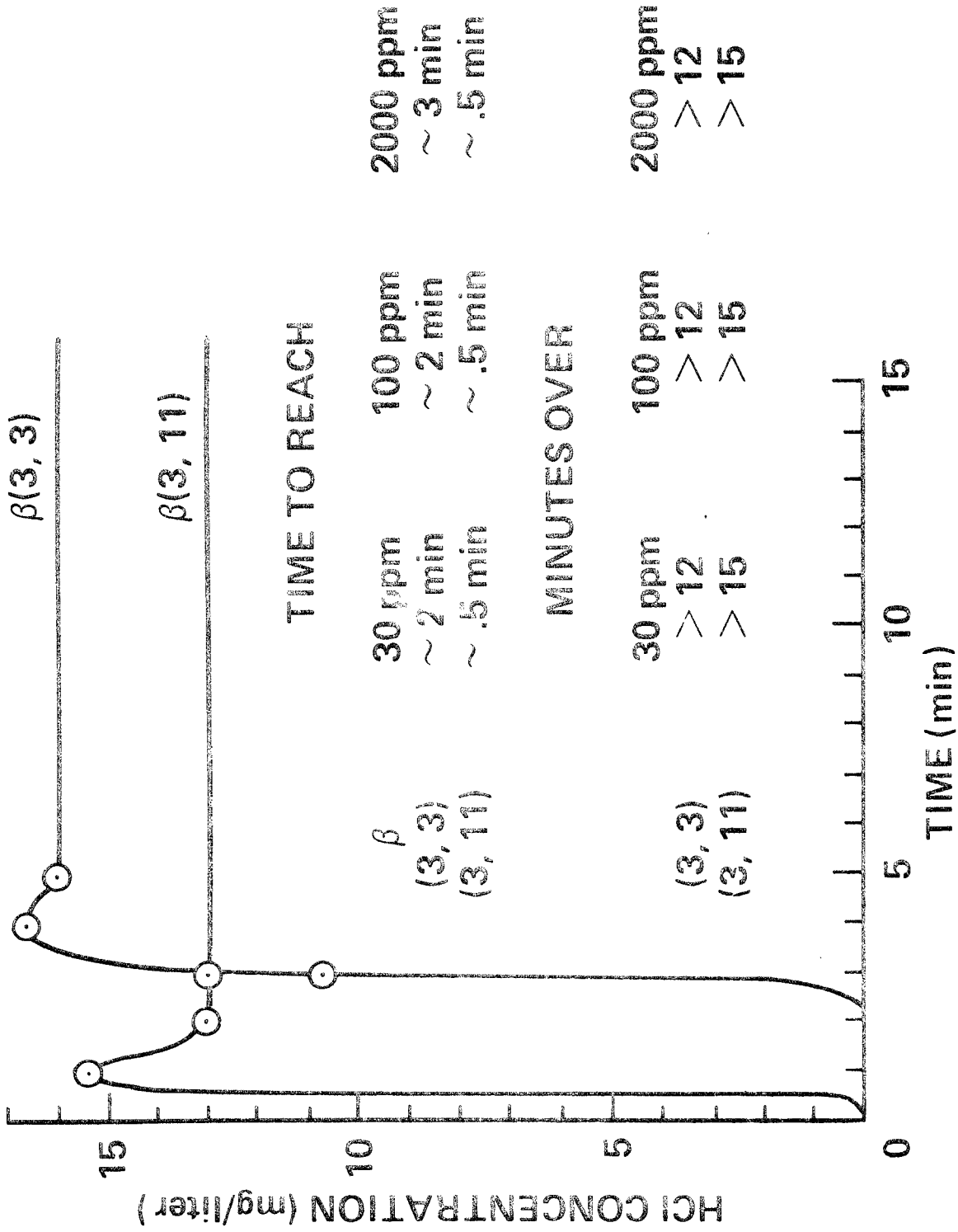


FIG. 9

TIME TO REACH 108kcal (400 Btu)

$\beta(3, 3)$ ∞

$\beta(3, 11)$ ~ 3 min

MINUTES OVER 108kcal (400 Btu)

$\beta(3, 3)$ 0

$\beta(3, 11)$ ~ 6 min

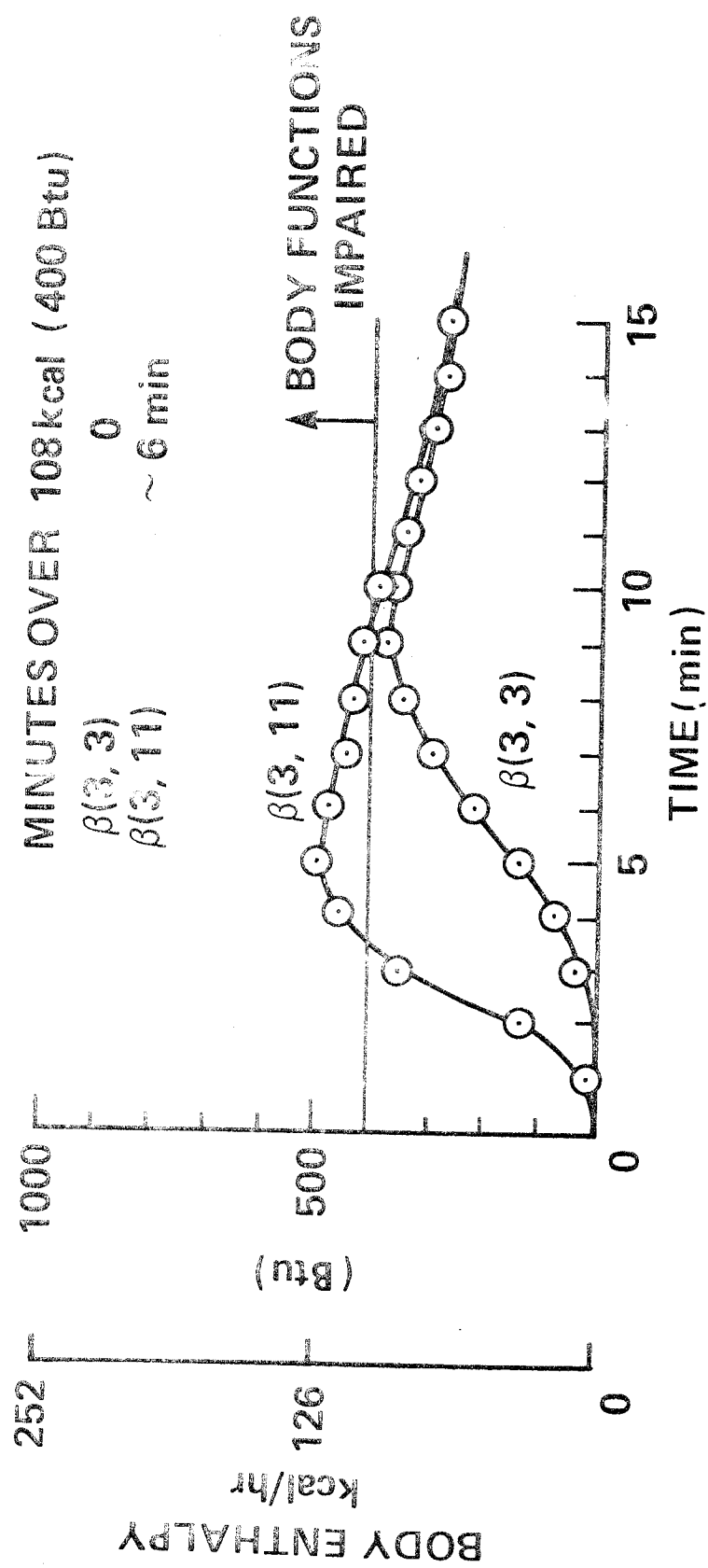


FIG. 10

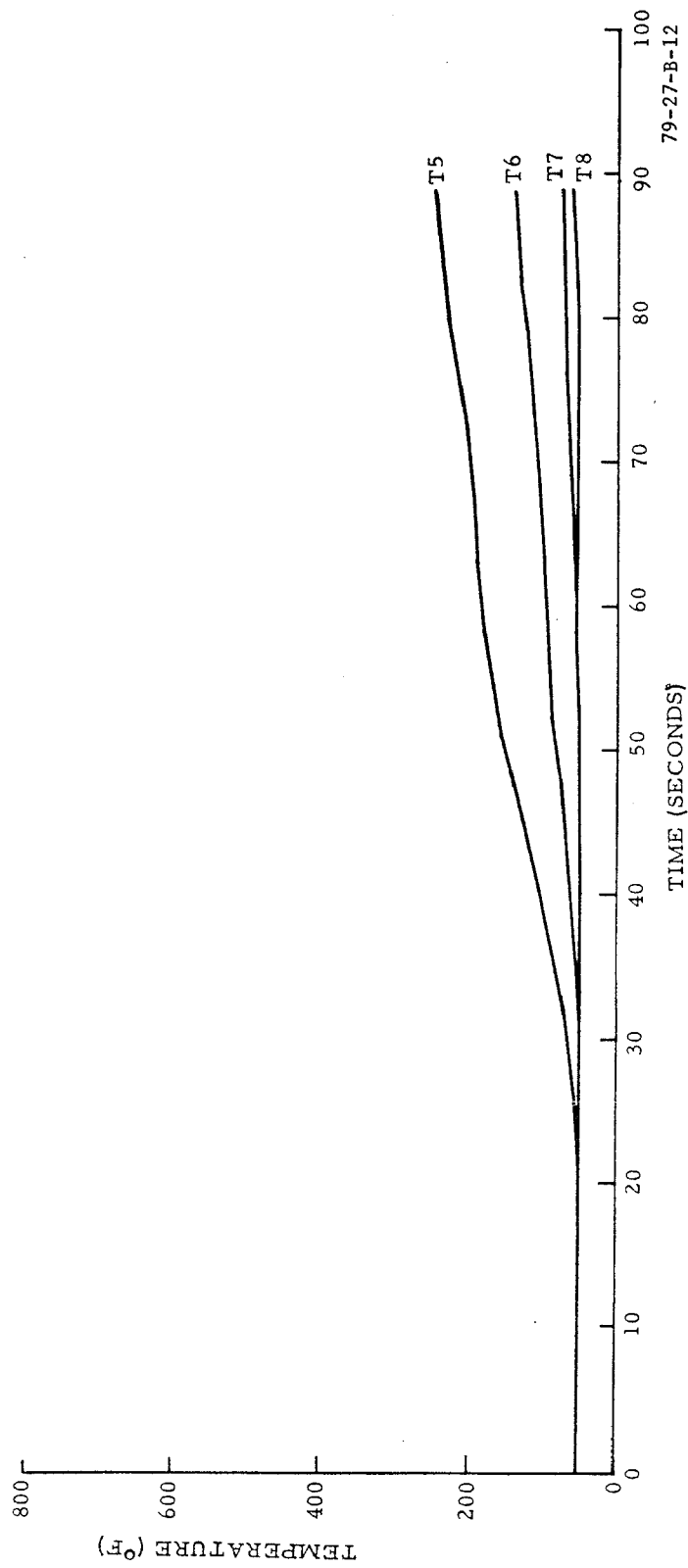


FIGURE B-12. TEST 14