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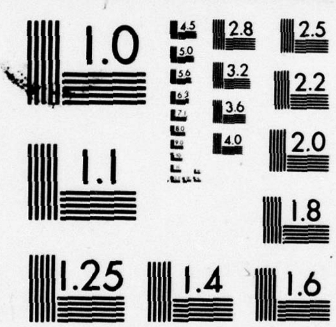


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NO. 495



A GENERAL MODEL FOR THE TRANSFER OF VAPOUR THROUGH CLOTHED SKIN FROM LIQUID ON AND IN CLOTHING (U)

by

Stanley B. Mellsen



PCN 13E01
WUD 13E19



June 1979

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# A GENERAL MODEL FOR THE TRANSFER OF VAPOUR THROUGH CLOTHED SKIN FROM LIQUID ON AND IN CLOTHING (U)

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ABSTRACT

A mathematical model which was developed by Monaghan at DRES was extended to predict the penetration of vapour through clothed skin for an initial liquid load on or in the clothing. The model and its associated computer program along with some sample calculations are described in this report.

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NOTATION

| | |
|---|---|
| $a$ | decomposition rate ($min^{-1}$) |
| $A_i$, $B_i$, $C_i$ | diffusive and absorptive coefficients for slice i |
| $C_s$ | saturated vapour concentration in air ($mg\ cm^{-3}$) |
| DELT | computer language for $\Delta t$ |
| $g$ | general boundary term introduced to account for vapour evolution in the inward direction from a vapour-liquid interface ($mg\ cm^{-2}$) |
| gf | same as g, except for vapour evolution in the outward direction ($mg\ cm^{-2}$) |
| $j$ | subscript for time increment number |
| MS | number of slices in a clothing layer |
| $m_i$ | mass per unit area in slice i ($mg\ cm^{-2}$) |
| $Q$ | total amount of surface liquid lost to vapour evolution ($mg\ cm^{-2}$) |
| $R_a$ | diffusive resistance of air ($min\ cm^{-1}$) |
| $R_i$ | diffusive resistance of slice i ($min\ cm^{-1}$) |
| $t$ | time (min) |
| $\Delta t$ | time increment size (min) |
| $U$ | total vapour loss to air ($mg\ cm^{-2}$) |
| $V_i$ | absorptive capacity of clothing or skin per unit area of slice i (cm) |

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# A GENERAL MODEL FOR THE TRANSFER OF VAPOUR THROUGH CLOTHED SKIN FROM LIQUID ON AND IN CLOTHING (U)

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## 1. INTRODUCTION

A mathematical model (Monaghan) was developed at DRES to predict the penetration of liquid or vapour through clothed skin. The essential features of the model are described as follows:

> The problem of agent penetration through clothed or bare skin is treated as a case of one-dimensional diffusion in a multilayer system where absorptive and diffusive properties may vary from one layer to another and agent may decay in the system as a result of decomposition. The flow of agent in such a system is analogous to the flow of heat through a series of slabs or the flow of current in a resistance-capacitance network when the resistance and capacitors are very numerous (Pattle and Monaghan, 1964).
>
> Experimental evidence suggests that the simplest model for the skin is a system in which two absorbent layers overlay a sink for agent, and only the layer next to the sink has a significant diffusional resistance. The two layers are broadly identifiable with the horny surface layer and the transitional layer of the epidermis and are so named in the model. The live epidermis and the dermis are ignored since both present no appreciable barrier to agent penetration and the latter is perfused by the blood which acts as the sink for agent. Similarly a clothing layer can be represented simply by a layer with a significant absorbence and diffusional resistance. Decom-

position of agent has been observed in both skin and cloth and is approximated by a first order reaction.

An electrical analogue was chosen as the basis of the model. The following table gives the analogues of electrical charge, potential, capacitance and resistance used in the model for a clothing or skin layer of thickness $\ell$, with a diffusion coefficient D, that has absorbed a mass of agent per unit volume C.

| | ANALOGUE | SYMBOL | UNITS |
|---|---|---|---|
| CHARGE | Mass absorbed per unit area = $C\ell$ | m | $mg/cm^2$ |
| POTENTIAL | Equilibrium concentration, vapour in air, $C_e = C/\beta$ | $C_e$ | $mg/cm^3$ |
| CAPACITANCE | Absorptive capacity per unit area = $\beta\ell = m/C_e$ | V | cm |
| RESISTANCE | Diffusional Resistance = $\ell/D\beta = \ell^2/DV$ | R | min/cm |

The coefficient $\beta$ and the capacitance V are assumed constant for a given agent and layer, but may vary from layer to layer. This assumption implies that V is independent of concentration.

The problem of agent penetration through skin is solved by deriving equations of flow from an analogous electric R-C network, in which each layer is divided into a sufficient number of uniform slices normal to the flow of agent to provide the required accuracy of solution. The equations of flow form a set of first order differential equations for each case considered and are solved numerically by means of a digital computer.

The computer program (McPherson) was written to calculate an approximate solution to the differential equations and to set up the initial and boundary conditions of the simulations.

In this program the model is subdivided into five submodels, two of which simulate cases where:

a) liquid is deposited on the top of the outside layer of clothing on a clothed person; and

b) liquid is pressed through the clothing.

In the first of these submodels, the initial liquid loading is specified, and in the second, the initial liquid loading in the cloth is specified, but both loadings cannot be specified at once. Also, the second submodel and its corresponding computer program did not produce reasonable results.

The objective of this paper is to describe an improved model which can handle the generalized initial condition of liquid on and in cloth.

## 2. FEATURES OF THE MODEL

The penetration model was developed in order to better understand the hazards to people posed by toxic chemicals in the liquid phase. In other words, this study deals with an attempt to describe mathematically the physical processes occurring, with time, when liquid droplets impact on the clothing of a person, or when liquid is forced into the clothing by applying pressure, e.g. by sitting. The passage of the contaminant through clothing and skin to the blood stream is a time dependent diffusion process.

In addition to the above, two other provisions are part of the model. If the challenge is to a clothing ensemble, then provision is made for the removal of this contaminated clothing at some point in time. This is accomplished by zeroing the mass that exists in each of the clothing layers at that time. Similarly, the model will simulate the decontamination of the outer clothing surface by zeroing the surface contaminant.

In its present form, the model can handle up to four layers of clothing over skin. Each layer of clothing is assumed to be homogeneous. The skin is divided into three distinct regimes, the horny surface layer, the transitional layer of the epidermis, and the blood stream (a sink).

## 3. CALCULATION OF VAPOUR PENETRATION

### a) Basic Mathematical Relationships

Penetration is described by a one-dimensional diffusion equation in a multi-layer system, i.e. clothing and skin, where absorptive and diffusion properties may vary from one layer to another and mass absorbed may decay with time in the system as a result of decomposition.

Each layer of the system is divided into several slices, the number of which is chosen to provide adequate computing accuracy.

A general expression for flow of agent vapour into a slice can be obtained by applying Kirchoff's law at a node in the analogous resistance capacitance network (Fig. 1). Note that Kirchoff's law states that at any junction in the circuit the total current flowing toward the junction must equal the total current flowing away. Considering flow into slice i we obtain:

$$\frac{dm_i}{dt} = \left(\frac{m_{i-1}}{V_{i-1}} - \frac{m_i}{V_i}\right)\frac{2}{R_{i-1}+R_i} + \left(\frac{m_{i+1}}{V_{i+1}} - \frac{m_i}{V_i}\right)\frac{2}{R_i+R_{i+1}} - am_i \qquad \text{(Eq. 1)}$$

where

$m_i$ is the mass per unit area in slice i (mg $cm^{-2}$)

$R_i$ is the diffusive resistance of slice i (min $cm^{-1}$)

$V_i$ is the absorptive capacity per unit area of slice i (cm)

a is the decomposition rate ($min^{-1}$)

A simple implicit difference method was used to solve the diffusion equation (Eq. 1). If we denote the mass per unit area of skin slice i at time $j\Delta t$ by $m_{i,j}$, and $m_{i,j+1}$ at the next increment of time, then Eq. 1 can be written in the following discretized form:

$$m_{i,j} = m_{i,j+1} - \left(\frac{m_{i-1,j+1}}{V_{i-1}} - \frac{m_{i,j+1}}{V_i}\right)\frac{2\Delta t}{R_{i-1}+R_i} - \left(\frac{m_{i+1,j+1}}{V_{i+1}} - \frac{m_{i,j+1}}{V_i}\right)\frac{2\Delta t}{R_i+R_{i+1}} + am_{i,j+1}\Delta t \qquad \text{(Eq. 2)}$$

Now let $A_i = \dfrac{-2\Delta t}{V_i(R_i + R_{i+1})}$ (Eq. 3)

$$B_i = 1 + \left[\frac{1}{V_i}\left(\frac{2}{R_{i-1} + R_i} + \frac{2}{R_i + R_{i+1}}\right) + a\right]\Delta t \qquad \text{(Eq. 4)}$$

$$C_i = \frac{-2\Delta t}{V_i(R_{i-1} + R_i)} \qquad \text{(Eq. 5)}$$

Then Eq. 2 can be written:

$$A_{i-1}m_{i-1,j+1} + B_i m_{i,j+1} + C_{i+1}m_{i+1,j+1} = m_{i,j} \qquad \text{(Eq. 6)}$$

Now the general expression for vapour diffusion in a skin-clothing system with n slices is given in the following matrix form:

$$\begin{bmatrix} B_1 & C_2 & 0 & \cdots & \cdots & \cdots & 0 \\ A_1 & B_2 & C_3 & 0 & \cdots & \cdots & \cdots \\ 0 & A_2 & B_3 & C_4 & 0 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & A_n & B_{n-1} & & C_n \\ 0 & \cdots & \cdots & 0 & A_{n-1} & & B_n \end{bmatrix} \begin{bmatrix} m_{1,j+1} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ m_{n,j+1} \end{bmatrix} = \begin{bmatrix} m_{i,j} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ m_{n,j} \end{bmatrix} \quad \text{(Eq. 7)}$$

b) Boundary and Initial Conditions

While the basic mathematics of the model appears quite simple, the elegance of it is attained through the control of the various boundary and initial conditions.

The initial conditions consist of the liquid loading on the outer clothing surface, and the magnitude and distribution of the liquid loading within each layer of clothing. The model does not allow gaps in the liquid loading. All the liquid loads must be contiguous.

Special conditions occur at the inside and outside boundaries of the clothed skin system and at liquid-vapour interfaces (Fig. 2). These are accounted for by modifying the corresponding equations in the general expression (Eq. 7) as follows:

(1) First equation in the system

The first slice in the clothed skin system represents the systemic sink, the potential and resistance of which are zero. Applying Kirchoff's law for flow into the slice gives:

$$\frac{dm_1}{dt} = \frac{2m_2}{V_2 R_2} \quad \text{(Eq. 8)}$$

Discretizing Eq. 8 in the same way as for Eq. 1 gives:

$$m_{1,j+1} + C_2 m_{2,j+1} = m_{1,j} \quad \text{(Eq. 9)}$$

Comparison to the general expression given by Eq. 4 and Eq. 6 then gives:

$$B_1 m_{1,j+1} + C_2 m_{2,j+1} = m_{ij} + gF \qquad \text{(Eq. 10)}$$

where $B_1 = 1$

gF is a general boundary term which was introduced to account for vapour evolution in the outward direction from a liquid-vapour interface. In Eq. 10, gF = 0.

(2) Inside of skin

The first inside slice of skin is represented by the second equation in the system. Noting that the resistance of the first slice is zero since it represents the systemic sink, application of Kirchoff's law for flow into the second slice gives:

$$\frac{dm_2}{dt} = -\frac{2m_2}{V_2 R_2} + \left(\frac{m_3}{V_3} - \frac{m_2}{V_2}\right)\frac{2}{R_2+R_3} + am_2 \qquad \text{(Eq. 11)}$$

Then discretizing as for Eq. 1 gives:

$$B_2 m_{2,j+1} + C_3 m_{3,j+1} = m_{2,j} \qquad \text{(Eq. 12)}$$

Comparison to the general expression given by Eq. 6 then shows $A_1 = 0$.

(3) Inside liquid-vapour interface

The last inside slice without liquid is designated i = nk (Fig. 2). The potential for flow from the adjacent liquid containing slice is given by the saturated vapour concentration, $C_s$. Application of Kirchoff's law for flow into slice nk gives:

$$\frac{dm_{nk}}{dt} = \left(\frac{m_{nk-1}}{V_{nk-1}} - \frac{m_{nk}}{V_{nk}}\right)\frac{2}{R_{nk-1}+R_{nk}} + \left(C_s - \frac{m_{nk}}{V_{nk}}\right)\frac{2}{R_{nk}} - am_{nk} \qquad \text{(Eq. 13)}$$

Discretizing as for Eq. 1 gives:

$$A_{nk-1} m_{nk-1,j+1} + B_{nk} m_{nk,j+1} = m_{nk} + g \qquad \text{(Eq. 14)}$$

where g is a general boundary term which was introduced to account for vapour evolution in the inward direction from a liquid-vapour interface. In Eq. 14, $g = \frac{2C_s\Delta t}{R_{nk}}$ (Eq. 15)

Comparison to the general expression given by Eq. 6 gives:

$$B_{nk} = 1 + \left[\frac{1}{V_{nk}}\left(\frac{2}{R_{nk-1}+R_{nk}} + \frac{2}{R_{nk}}\right) + a\right]\Delta t \quad \text{(Eq. 16)}$$

For the special case of liquid in the clothing slice adjacent to the skin, Eq. 15 and Eq. 16 show that g and $B_{nk}$ become infinite because the outer skin slice has no resistance. This is not a reasonable physical representation. To adjust this, the assumption was made that, over a finite time interval, the clothing dries from the inside so that there is a non-zero resistance to vapour transport. This resistance was assumed to increase from 0 to $R_{nk+1}$ with time as the clothing dries. Then the average value of the resistance was used in the discretization, so that for the outer skin slice Eq. 15 and Eq. 16 become:

$$g = \frac{2C_s\Delta t}{R_{nk+1}} \quad \text{(Eq. 17)}$$

and $$B_{nk} = 1 + \left[\frac{1}{V_{nk}}\left(\frac{2}{R_{nk-1}} + \frac{2}{R_{nk+1}}\right) + a\right]\Delta t \quad \text{(Eq. 18)}$$

(4) <u>Outside liquid-vapour interface within clothing</u>

The first outside slice without liquid is designated $i = n\ell$ (Fig. 2). As for the previously mentioned interface, the potential for vapour transport from the adjacent slice containing liquid is the saturated vapour concentration, $C_s$. Application of Kirchoff's law for flow into slice $n\ell$ gives:

$$\frac{dm_{n\ell}}{dt} = \left(C_s - \frac{m_{n\ell}}{V_{n\ell}}\right)\frac{2}{R_{n\ell}} + \left(\frac{m_{n\ell+1}}{V_{n\ell+1}} - \frac{m_{n\ell}}{V_{n\ell}}\right)\frac{2}{R_{n\ell}+R_{n\ell+1}} - am_{n\ell} \quad \text{(Eq. 19)}$$

Discretizing as for Eq. 1 gives:

$$B m_{n\ell,j+1} + C_{n\ell+1} m_{n\ell+1,j+1} = m_{n\ell,j} + gF \qquad \text{(Eq. 20)}$$

where $$gF = \frac{2C_s \Delta t}{R_{n\ell}} \qquad \text{(Eq. 21)}$$

Comparison to the general case by referring to Eq. 4 and Eq. 6 shows that the value B is given by:

$$B_{n\ell} = 1 + \left[ \frac{1}{V_{n\ell}} \left( \frac{2}{R_{n\ell}} + \frac{2}{R_{n\ell}+R_{n\ell+1}} \right) a \right] \Delta t \qquad \text{(Eq. 22)}$$

(5) Outside clothing slice

The outside clothing slice is designated by i = nn (Fig. 2). The vapour transport equation for this slice is the last in the system of n equations. Liquid may or may not be present on the surface. This must be accounted for in the equations for this slice. Also, there is the special case of only one slice without liquid, which must be treated separately.

(5a) Two or more slices without liquid

1. Liquid on the surface. Application of Kirchoff's law for flow into slice nn gives:

$$\frac{dm_{nn}}{dt} = \left( \frac{m_{nn-1}}{V_{nn-1}} - \frac{m_{nn}}{V_{nn}} \right) \frac{2}{R_{nn-1}+R_{nn}} + \left( C_s - \frac{m_{nn}}{V_{nn}} \right) \frac{2}{R_{nn}} - am_{nn} \qquad \text{(Eq. 23)}$$

Discretizing as for Eq. 1 gives:

$$A_{nn-1} m_{nn-1,j+1} + B_{nn} m_{nn,j+1} = m_{nn,j} + g \qquad \text{(Eq. 24)}$$

where $$g = \frac{2C_s \Delta t}{R_{nn}} \qquad \text{(Eq. 25)}$$

Comparison to Eq. 4 and Eq. 6 gives the modified value of B as follows:

$$B_{nn} = 1 + \left[ \frac{1}{V_{nn}} \left( \frac{2}{R_{nn-1}+R_{nn}} + \frac{2}{R_{nn}} \right) + a \right] \Delta t \qquad \text{(Eq. 26)}$$

2. No liquid on the surface. In Eq. 23 there is zero potential in place of $C_s$ and resistance for flow rate into the slice from the outside is changed from $\frac{R_{nn}}{2}$ to $\frac{R_{nn}}{2} + R_a$ where $R_a$ is the diffusive resistance of air.

Then g = 0 (Eq. 27)

$$\text{and } B_{nn} = 1 + \left[\frac{1}{V_{nn}}\left(\frac{2}{R_{nn-1}+R_{nn}} + \frac{2}{R_{nn}+2R_a}\right) + a\right]\Delta t \qquad \text{(Eq. 28)}$$

(5b) Special case when only one outside slice does not contain liquid

Application of Kirchoff's law for flow of vapour into slice nn gives the following equation:

$$\frac{dm_{nn}}{dt} = \left(C_s - \frac{m_{nn}}{V_{nn}}\right)\frac{2}{R_{nn}} + \left(0 - \frac{m_{nn}}{V_{nn}}\right)\frac{2}{R_n+2R_{a2}} - am_{nn} \qquad \text{(Eq. 29)}$$

Discretizing as for Eq. 1 gives:

$$B_{nn}m_{nn,j+1} = m_{nn,j} + gF + g \qquad \text{(Eq. 30)}$$

where g = 0 (Eq. 31)

$$\text{and } gF = \frac{2c_s\Delta t}{R_{nn}} \qquad \text{(Eq. 32)}$$

Comparison to Eq. 4 and Eq. 6 gives:

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}}\left(\frac{2}{R_{nn}} + \frac{2}{R_{nn}+2R_a}\right) + a\right]\Delta t \qquad \text{(Eq. 33)}$$

c) Complete System of Equations in Matrix Form

The equations of vapour transport can now be written in the form of Eq. 7 with all the modifications to account for the various boundary conditions.

Considering boundary conditions (1) to (3) the equations of vapour transport in the inside slices are written as follows:

$$\begin{bmatrix} B_1 & C_2 & 0 & .. & .. & 0 \\ A_1 & B_2 & C_3 & 0 & .. & .. \\ 0 & A_2 & B_3 & C_4 & 0 & .. \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & .. \\ .. & 0 & A_{nk-1} & B_{nk-1} & C_{nk} & \\ 0 & .. & .. & 0 & A_{nk-1} & B_{nk} \end{bmatrix} \begin{bmatrix} m_{1,j+1} \\ .. \\ .. \\ .. \\ .. \\ .. \\ m_{nk,j+1} \end{bmatrix} = \begin{bmatrix} m_{1,j} \\ .. \\ .. \\ .. \\ .. \\ .. \\ m_{nk,j} \end{bmatrix} + \begin{bmatrix} gF \\ 0 \\ .. \\ .. \\ .. \\ 0 \\ g \end{bmatrix} \qquad \text{(Eq. 34)}$$

where $A_1 = 0$ (Eq. 35)

$B_1 = 1$ (Eq. 36)

$gF = 0$ (Eq. 37)

$$g = \frac{2C_s \Delta t}{R_{nk}} \qquad \text{(Eq. 38)}$$

$$B_{nk} = 1 + \left[\frac{1}{V_{nk}}\left(\frac{2}{R_{nk-1}+R_{nk}} + \frac{2}{R_{nk}}\right) + a\right]\Delta t \qquad \text{(Eq. 39)}$$

except when the slice adjacent to the skin contains liquid. Then:

$$g = \frac{2C_s \Delta t}{R_{nk+1}} \qquad \text{(Eq. 40)}$$

and $$B_{nk} = 1 + \left[\frac{1}{V_{nk}}\left(\frac{2}{R_{nk-1}} + \frac{2}{R_{nk+1}}\right) + a\right]\Delta t \qquad \text{(Eq. 41)}$$

which is identical to Eq. 4 because $R_{nk} = 0$.

Considering boundary equations (4) and (5) the matrix system for vapour transport in the outside slices is written as follows:

$$\begin{bmatrix} B_{n\ell} & C_{n\ell+1} & 0 & & 0 \\ A_{n\ell} & B_{n\ell+1} & C_{n\ell+2} & 0 & \\ 0 & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \\ .. & 0 & A_{nn-1} & B_{nn-1} & C_{nn} \\ 0 & .. & 0 & A_{nn-1} & B_{nn} \end{bmatrix} \begin{bmatrix} m_{n\ell,j+1} \\ .. \\ .. \\ .. \\ .. \\ .. \\ m_{nn,j+1} \end{bmatrix} = \begin{bmatrix} m_{n\ell,j} \\ .. \\ .. \\ .. \\ .. \\ .. \\ m_{n\ell,j} \end{bmatrix} + \begin{bmatrix} gF \\ 0 \\ .. \\ .. \\ .. \\ 0 \\ g \end{bmatrix} \qquad \text{(Eq. 42)}$$

where $$gF = \frac{2C_s \Delta t}{R_{n\ell}} \qquad \text{(Eq. 43)}$$

$$B_{n\ell} = 1 + \left[ \frac{1}{V_{n\ell}} \left( \frac{2}{R_{n\ell}} + \frac{2}{R_{n\ell} + R_{n\ell+1}} + \right) a \right] \Delta t \qquad \text{(Eq. 44)}$$

1) Liquid on Surface

$$g = \frac{2C_s \Delta t}{R_{nn}} \qquad \text{(Eq. 45)}$$

$$B_{nn} = 1 + \left[ \frac{1}{V_{nn}} \left( \frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn}} \right) + a \right] \Delta t \qquad \text{(Eq. 46)}$$

2) No Liquid on Surface

$$g = 0 \qquad \text{(Eq. 47)}$$

$$B_{nn} = 1 + \left[ \frac{1}{V_{nn}} \left( \frac{2}{R_{nn-1} + R_{nn}} + \frac{2}{R_{nn} + 2R_a} \right) + a \right] \Delta t \qquad \text{(Eq. 48)}$$

When there is only one outside slice which does not contain liquid the matrix system of Eq. 42 reduces to a single equation as follows:

$$B_{nn} m_{nn,j+1} = m_{nn,j} + gF + g \qquad \text{(Eq. 49)}$$

where $$gF = \frac{2C_s \Delta t}{R_{nn}} \qquad \text{(Eq. 50)}$$

and $$g = 0 \qquad \text{(Eq. 51)}$$

$$B_{nn} = 1 + \left[ \frac{1}{V_{nn}} \left( \frac{2}{R_{nn}} + \frac{2}{R_{nn} + 2R_{a2}} \right) + a \right] \Delta t \qquad \text{(Eq. 52)}$$

When there is no liquid at all in the clothing, the equations for vapour transport can be expressed by one matrix system as follows:

$$\begin{bmatrix} B_1 & C_2 & 0 & .. & .. & 0 \\ A_1 & B_2 & C_3 & 0 & .. & .. \\ 0 & A_2 & B_3 & B_4 & 0 & .. \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & A_{nn-1} & B_{nn-1} & C_{nn} \\ 0 & .. & .. & 0 & A_{nn-1} & B_{nn} \end{bmatrix} \begin{bmatrix} m_{1,j+1} \\ .. \\ .. \\ .. \\ .. \\ .. \\ m_{nn,j+1} \end{bmatrix} = \begin{bmatrix} m_{1,j} \\ .. \\ .. \\ .. \\ .. \\ .. \\ m_{nn,j} \end{bmatrix} + \begin{bmatrix} gF \\ 0 \\ .. \\ .. \\ .. \\ 0 \\ g \end{bmatrix} \qquad \text{(Eq. 53)}$$

where

$$A_1 = 0 \qquad \text{(Eq. 54)}$$

$$B_1 = 0 \qquad \text{(Eq. 55)}$$

$$gF = 0 \qquad \text{(Eq. 56)}$$

1) Liquid on Surface

$$g = \frac{2C_s \Delta t}{R_{nn}} \qquad \text{(Eq. 57)}$$

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}}\left(\frac{2}{R_{nn-1}+R_{nn}} + \frac{2}{R_{nn}}\right) + a\right]\Delta t \qquad \text{(Eq. 58)}$$

2) No Liquid on Surface

$$g = 0 \qquad \text{(Eq. 59)}$$

$$B_{nn} = 1 + \left[\frac{1}{V_{nn}}\left(\frac{2}{R_{nn-1}+R_{nn}} + \frac{2}{R_{nn}+2R_a}\right) + a\right]\Delta t \qquad \text{(Eq. 60)}$$

All three matrices given by Eq. 34, Eq. 42 and Eq. 53 are of the same form and can be written in matrix notation as follows:

$$\tilde{A}\,\vec{M}_{j+1} = \vec{M}_j + \vec{G} \qquad \text{(Eq. 61)}$$

where

$\vec{M}_j$ is the mass of vapour per unit area in each slice of the system at a given point in time $j\Delta t$

$\vec{M}_{j+1}$ is the vector of mass per unit area after the next time increment

$\tilde{A}$ is the tridiagonal matrix of coefficients of the absorptive and diffusive properties of the system

$\vec{G}$ is the vector of boundary conditions

For a given set of initial conditions, the solution to the problem, which can readily be obtained by the Gauss elimination method (Westlake), is then:

$$\vec{M}_{j+1} = \tilde{A}^{-1} (\vec{M}_j + \vec{G}) \quad \text{(Eq. 62)}$$

for the two matrices given by Eq. 34 and Eq. 42 when the clothing contains liquid and for the matrix of Eq. 53 when the clothing contains only vapour, except when only one outside slice does not contain liquid. Then the solution for this slice is:

$$m_{nn,j+1} = \frac{m_{nn,j} + gF}{B_{nn}} \quad \text{(Eq. 63)}$$

## 4. AUXILIARY RELATIONSHIPS

### a) Loss of Liquid

As vapour is transported away from liquid-vapour interfaces, the amount of liquid in the liquid containing slice must be reduced to balance it. In addition, there is a loss due to decomposition, which also occurs in internal slices within the clothing layers containing liquid. The liquid initially on the clothing surface is gradually lost due to evaporation to the air, and when the slice of clothing next to the surface contains no liquid, there is an additional loss due to vapour transport into the clothing.

The liquid losses were accounted for in each time step along with the vapour transport, previously described, as follows.

#### (1) First inside slice containing liquid

The first inside slice containing liquid is designated nk + 1 (Fig. 2). The loss of liquid from this slice was determined using the electrical analogy (Fig. 1) for vapour transport. Application of Kirchoff's law for flow into slice nk + 1 gives:

$$\frac{dm_{nk+1}}{dt} = \left(\frac{m_{nk}}{V_{nk}} - C_s\right)\frac{2}{R_{nk}} - aC_sV_{nk+1} \qquad \text{(Eq. 64)}$$

Discretizing for time step $j\Delta t$ to $(j+1)\Delta t$ then gives:

$$m_{nk+1,j+1} = m_{nk+1,j} + \frac{2m_{nk,j}\Delta t}{V_{nk}R_{nk}} - \frac{2C_s\Delta t}{R_{nk}} - aC_sV_{nk+1}\Delta t \qquad \text{(Eq. 65)}$$

There is a special case when the first inside slice containing liquid is adjacent to the skin. The value of $R_{nk}$ is zero for the outer skin slice, which gives rise to terms of infinite value in Eq. 65. This was adjusted in the same manner as for vapour transport, described in section 3.b)(3). Thus, for slice nk+1, (Eq. 65) is replaced by the following equation:

$$m_{nk+1,j+1} = m_{nk+1,j} + \frac{2m_{nk,j}\Delta t}{V_{nk}R_{nk+1}} - \frac{2C_s\Delta t}{R_{nk+1}} - aC_sV_{nk+1}\Delta t \qquad \text{(Eq. 66)}$$

(2) First outside slice containing liquid

The first outside slice containing liquid is designated $n\ell-1$ (Fig. 2). Application of Kirchoff's law for flow into this slice gives:

$$\frac{dm_{n\ell-1}}{dt} = \left(\frac{m_{n\ell}}{V_{n\ell}} - C_s\right)\frac{2}{R_{n\ell}} - aC_sV_{nk+1} \qquad \text{(Eq. 67)}$$

Discretizing for time step $j\Delta t$ to $(j+1)\Delta t$ then gives:

$$m_{n\ell-1,j+1} = m_{n\ell-1,j} + \frac{2m_{n\ell,j}\Delta t}{V_{n\ell}R_{n\ell}} - \frac{2C_s\Delta t}{R_{n\ell}} - aC_sV_{n\ell-1}\Delta t \qquad \text{(Eq. 68)}$$

There is also a special case for the first outside slice containing liquid. This occurs at the outside slice of clothing, which is designated i = nn (Fig. 2). When there is no liquid on the surface Kirchoff's law for flow into slice nn gives:

$$\frac{dm_{nn}}{dt} = -\frac{C_s\Delta t}{R_a} - aC_sV_{nn}\Delta t \qquad \text{(Eq. 69)}$$

Discretizing gives:

$$m_{nn,j+1} = m_{nn,j} - \frac{C_s \Delta t}{R_a} - aC_s V_{nn} \Delta t \quad \text{(Eq. 70)}$$

When there is liquid on the surface, Eq. 70 reduces to:

$$m_{nn,j+1} = m_{nn,j} - aC_s V_{nn} \Delta t \quad \text{(Eq. 71)}$$

(3) Middle slices

The middle slices in the clothing are designated i, where nk + 1 < i < nℓ - 1 (Fig. 2). Since the reduction of liquid in these slices is by decomposition only, Kirchoff's law for flow into one of these is:

$$\frac{dm_i}{dt} = - aC_s V_i \qquad nk + 1 < i < n\ell - 1 \quad \text{(Eq. 72)}$$

Discretizing gives:

$$m_{i,j+1} + m_{i,j} - aC_s V_i \qquad nk + 1 < i < n\ell - 1 \quad \text{(Eq. 73)}$$

Note that the rate of loss by decomposition throughout the model is assumed to be $aC_s V_i$ whenever $m_i/V_i \geq C_s$. Also note that $C_s$ is only used as a potential whenever $m_i/V_i \geq C_s$.

(4) Only one slice containing liquid

When there is only one slice in the clothing which contains liquid nk + 1 = nℓ - 1 (Fig. 2). The loss to the inside is given by Eq. 65 or Eq. 66, and the loss to the outside is given by one of Eq. 68, 70 or 71. However, in order not to apply the decomposition twice the quantity $aC_s V_{n\ell+1} \Delta t$ was added to the equation for the outside slice whenever nk + 1 = nℓ - 1.

(5) Loss of liquid from outside clothing surface

When there is no liquid in the outer slice of clothing, Kirchoff's law for the flow of vapour away from the liquid on the clothing surface gives:

$$\frac{dQ}{dt} = \left(C_s - \frac{m_{nn}}{V_{nn}}\right)\frac{2}{R_{nn}} + \frac{C_s}{R_a} \qquad \text{(Eq. 74)}$$

where Q is the total amount of surface liquid lost to vapour evolution.

Discretizing gives:

$$Q_{j+1} = Q_j + \frac{2C_s\Delta t}{R_{nn}} - \frac{2m_{nn}\Delta t}{V_{nn}R_{nn}} + \frac{C_s\Delta t}{R_a} \qquad \text{(Eq. 75)}$$

When there is liquid in the outer slice of clothing Eq. 75 reduces to:

$$Q_{j+1} = Q_j + \frac{C_s\Delta t}{R_a} \qquad \text{(Eq. 76)}$$

b) Total Loss of Vapour to Air

The initial liquid on and in clothing is lost to air, to vapour in clothing, to the systemic sink and to decomposition. After the liquid is gone from the surface, there is a further vapour loss to air from the clothing. Now, if the vapour loss to air is accounted for, it is possible to calculate the loss due to decomposition, because this is the mass deficiency in the sums of the vapour and liquid in the total system. Alternatively, if the decomposition is set to zero, the calculation of vapour transport can be checked at each time step by observing that the total mass in the system must be constant.

The loss of vapour to air was accounted for in each time step as follows:

(1) No liquid in the outside clothing slice or on the surface

Application of Kirchoff's law using the electrical analogy (Fig. 1) for vapour transport to air from the outside clothing slice gives:

$$\frac{dU}{dt} = \frac{m_{nn}}{V_{nn}}\left(\frac{2}{R_{nn}+R_a}\right) \qquad \text{(Eq. 77)}$$

where U is the total vapour loss to air.

Discretizing gives:

$$U_{j+1} = U_j = \frac{2m_{nn}\Delta t}{V_{nn}(R_{nn}+2R_a)} \qquad \text{(Eq. 78)}$$

(2) Liquid in the outside clothing slice or on the surface

Kirchoff's law gives: $\frac{dU}{dt} = \frac{C_s}{R_a}$ (Eq. 73)

Discretizing gives: $U_{j+1} = U_j + \frac{C_s \Delta t}{R_a}$ (Eq. 74)

c) Maximum Allowable Size of Time Increment

**The chosen time increment for the calculation of vapour transport must be such that the mass in a slice never becomes negative, otherwise solutions become unstable. Experience has shown that this can occur for liquid reduction in slice nk+1 as calculated from Eq. 65 when the increment is too large. Analysis of Eq. 65 then provided a relationship for predetermining an approximate upper limit for the time step size. This was done in the following way:**

**For** $m_{nk+1,j+1} \geq 0$ **in Eq. 65 we must have:**

$$\Delta t \left( \frac{2_{nk,j}}{V_{nk}R_{nk}} - \frac{2C_s}{R_{nk}} - aC_s V_{nk+1} \right) \leq m_{nk+1,j} \qquad \text{(Eq. 81)}$$

**Liquid must be present whenever Eq. 65 is used. Therefore:**

$$m_{nk+1,j} \geq C_s V_{nk+1} \qquad \text{(Eq. 82)}$$

**Substitution of Eq. 82 into Eq. 81 and rearranging gives:**

$$\Delta t \leq \frac{C_s V_{nk+1}}{C_s\left( \frac{2}{R_{nk}} + aV_{nk+1} \right) - \frac{2m_{nk}}{V_{nk}R_{nk}}} \qquad \text{(Eq. 83)}$$

**A simplified but slightly stronger restriction on the maximum**

size of the time increment is obtained by setting the second term in the denominator of Eq. 83 to zero.

Thus
$$\Delta t \leq \frac{R_{nk}V_{nk+1}}{2+aR_{nk}V_{nk+1}} \qquad \text{(Eq. 84)}$$

## 5. COMPUTER PROGRAM

A computer program was written to solve the problem of vapour transport by means of the mathematical model described in the previous sections. A listing of the program along with one set of output results is shown in Appendix A. The listing is annotated in detail to describe the function of each part of the program and the input data required.

The program is written in the basic Fortran IV language of the DRES 1130 model 2C computer which has 16K words of core storage. The program in its present form requires approximately 9K of core storage. It will allow up to four layers of clothing to be simulated over skin with a total of fifty slices in the system. The skin is usually divided into seven slices, which leaves forty three slices for the clothing layers.

## 6. RESULTS

The computer program was applied to compare the systemic dose for various distributions of a 1.2 mg cm$^{-2}$ initial load on and in two layers of clothing. The absorptive and diffusive properties used were chosen for test purposes only, and, in the author's knowledge, do not represent any real liquid and clothed skin system. The resistance, capacitance and saturated vapour concentration used are those shown in the sample computer output (Appendix A). The calculations were done for two different windspeeds to show the effect of varying windspeed on the total systemic dose for various load distributions. The results for five load distributions are shown in Table 1 and Table 2 for windspeeds of 6.87 cm sec$^{-1}$ and 100 cm sec$^{-1}$ respectively.

Also, using the same five initial load distributions, the program was applied for 5, 10 and 20 slices in each of two layers and times of 1.0 and 0.1 minutes combined as shown in Table 3. The systemic dose and percentage of initial mass are also recorded in Table 3 to show the effect of varying the number of clothing slices and the time increment size on the results. In these tests, the decomposition was set to zero so that the total mass of agent should theoretically remain constant. The mass deficiency indicated in Table 3 is then only due to approximations caused by discretizing the skin clothing system.

## 7. DISCUSSION

The results shown in Table 1 and Table 2 indicate that the windspeed over the clothing surface has a considerable effect on the systemic dose for all five loading configurations tested. The largest effect occurs when the initial load is placed at the surface, and the effect decreases as the initial load is distributed closer to the skin. Also, the systemic dose is increased as the initial load is distributed closer to the skin, as one would intuitively expect.

The results in Table 3 for various time step sizes and number of clothing slices indicate that, for practical purposes, even the most coarse discretization produces sufficient accuracy. Another method of discretization was tried for the slices at liquid-vapour interfaces. Instead of assuming that the diffusive resistance started exactly at the interface as was done in the present model, except for the skin-clothing interface, the assumed resistance included half that of the liquid containing slice. The difference in results between these two methods was found to be less than one percent, for the test data used to obtain the results in Table 1. Therefore, either method produces sufficiently accurate results for practical purposes.

## 8. CONCLUSIONS

A mathematical model and an associated computer program have been produced to calculate the systemic dose for an initial liquid loading on or in the clothing of a clothed skin system. The program can be applied to practical problems for any liquid agent, when the diffusive and absorptive properties of a given system are known.

## REFERENCES


1. McPherson, W.R. 1972 "A Computer Program for the Calculation of Liquid or Vapour Penetration Through Bare and Clothed Skin (U)". Suffield Technical Note No. 310. UNCLASSIFIED.

2. Monaghan, J. 1970 Private Communication

3. Pattle, R.E. and J. Monaghan 1964 "The Calculation of Time-Lag in Thermal and Electrical Conduction, and in Diffusion". Quarterly Journal of Mechanics and Applied Mathematics. Vol. XVII, Part 1.

4. Westlake, Joan R. 1968 "A Handbook of Numerical Matrix Inversion and Solution of Linear Equations". John Wiley and Sons Inc.

TABLE 1

COMPARISON OF SYSTEMIC DOSES FOR VARIOUS DISTRIBUTIONS OF 1.2 mg $cm^{-2}$ LOADING AND WINDSPEED OF 6.87 cm $sec^{-1}$

| INPUT DATA | | | | | | RESULTS |
|---|---|---|---|---|---|---|
| Loading mg $cm^{-2}$ | | | Decay | MS | DELT | Systemic Dose |
| Surface | Top Layer | Bottom Layer | $min^{-1}$ | No. | min | at 29 Hours mg $cm^{-2}$ |
| 1.2 | 0 | 0 | 0.003 | 20 | 0.1 | 0.01297 |
| 0.8 | 0.4 | 0 | 0.003 | 20 | 0.1 | 0.01359 |
| 0.4 | 0.8 | 0 | 0.003 | 20 | 0.1 | 0.01417 |
| 0 | 1.2 | 0 | 0.003 | 20 | 0.1 | 0.01473 |
| 0.4 | 0.4 | 0.4 | 0.003 | 20 | 0.1 | 0.01541 |

TABLE 2

COMPARISON OF SYSTEMIC DOSES FOR VARIOUS DISTRIBUTIONS OF 1.2 mg $cm^{-2}$ LOADING AND WINDSPEED OF 100 cm $sec^{-1}$

| INPUT DATA | | | | | | RESULTS |
|---|---|---|---|---|---|---|
| Loading mg $cm^{-2}$ | | | Decay | MS | DELT | Systemic Dose |
| Surface | Top Layer | Bottom Layer | $min^{-1}$ | No. | min | at 29 Hours mg $cm^{-2}$ |
| 1.2 | 0 | 0 | 0.003 | 20 | 0.1 | 0.00260 |
| 0.8 | 0.4 | 0 | 0.003 | 20 | 0.1 | 0.00345 |
| 0.4 | 0.8 | 0 | 0.003 | 20 | 0.1 | 0.00430 |
| 0 | 1.2 | 0 | 0.003 | 20 | 0.1 | 0.00516 |
| 0.4 | 0.4 | 0.4 | 0.003 | 20 | 0.1 | 0.00600 |

TABLE 3

COMPARISON OF RESULTS FOR VARIOUS TIME STEP SIZES AND NUMBER OF SLICES IN EACH CLOTHING LAYER

| INPUT DATA | | | | | | CALCULATED RESULTS FOR WINDSPEED 6.87 cm $sec^{-1}$ | | |
|---|---|---|---|---|---|---|---|---|
| Loading mg $cm^{-2}$ | | | Decay | MS | DELT | Results at 29 Hours mg $cm^{-2}$ | | |
| Surface | Top Layer | Bottom Layer | $min^{-1}$ | No. | min | Systemic Dose | Total Mass | % of Initial Mass |
| 1.2 | 0 | 0 | 0 | 5 | 1.0 | 0.04734 | 1.1699 | 97.49 |
| 0.8 | 0.4 | 0 | 0 | 5 | 1.0 | 0.04948 | 1.1707 | 97.56 |
| 0.4 | 0.8 | 0 | 0 | 5 | 1.0 | 0.05056 | 1.1691 | 97.43 |
| 0 | 1.2 | 0 | 0 | 5 | 1.0 | 0.05150 | 1.1707 | 97.56 |
| 0.4 | 0.4 | 0.4 | 0 | 5 | 1.0 | 0.05323 | 1.1637 | 96.97 |
| 1.2 | 0 | 0 | 0 | 5 | 0.1 | 0.04796 | 1.1970 | 99.75 |
| 0.8 | 0.4 | 0 | 0 | 5 | 0.1 | 0.05029 | 1.1974 | 99.78 |
| 0.4 | 0.8 | 0 | 0 | 5 | 0.1 | 0.05129 | 1.1972 | 99.76 |
| 0 | 1.2 | 0 | 0 | 5 | 0.1 | 0.05206 | 1.1973 | 99.77 |
| 0.4 | 0.4 | 0.4 | 0 | 5 | 0.1 | 0.05409 | 1.1975 | 99.79 |
| 1.2 | 0 | 0 | 0 | 10 | 0.1 | 0.04790 | 1.1940 | 99.50 |
| 0.8 | 0.4 | 0 | 0 | 10 | 0.1 | 0.05013 | 1.1945 | 99.54 |
| 0.4 | 0.8 | 0 | 0 | 10 | 0.1 | 0.05125 | 1.1945 | 99.54 |
| 0 | 1.2 | 0 | 0 | 10 | 0.1 | 0.05207 | 1.1945 | 99.54 |
| 0.4 | 0.4 | 0.4 | 0 | 10 | 0.1 | 0.05413 | 1.1955 | 99.63 |
| 1.2 | 0 | 0 | 0 | 20 | 0.1 | 0.04777 | 1.1881 | 99.00 |
| 0.8 | 0.4 | 0 | 0 | 20 | 0.1 | 0.04995 | 1.1896 | 99.13 |
| 0.4 | 0.8 | 0 | 0 | 20 | 0.1 | 0.05108 | 1.1876 | 98.97 |
| 0 | 1.2 | 0 | 0 | 20 | 0.1 | 0.05196 | 1.1823 | 98.94 |
| 0.4 | 0.4 | 0.4 | 0 | 20 | 0.1 | 0.05367 | 1.1758 | 97.98 |

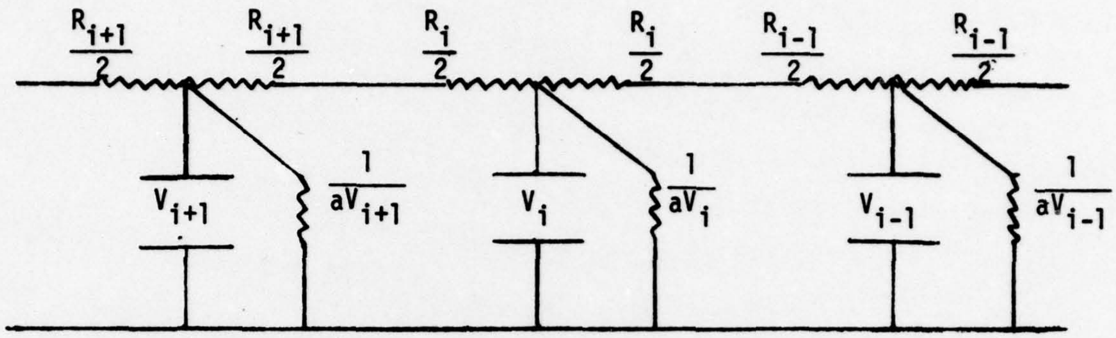


Figure 1: Analogous Electrical Network for Non-Boundary Slices

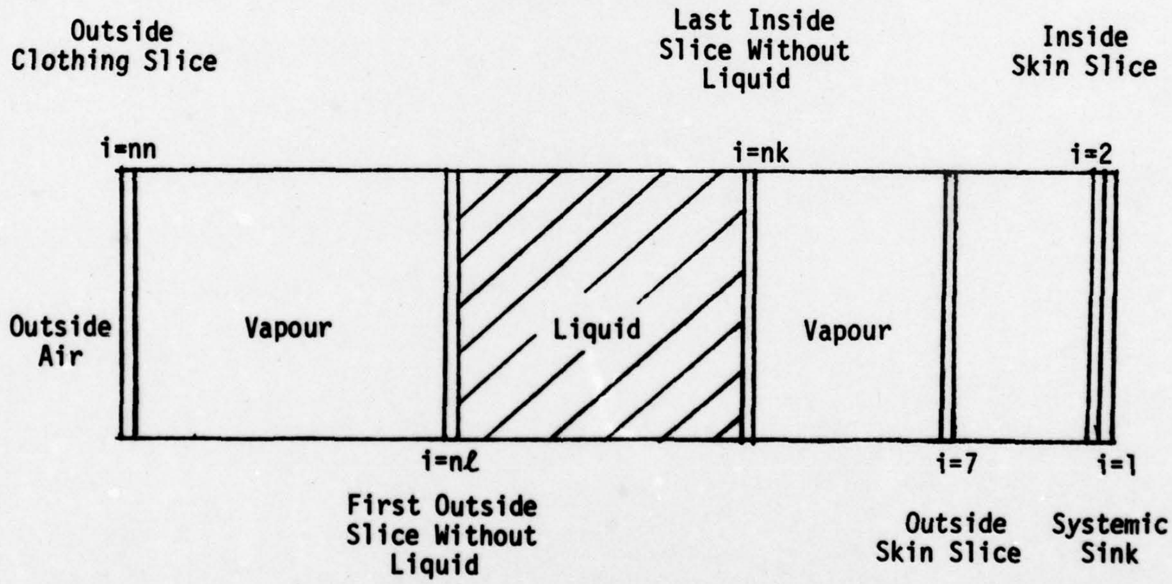


Figure 2: Clothed Skin System Showing Designation of Boundary Slices

# APPENDIX A

## COMPUTER PROGRAM WITH RESULTS FOR ONE SET OF DATA

```
// JOB T

LOG DRIVE   CART SPEC   CART AVAIL  PHY DRIVE
  0000        0206        0206        0000

V2 M11   ACTUAL 16K  CONFIG 16K

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE AGENT(RTHIN,VTHIN,RAVEG,VAVEG,U,R,V,RA1,RA2,N,NS,DECAY,
     1INDEX)
C
C     THIS SUBROUTINE CALCULATES THE RESISTANCE AND CAPACITANCE OF A
C     SLICE OF THE TRANSITIONAL LAYER OF SKIN AND OF THE AIR.
C
      DIMENSION R(2),V(2),INDEX(5),A(80)
      WRITE(3,200)
      READ(2,100)(A(I),I=1,80)
C
      WRITE(3,201)
      WRITE (3,205) (A(I),I=1,80)
      GO TO (3,4),NS
    3 R(2)=RAVEG/FLOAT(N-2)
      V(2)=VAVEG/FLOAT(N-2)
      WRITE(3,202) RAVEG,VAVEG
      GO TO 5
    4 R(2) = RTHIN/FLOAT(N-2)
      V(2) = VTHIN/FLOAT(N-2)
      WRITE(3,203) RTHIN,VTHIN
    5 RA1 = 0.9/U**0.78
      RA2 = RA1
      WRITE(3,204) U,RA1,DECAY
      DO 6 I = 1,5
    6 INDEX(I) = 0
C
C     FORMATS FOR INPUT AND OUTPUT STATEMENTS
C
  100 FORMAT(80A1)
  200 FORMAT('1',33X,'A MATHEMATICAL MODEL FOR THE PENETRATION')
  201 FORMAT(48X,'OF CLOTHING AND SKIN')
  202 FORMAT(//,42X,'SKIN TYPE - AVERAGE',/,44X,'RESISTANCE  =',F7.3,3X,
     1'(MIN/CM)',/,44X,'CAPACITANCE =',F7.1,3X,'(CM)')
  203 FORMAT(//,42X,'SKIN TYPE - THIN',/,44X,'RESISTANCE  =',F7.3,3X,'(M
     1IN/CM)',/,44X,'CAPACITANCE =',F7.1,3X,'(CM)')
```

```
  204 FORMAT(/,42X,'WINDSPEED = ',F6.2,6X,'(CM/SEC)',/,42X,'BOUNDARY LAY
     1ER RESISTANCE',F9.3,2X,'(MIN/CM)',/,42X,'DECOMPOSITION RATE',10X,F
     25.3, 2X,'(1/MIN)')
  205 FORMAT(/,20X,80A1,/)
C
      RETURN
      END
VARIABLE ALLOCATIONS
     A(R )=00FD-0000      I(I )=00F3

STATEMENT ALLOCATIONS
 100  =0102  200  =0105  201  =011E  202  =012B  203  =015A  204  =0187  205  =01C3  3    =022D  4    =0255  5    =027B
 6    =0296

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 FAXB    ELD     ESTO    ESTOX   EDVR    FLOAT   SRED    SWRT    SCOMP   SIOFX   SIOF    SUBSC   SUBIN

REAL CONSTANTS
   .900000000E 00=00F6     .780000000E 00=00F9

INTEGER CONSTANTS
     3=00FC     2=00FD     1=00FE     80=00FF     5=0100     0=0101

CORE REQUIREMENTS FOR AGENT
 COMMON       0  VARIABLES      246  PROGRAM      436

RELATIVE ENTRY POINT ADDRESS IS 01C9 (HEX)

END OF COMPILATION

// DUP

*STORE      WS  UA  AGENT
CART ID 0206   DB ADDR  4D20   DB CNT   001C

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE INDXX(DELT,TOTAL,TN,TD,TR,NTOTL,NTN,NTD,NTR)
C     THIS SUBROUTINE CHANGES THE VARIOUS INPUT TIMES TO INTEGER FORM.
C
```

```
      NTOTL = IFIX(TOTAL*60.0/DELT + 0.00001)
      NTN = IFIX(TN*60.0/DELT + 0.00001)
      NTD = IFIX(TD*60.0/DELT + 0.00001)
      NTR = IFIX(TR*60.0/DELT + 0.00001)
      WRITE(3,200) TOTAL,TD,TN,DELT
  200 FORMAT(//,42X,'TIME CONSTANTS',/,44X,'TOTAL TIME',8X,'=',F7.2,3X,'
     1(HOURS)',/,44X,'TIME OF DECONTAM   =',F7.2,3X,'(HOURS)',/,44X,'TIME
     2 INCREMENT      =',F7.2,3X,'(HOURS)',/,44X,'DELT     =',F6.3,3X,'(MINU
     3TES)',///)
C
      RETURN
      END

STATEMENT ALLOCATIONS
 200  =000B

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 EADD     EMPY     EDIV     ELD      ESTO     IFIX     SWRT     SCOMP    SIOF     SUBIN

REAL CONSTANTS
   .600000000E 02=0004      .100000000E-04=0007

INTEGER CONSTANTS
    3=000A

CORE REQUIREMENTS FOR INDXX
 COMMON       0  VARIABLES        4  PROGRAM     198

RELATIVE ENTRY POINT ADDRESS IS 0063 (HEX)

END OF COMPILATION

// DUP

*STORE      WS  UA  INDXX
CART ID 0206    DB ADDR  4D3C    DB CNT    000E

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE CONST(N,NN,NUM,NK,DELT,DECAY,RA1,RA2,R,V,RT,VT,MS,A,B,C
```

```
      1)
C
C     THIS SUBROUTINE CALCULATES THE RESISTANCE AND CAPACITANCE OF EACH
C     SLICE OF CLOTHING AND SKIN AND ALSO CALCULATES THE COMPONENTS OF
C     THE MATRIX OF COEFFICIENTS.
C
      DIMENSION V(50),R(50),VT(5),RT(5),MS(4),A(50),B(50),C(50)
C
C     SKIN LAYERS
C
      R(1) = 0.0
      NK=N-1
      DO 10 I=3,NK
      V(I)=V(2)
   10 R(I) = R(2)
C
C     HORNY LAYER
C
      V(N)=5.*V(2)
      R(N) = 0.0
C
C     CLOTH LAYERS
C
      NK=N+1
      DO 16 J=1,NUM
      M1 = MS(J) + NK - 1
      DO 13 I=NK,M1
      R(I)=RT(J)/FLOAT(MS(J))
   13 V(I)=VT(J)/FLOAT(MS(J))
   16 NK = M1 + 1
C
C     OUTSIDE SLICE OF OUTER LAYER
C
      NN = M1
      NK=NN
C
C     SURFACE
C
      R(NN+1) = RA2
C
C     TRIDIAGONAL MATRIX OF COEFFICIENTS IN DIFFERENTIAL EQUATIONS OF
C     MASS TRANSPORT
C
      B(1)=1.0
      A(2)=0.0
      B(NK) = 1.0 + DELT*((2.0/(R(NK-1)+R(NK)) + 2.0/R(NK))/V(NK)+DECAY)
```

```
      DO 25 I=2,NK
      C(I-1) = -DELT*2.0/(V(I)*(R(I-1)+R(I)))
      IF(I-NK) 24,25,25
   24 A(I+1) = -DELT*2.0/(V(I)*(R(I)+R(I+1)))
      B(I) = 1.0 + DELT*((2.0/(R(I-1)+R(I))+2.0/(R(I) + R(I+1)))
     1/V(I) + DECAY)
   25 CONTINUE
C
      RETURN
      END
VARIABLE ALLOCATIONS
      I(I )=0003      J(I )=0004           M1(I )=0005

STATEMENT ALLOCATIONS
 10   =0089  13   =00EB  16   =010B  24   =0186  25   =01CC

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 EADD    EADDX   EMPY    EMPYX   EDIVX   ELD     ELDX    ESTO    ESTOX   EDVR    EDVRX   FLOAT   SUBSC   SNR     SUBIN

REAL CONSTANTS
   .000000000E 00=000C    .500000000E 01=000F.    .100000000E 01=0012     .200000000E 01=0015

INTEGER CONSTANTS
      1=0018      3=0019      2=001A

CORE REQUIREMENTS FOR CONST
 COMMON       0  VARIABLES      12  PROGRAM     460

RELATIVE FNTRY POINT ADDRESS IS 001B (HEX)

END OF COMPILATION

// DUP

*STORE        WS  UA  CONST
CART ID 0206    DB ADDR  404A   DB CNT   0020

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE CLOTH(N,NN,NUM,NTIME,NTR,NK,INDEX,ITHLY,KTHSL,M,
```

```
     1R,B,G,U,DELT,RA2,DECAY,MASS,CS,MS,V,KIN,A,C,LIN,LTHLY,NL,LTHSL,
     2NSURF,Q)
C
C     THIS SUBROUTINE DETERMINES WHEN THE LIQUID IS GONE IN SUCCESSIVE
C     SLICES AND CHANGES THE APPROPRIATE CONSTANTS
C     AT LIQUID-VAPOR INTERFACES.
C
      REAL M(50),MASS(5)
      DIMENSION INDEX(5),R(50),B(50),MS(4),V(50),A(50),C(50)
      IF(INDEX(1))1,1,2
C
C     SET INITIAL CONDITIONS
C
    1 CALL LIQPC(CS,NUM,N,MS,M,ITHLY,KTHSL,KIN,INDEX,
     1LIN,LTHLY,U,NL,LTHSL,NSURF,Q,MASS)
    2 IF(INDEX(4))3,3,310
C
C     REPLACE CLOTHING AT DESIGNATED TIME
C
    3 IF(NTR -NTIME)310,4,310
    4 CALL CLREM(NTIME,N,NN,M,DELT,NK,INDEX,MASS,NSURF)
C
C     CHECK FOR LIQUID ON SURFACE
C
  310 IF(INDEX(5))5,5,10
    5 IF(M(NN)-CS*V(NN))6,6,7
    6 Q = Q + DELT*(CS*(R(NN)+2.0*RA2)/(R(NN)*RA2)- M(NN)/(V(NN)*R(NN)/
     12.0))
      GO TO 8
    7 Q=Q+DELT*CS/RA2
    8 IF(Q-MASS(NSURF))10,9,9
    9 IF(NTIME-1)312,312,311
  311 TIME = FLOAT(NTIME)*DELT/60.0
      WRITE(3,202)TIME
  312 B(NN) = 1.0 + DELT*((2.0/(R(NN-1)+R(NN)) + 2.0/(R(NN) +
     12.0*RA2))/V(NN)+ DECAY)
C
C     SET INDEX FOR LIQUID ALL GONE FROM SURFACE
C
      INDEX(5)=INDEX(5)+1
C
C     IF LIQUID ALL GONE IN CLOTHING USE TRID ACCORDINGLY
C
   10 IF(INDEX(2)) 11,11,60
C
C     FIND INNERMOST SLICE WHICH STILL CONTAINS LIQUID
```

```
C
   11 IF(M(KTHSL)-CS*V(KTHSL)) 12,12,15
   12 KTHSL=KTHSL+1
      IF(KTHSL-NL)13,14,14
   13 GO TO 11
C
C     SET INDEX FOR LIQUID ALL GONE
C
   14 INDEX(2)=INDEX(2) + 1
      KTHSL=KTHSL-1
      TIME=FLOAT(NTIME)*DELT/60.0
      WRITE (3,201) TIME
      IF(INDEX(4))314,314,60
  314 CONTINUE
      WRITE(3,204)KTHSL
      GO TO 60
C
C     FIND OUTERMOST SLICE WHICH STILL CONTAINS LIQUID
C
   15 IF(M(LTHSL) - CS*V(LTHSL))16,16,26
   16 LTHSL = LTHSL - 1
      GO TO 11
C
C     RECORD TIME AT WHICH LIQUID IS GONE FROM EACH SUCCESSIVE LAYER
C
   26 IF((KTHSL-KIN)-MS(ITHLY)) 28,27,27
   27 TIME=FLOAT(NTIME)*DELT/60.0
      WRITE(3,200) ITHLY,TIME
      KIN=KIN+ MS(ITHLY)
      ITHLY=ITHLY + 1
      GO TO 26
   28 IF((LIN-LTHSL)-MS(LTHLY))30,29,29
   29 TIME=FLOAT(NTIME)*DELT/60.0
      WRITE(3,200)LTHLY,TIME
      LIN=LIN-MS(LTHLY)
      LTHLY=LTHLY-1
      GO TO 28
C
C     FIRST OUTER SLICE WHICH CONTAINS NO LIQUID
C
   30 NL = LTHSL + 1
C
C     VAPOUR TRANSPORT IN INNER SLICES
C
C     SET NUMBER OF EQUATIONS IN TRID TO OUTER SLICE OF INSIDE SLICES
C     CONTAINING NO LIQUID
```

```
C
      NK=KTHSL-1
      NJ = 1
      GF = 0.0
C
C     SPECIAL CASE OF LIQUID IN SLICE NEXT TO SKIN
C
      IF(NK-N)35,34,35
   34 G = 2.0 * DELT*CS/R(N+1)
      M(N+1)= M(N+1) - DELT*(CS*(2./R(N+1)  + DECAY*V(N+1)) -M(N)/
     1(V(N)*R(N+1)/2.0))
      GO TO 36
   35 G = 2.0 * DELT*CS/R(NK)
C
C     REDUCE MASS OF LIQUID IN INNER SLICE
C
      M(NK+1) = M(NK+1) - DELT*(CS*(2./R(NK) +DECAY*V(NK+1))- M(NK)/
     1(V(NK)*R(NK)/2.0))
      B(NK) = 1.0 + DELT*((2.0/(R(NK-1)+R(NK)) + 2.0/R(NK))/V(NK)+DECAY)
   36 CALL TRID(M,A,B,C,NK,G,NJ,GF)
      B(NK) = 1.0 + DELT*((2.0/(R(NK-1)+R(NK)) + 2.0/(R(NK) + R(NK+1)))/
     1V(NK)+ DECAY)
C
C     VAPOUR TRANSPORT IN OUTER SLICES
C
      NK = NN
      IF(Q-MASS(NSURF))41,42,42
   41 G = 2.0*DELT*CS/R(NN)
      GO TO 43
   42 G = 0.0
C
C     SET STARTING POINT OF TRID TO FIRST OUTER SLICE CONTAINING NO
C     LIQUID
C
   43 NJ=NL
      GF = 2.0*DELT*CS/R(NL)
C
C     REDUCE MASS OF LIQUID IN OUTER SLICE
C
      IF(KTHSL - LTHSL)344,44,344
   44 TEMP = DECAY
      DECAY = 0.0
  344 IF(NL-(NN+1))52,45,45
   45 IF(Q-MASS(NSURF))46,49,49
   46 M(NN)=M(NN)-DELT*DECAY*CS*V(NN)
      U=U+DELT*CS/RA2
```

```
      GO TO 56
   49 M(NN) = M(NN) - DELT*CS*(1./RA2 + DECAY*V(NN))
      U = U + DELT*CS/RA2
      GO TO 56
   52 IF(NL - NN) 54,53,53
   53 M(NN-1) = M(NN-1) - DELT*(CS*(2./R(NN)+ DECAY*V(NN-1))-M(NN)/
     1(V(NN)*R(NN)/2.0))
      IF(KTHSL - LTHSL)346,345,346
  345 DECAY = TEMP
  346 U = U + DELT*M(NN)/(V(NN)*(R(NN)/2.0 + RA2))
      B(NN) = 1.C + DELT*((2.0/(R(NN)) + 2.0/(R(NN) +
     12.0*RA2))/V(NN)+ DECAY)
C
C     SOLVE EQUATION FOR ONE SLICE INSTEAD OF CALLING TRID
C
      M(NN) = (M(NN) + GF)/B(NN)
      B(NN) = 1.0 + DELT*((2.0/(R(NN-1)+R(NN)) + 2.0/(R(NN) +
     12.0*RA2))/V(NN)+ DECAY)
      GO TO 356
   54 M(NL-1) = M(NL-1) - DELT*(CS*(2./R(NL)+ DECAY*V(NL-1))-M(NL)/
     1(V(NL)*R(NL)/2.0))
      IF(KTHSL - LTHSL)351,350,351
  350 DECAY = TEMP
  351 U = U + DELT*M(NN)/(V(NN)*(R(NN)/2.0 + RA2))
      B(NJ) = 1.0 + DELT*((2.0/R(NJ) + 2.0/(R(NJ) + R(NJ+1)))
     1/V(NJ)+ DECAY)
C
C     SOLVE EQUATIONS FOR TWO OR MORE SLICES
C
      CALL TRID(M,A,B,C,NK,G,NJ,GF)
      B(NJ) = 1.0 + DELT*((2.0/(R(NJ-1) + R(NJ)) + 2.0/(R(NJ) +
     1R(NJ+1)))/V(NJ)+ DECAY)
      GO TO 356
C
C     REDUCE LIQUID MASS IN MIDDLE SLICES BY DECOMPOSITION ONLY
C
   56 IF(KTHSL - LTHSL)356,355,356
  355 DECAY = TEMP
  356 L = KTHSL +2
      IF(L-LTHSL)57,57,99
   57 CONTINUE
      DO 58 I = L,LTHSL
   58 M(I-1) = M(I-1) - DELT*DECAY*CS*V(I-1)
      GO TO 99
C
C     LIQUID ALL GONE IN CLOTHING
```

```
C
   60 NK = NN
      IF(Q-MASS(NSURF))61,62,62
   61 G = 2.0*DELT*CS/R(NN)
      U=U+DELT*CS/RA2
      GO TO 63
   62 G=0.0
      U = U + DELT*M(NN)/(V(NN)*(R(NN)/2.0 + RA2))
   63 NJ=1
      GF = 0.0
      CALL TRID(M,A,B,C,NK,G,NJ,GF)
   99 RETURN
C
C     FORMATS FOR OUTPUT STATEMENTS
C
  200 FORMAT(/,22X,'LIQUID ALL GONE IN LAYER ', I2,' AT T=',F6.2,2X,'(HO
     1URS)',/)
  201 FORMAT(/,22X,'LIQUID ALL GONE IN CLOTHING AT T=',
     1F6.2,2X,'(HOURS)',/)
  202 FORMAT(/,22X,'LIQUID ALL GONE FROM SURFACE AT T=',F6.2,2X,
     1'(HOURS)',/)
  204 FORMAT(  22X,'LAST SLICE TO CONTAIN LIQUID WAS',I3,/)
      END
VARIABLE ALLOCATIONS
  TIME(R )=0000     GF(R )=0003     TEMP(R )=0006     NJ(I )=000F     L(I )=0010     I(I )=0011

STATEMENT ALLOCATIONS
 200 =0025 201 =0043 202 =0060 204 =007D 1   =0223 2   =0236 3   =023C 4   =0242 310 =024D 5   =0253
 6   =0261 7   =028A 8   =0294 9   =02A0 311 =02A6 312 =02B5 10  =02E5 11  =02EB 12  =02F9 13  =0305
 14  =0307 314 =032A 15  =0332 16  =0340 26  =0348 27  =0355 28  =0379 29  =0386 30  =03AA 34  =03C4
 35  =0402 36  =045D 41  =04A8 42  =04B9 43  =04BD 44  =04D6 344 =04DE 45  =04E8 46  =04F4 49  =0511
 52  =053A 53  =0540 345 =0576 346 =057A 54  =05DE 350 =0614 351 =0618 56  =0696 355 =069C 356 =06A0
 57  =06AC 58  =06B0 60  =06CC 61  =06DC 62  =06F7 63  =0714 99  =0726

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 LIOPC  CLREM  TRID   EADD   EADDX  FSUBX  EMPY   EMPYX  EDIV   EDIVX  ELD    ELDX   ESTO   ESTOX  ESBR
 ESBRX  FDVR   EDVRX  FLCAT  SWRT   SCOMP  SIOF   SIOI   SUBSC  SUBIN

REAL CONSTANTS
  .200000000E 01=0016     .600000000E 02=0019     .100000000E 01=001C     .000000000E 00=001F

INTEGER CONSTANTS
   1=0022      3=0023      2=0024
```

```
CORE REQUIREMENTS FOR CLOTH
 COMMON       0  VARIABLES      22  PROGRAM    1810

RELATIVE ENTRY POINT ADDRESS IS 0092 (HEX)

END OF COMPILATION

// DUP

*STORE      WS  UA  CLOTH
CART ID 0206    DB ADDR  4D6A   DB CNT    007E

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE LIQPC(CS,NUM,N,MS,M,ITHLY,KTHSL,KIN,INDEX,
     1LIN,LTHLY,U,NL,LTHSL,NSURF,Q,MASS)
C
C     THIS SUBROUTINE SETS THE INITIAL CONDITIONS.
C
      REAL M(50),MASS(5)
      DIMENSION MS(4),INDEX(5)
C
C     INPUT SATURATED VAPOR CONCENTRATION AND MASS OF LIQUID IN EACH
C     LAYER
C
      NSURF=NUM+1
      READ(2,100) CS,(MASS(I),I=1,NSURF)
      WRITE(3,200) CS,(I,MASS(I),I=1,NUM)
      WRITE(3,201)MASS(NSURF)
      DO 30 I=1,NUM
      IF(MASS(I)) 30,30,31
   30 CONTINUE
C
C     INDEX FIRST LAYER CONTAINING LIQUID
C
   31 ITHLY=I
C
C     INDEX INSIDE SLICE OF FIRST LAYER CONTAINING LIQUID
C
      KTHSL=N+1
      IF(ITHLY-1) 32,32,33
   33 DO 34 I=2,ITHLY
```

```
C
C     INDEX INSIDE SLICE OF FIRST LAYER CONTAINING LIQUID
C
   34 KTHSL=KTHSL + MS(I-1)
C
C     SET INDEX OF INSIDE SLICE OF FIRST LAYER CONTAINING LIQUID
C
   32 KIN=KTHSL
C
C     SET MASS EQUAL ZERO IN EACH LAYER WHICH CONTAINS NO LIQUID
C
      DO 35 I=2,KTHSL
   35 M(I-1)=0.0
C
C     INDEX SLICE AT BEGINNING OF FIRST LAYER WHICH CONTAINS LIQUID
C
      NN=KTHSL
C
C     SET INDEX IF NO LIQUID IN CLOTHING
C
      IF(ITHLY-NUM)39,39,38
   38 INDEX(2) = INDEX(2) + 1
      GO TO 40
   39 CONTINUE
C
C     INDEX OUTSIDE SLICE OF EACH LAYER IN TURN
C
      DO 36 J=ITHLY,NUM
      NK=MS(J)+NN-1
C
C     SET MASS IN EACH SLICE OF LAYERS WHICH CONTAIN LIQUID
C
      DO 37 L=NN,NK
   37 M(L)=MASS(J)/FLOAT(MS(J))
C
C     INDEX SLICE AT BEGINNING OF NEXT LAYER
C
   36 NN=NK+1
C
C     SET INDICES AT OUTSIDE BOUNDARY
C
      LIN = NN-1
      LTHLY = NUM
      LTHSL = NN-1
      NL = NN
```

```
C
C     MASS LOSS TO ATMOSPHERE
C
   40 U=0.0
      Q=0.0
C
C     INITIAL CONDITIONS HAVE BEEN SET
C
      INDEX(1)=INDEX(1) + 1
C
C     FORMATS FOR OUTPUT STATEMENTS
C
  100 FORMAT(8F10.0)
  200 FORMAT(/,42X,'SATURATED VAPOR CONCENTRATION', / ,58X,'SVC =',E11.4
     1,2X,'(MG/CM**3)',//,49X,'INITIAL LIQUID LOADING',//,
     2(42X,'MASS IN LAYER   ',I1,7X,F7.3,'  MG/CM**2'))
  201 FORMAT(/,42X,'MASS ON SURFACE',8X,F7.3,'  MG/CM**2'/)
      RETURN
      END
VARIABLE ALLOCATIONS
    I(I )=0000        NN(I )=0001           J(I )=0002          NK(I )=0003          L(I )=0004

STATEMENT ALLOCATIONS
 100   =000E  200  =0011  201   =0056  30   =00FD  31   =0106  33   =0116  34   =011A  32   =012E  35   =0136  38   =0152
 39    =015C  37   =0171  36    =019B  40   =01BE

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 ELD      FLDX     ESTO     ESTOX    EDVRX    FLOAT    SRED     SWRT     SCOMP    SIOFX    SIOF     SIOI     SUBSC    SUBIN

REAL CONSTANTS
  .000000000E 00=0008

INTEGER CONSTANTS
    1=0008      2=000C        3=000D

CORE REQUIREMENTS FOR LIQPC
 COMMON        0  VARIABLES        8  PROGRAM    456

RELATIVE ENTRY POINT ADDRESS IS 006B (HEX)

END OF COMPILATION
```

```
// DUP

*STORE      WS  UA  LIQPC
CART ID 0206   DB ADDR  4DE8   DB CNT   001D
// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE CLREM(NTIME,N,NN,M,DELT,NK,INDEX,MASS,NSURF)
C
C     THIS SUBROUTINE SETS THE MASS OF AGENT ON AND IN CLOTHING TO
C     ZERO AT TIME OF CLOTHING REPLACEMENT.
C
      REAL  M(50),MASS(5)
      DIMENSION INDEX(5)
      K = N+1
      TIME = FLOAT(NTIME)*DELT/60.0
      WRITE(3,200) TIME
      DO 2 I = K,NN
    2 M(I) = 0.0
      MASS(NSURF) = 0.0
      INDEX(4) = INDEX(4) + 1
C
C     FORMAT FOR OUTPUT STATEMENT
C
  200 FORMAT(/,22X,'CLOTHING REPLACED AT T=',F6.2,2X,'(HOURS)',/)
      RETURN
      END
VARIABLE ALLOCATIONS
  TIME(R )=0000          K(I )=0003          I(I )=0004

STATEMENT ALLOCATIONS
 200  =0010  2     =0056

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 EMPY     FDIV     ELD      ESTO     ESTOX    FLOAT    SWRT     SCOMP    SIOF     SUBSC    SUBIN

REAL CONSTANTS
  .600000000E 02=0008      .000000000E 00=000B

INTEGER CONSTANTS
    1=000E       3=000F
```

```
CORE REQUIREMENTS FOR CLREM
 COMMON      0  VARIABLES       8  PROGRAM     116

RELATIVE ENTRY POINT ADDRESS IS 0028 (HEX)

END OF COMPILATION

// DUP

*STORE      WS  UA  CLREM
CART ID 0206   DB ADDR  4E05   DB CNT    0009

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE DECON(NTIME,MASS,NSURF,Q,EFFIC,DELT)
C
C     THIS SUBROUTINE REDUCES THE MASS ON THE OUTER CLOTHING SURFACE
C     AT THE TIME OF DECONTAMINATION.
C
      REAL MASS(5)
      TIME = FLOAT(NTIME)*DELT/60.0
      WRITE(3,200)TIME
      Q = Q + EFFIC*MASS(NSURF)
      MASS(NSURF) = (1.0 - EFFIC)*MASS(NSURF)
C
C     FORMAT FOR OUTPUT STATEMENT
C
  200 FORMAT(/,42X,'DECONTAMINATION AT T=',F6.2,2X,'(HOURS)',/)
C
      RETURN
      END
VARIABLE ALLOCATIONS
  TIME(R )=0000

STATEMENT ALLOCATIONS
 200    =000R

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 EADD    ESUB    EMPY    EMPYX   EDIV    ELD     ESTO    ESTOX   FLOAT   SWRT    SCOMP   SIOF    SUBSC   SUBIN
```

```
REAL CONSTANTS
   .600000000E 02=0004      .100000000E 01=0007

INTEGER CONSTANTS
   3=000A

CORE REQUIREMENTS FOR DECON
 COMMON       0  VARIABLES       4  PROGRAM      90

RELATIVE ENTRY POINT ADDRESS IS 0022 (HEX)

END OF COMPILATION

// DUP

*STORE      WS  UA  DECON
CART ID 0206   DB ADDR  4E0E   DB CNT    0007

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE TRID(M,A,B,C,NK,GG,NJ,GF)
C
C     THIS SUBROUTINE CALCULATES THE MASS OF VAPOUR IN EACH LAYER AS A
C     FUNCTION OF TIME BY SOLUTION OF THE EQUATIONS OF MASS TRANSFER.
C     GAUSSIAN ELIMINATION IS USED TO GET THE SOLUTION VECTOR FROM THE
C     MATRIX OF COEFFICIENTS.
C
      REAL M(50)
      DIMENSION A(50),B(50),C(50),Q(200),W(200),G(200)
C
C     VAPOUR IN OUTSIDE SLICE
C
      M(NK) = M(NK) + GG
C
C     COEFFICIENT FOR INSIDE SLICE
C
      M(NJ) = M(NJ) + GF
      W(NJ) = B(NJ)
      G(NJ) = M(NJ)/W(NJ)
C
C     REDUCTION TO TRIANGULAR FORM
C
```

```
C      THE NEW VALUES OF A ARE ZERO
C      THE NEW VALUES OF B ARE ONE
C      Q IS THE NEW VALUE OF C
C      G IS THE NEW VALUE OF D
C      D IS THE VALUE OF M INITIALLY
C
       JJ = NJ + 1
       DO 1 I=JJ,NK
       Q(I-1)= C(I-1)/W(I-1)
       W(I) =B(I)-A(I)*Q(I-1)
     1 G(I) =(M(I) - A(I)*G(I-1))/W(I)
C
C      BACK SUBSTITUTION TO OBTAIN SOLUTION VECTOR
C
       JJ = NK-NJ+1
       M(NK) = G(NK)
       DO 2 I = 2,JJ
       K = NK + 1-I
     2 M(K) = G(K) - Q(K)*M(K+1)
C
       RETURN
       END
VARIABLE ALLOCATIONS
   Q(R )=0255-0000     W(R )=04AD-0258     G(R )=0705-04B0     JJ(I )=0708     I(I )=0709     K(I )=070A

STATEMENT ALLOCATIONS
 1     =077D  2     =07B3

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 EADD     EMPYX    EDIVX    ELDX     ESTOX    ESBRX    SUBSC    SUBIN

INTEGER CONSTANTS
     1=070E      2=070F

CORE REQUIREMENTS FOR TRID
 COMMON        0  VARIABLES    1806  PROGRAM    200

RELATIVE ENTRY POINT ADDRESS IS 0710 (HEX)

END OF COMPILATION
```

```
// DUP

*STORE      WS  UA  TRID
CART ID 0206    DB ADDR  4E15    DB CNT    000F

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*LIST ALL
      SUBROUTINE PROUT(NUM,N,NTIME,M,MS,U,DELT,INDEX)
C
C     THIS SUBROUTINE PRINTS THE CALCULATED MASS OF AGENT IN EACH
C     LAYFR AS A FUNCTION OF TIME.
C
      REAL M(50)
      DIMENSION INDEX(5),SUM(5),MS(4)
C
      TIME=FLOAT(NTIME)*DELT/60.0 + 0.00001
      DO 20 I=1,5
   20 SUM(I)=C.0
C
      IF(INDEX(3)) 21,21,40
   21 WRITE(3,200)
      INDEX(3)=INDEX(3) + 1
      IF(NUM-4) 27,27,28
   27 NM=NUM
      GO TO 29
   28 NM=4
   29 GO TO (30,31,32,33),NM
   30 WRITE(3,201)
      GO TO 40
   31 WRITE(3,202)
      GO TO 40
   32 WRITF(3,203)
      GO TO 40
   33 WRITF(3,204)
   40 DO 47 I=3,N
   47 SUM(1)=SUM(1) + M(I-1)
      K=N+1
      KNK=NM + 1
      DO 55 J=2,KNK
      KK=K-1+MS(J-1)
      DO 56 I=K,KK
   56 SUM(J)=SUM(J) + M(I)
   55 K=KK+1
C
```

```
C     FORMATS FOR OUTPUT STATEMENTS
C
      WRITE(3,205)TIME,U,M(1),SUM(1),M(N),(SUM(I),I=2,KNK)
  200 FORMAT('1',44X,'MASS IN EACH LAYER IN MG/CM**2',//)
  201 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
     1,'MASS IN',/,1X,'HOURS',1X,'MG/CM**2',4X,'DOSE',9X,'TRANSITIONAL',
     26X,'HORNY',7X,'FIRST CLOTH',/,35X,3('LAYER',10X),/)
  202 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
     1,'MASS IN',8X,'MASS IN',/,1X,'HOURS',1X,'MG/CM**2',4X,'DOSE',9X,'T
     2RANSITIONAL',6X,'HORNY',7X,'FIRST CLOTH',4X,'SECOND CLOTH',/,35X,4
     3('LAYER',10X),/)
  203 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
     1,'MASS IN',8X,'MASS IN',8X,'MASS IN',/,1X,'HOURS',1X,'MG/CM**2',4X
     2,'DOSE',9X,'TRANSITIONAL',6X,'HORNY',7X,'FIRST CLOTH',4X,'SECOND C
     3LOTH',3X,'THIRD CLOTH',/,35X,5('LAYER',10X),/)
  204 FORMAT(2X,'TIME',4X,'U',6X,'SYSTEMIC',9X,'MASS IN',8X,'MASS IN',8X
     1,'MASS IN',8X,'MASS IN',8X,'MASS IN',8X,'MASS IN',/,1X,'HOURS',1X,'
     2MG/CM**2',4X,'DOSE',9X,'TRANSITIONAL',6X,'HORNY',7X,'FIRST CLOTH',
     34X,'SECOND CLOTH',3X,'THIRD CLOTH',4X,'FOURTH CLOTH',/,35X,5('LAYE
     4R',10X),'LAYER',/)
  205 FORMAT(F7.3,F8.5,7(2X,F10.7,3X))
C
      RETURN
      END
VARIABLE ALLOCATIONS
  SUM(R )=000C-0000  TIME(R )=000F     I(I )=0012       NM(I )=0013        K(I )=0014       KNK(I )=0015
    J(I )=0016          KK(I )=0017

STATEMENT ALLOCATIONS
 200  =002A  201  =0040  202  =008F  203  =00EC  204  =0157  205  =01D4  20   =0206  21   =021E  27   =0230  28   =0236
 29   =023A  30   =0242  31   =0248  32   =024E  33   =0254  40   =0258  47   =025C  56   =0297  55   =0286

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION

CALLED SUBPROGRAMS
 EADD    EADDX   EMPY    EDIV    ELD     ELDX    ESTO    ESTOX   FLOAT   SWRT    SCOMP   SIOFX   SIOF    SUBSC   SUBIN

REAL CONSTANTS
  .600000000E 02=001C     .100000000E-04=001F     .000000000E 00=0022

INTEGER CONSTANTS
    1=0025       5=0026       3=0027       4=0028       2=0029

CORE REQUIREMENTS FOR PROUT
 COMMON       0  VARIABLES      28  PROGRAM     724
```

```
RELATIVE ENTRY POINT ADDRESS IS 01DC (HEX)

END OF COMPILATION

// DUP

*STORE      WS  UA  PROUT
CART ID 0206    DB ADDR  4E24    DB CNT    002C

// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
*IOCS(CARD)
*IOCS(1132 PRINTER)
*IOCS(DISK)
*LIST ALL
C
C      INPUT DATA FOR LIQUID ON AND IN CLOTH PROGRAM
C
C      CARD 1 - 2I3
C         N,NS
C         N - TOTAL NUMBER OF SLICES SKIN IS DIVIDED INTO
C         NS=1 AVERAGE SKIN
C         NS=2 THIN SKIN
C
C      CARD 2 - 8F10.3
C         RTHIN,VTHIK,RAVEG,VAVEG,U,DECAY,DELT,EFFIC
C         RTHIN,RAVEG - RESISTANCE OF SKIN TYPES (MIN/CM)
C         VTHIN,VAVEG - CAPACITANCE OF SKIN TYPES (CM)
C         U - WIND SPEED (CM/SEC)
C         DECAY - DECAY FACTOR (PER CENT*10**-2 PER MINUTE)
C         DELT - TIME INCREMENT IN MINUTES
C         EFFIC - EFFICIENCY OF DECONTAMINATION
C
C      CARD 3 - 8F10.3
C         TOTAL,TN,TD,TR
C         TOTAL - TOTAL TIME PERIOD (HOURS)
C         TN - TYPE OUT INCREMENT (HOURS)
C         TD - TIME OF DECONTAMINATION (HOURS)
C         TR - TIME OF REMOVAL OF CLOTHING (IF APPLICABLE),(HOURS)
C
C      CARD 4 - 80A1 (IN SUBROUTINE AGENT)
C         A(I)
C         A(I) - IDENTICATION OF AGENT AND APPLICATION
C
```

```
C     CARD 5 - I3
C         NUM
C         NUM - NUMBER OF LAYERS OF CLOTHING.  THE PROGRAM WILL ACCEPT
C         ANY NUMBER OF LAYERS BUT ONLY THE CONTENTS OF THE INNERMOST 4
C         WILL BE PRINTED.  FOR MORE THAN 5 LAYERS, THE DIMENSION
C         STATEMENTS MUST BE ALTERED.
C     CARD 6A - I3,2F10.0
C         MS(I),RT(I),VT(I)
C         ONE CARD PER CLOTHING LAYER (STARTING WITH THE INNERMOST)
C         MS - NUMBER OF SLICES THAT EACH LAYER IS SUBDIVIDED INTO
C         RT - RESISTANCE OF EACH LAYER (MIN/CM)
C         VT - CAPACITANCE OF EACH LAYER (CM)
C
C     CARD 7 - 8F10.0 (IN SUBROUTINE LIQPC)
C     CS,MASS(I)
C         CS - SATURATED VAPOUR CONCENTRATION (MG/CM**3)
C         MASS(I) - MASS IN CLOTHING AT T=0 (MG/CM**2)    I=1,NUM
C                   AND ON CLOTHING    I=NUM+1
C
C     CARD 8 - 2I3
C         START OF ANOTHER SET OF DATA OR CALL EXIT
C         N - CALLS EXIT IF ZERO OR NEGATIVE
C
      REAL M(50), MASS(5)
      DIMENSION A(50),B(50),C(50),R(50),V(50),RT(5),VT(5),MS(4),INDEX(5)
C
    1 READ(2,100) N,NS
      IF(N)99,99,2
C
    2 READ(2,101) RTHIN,VTHIN,RAVEG,VAVEG,U,DECAY,DELT,EFFIC
      READ(2,101) TOTAL,TN,TD,TR
      CALL AGENT(RTHIN,VTHIN,RAVEG,VAVEG,U,R,V,RA1,RA2,N,NS,DECAY,INDEX)
      DO 3 I=1,4
    3 MS(I) = 0
      READ(2,102)NUM,(MS(I),RT(I),VT(I),I=1,NUM)
      WRITE(3,200)
      WRITE(3,201) (I,MS(I),RT(I),VT(I),I=1,NUM)
C
      CALL INDXX(DELT,TOTAL,TN,TD,TR,NTOTL,NTN,NTD,NTR)
      CALL CONST(N,NN,NUM,NK,DELT,DECAY,RA1,RA2,R,V,RT,VT,MS,A,B,C)
C
      NTT = NTN
C
      NTIME = 1
C
```

```
   14 CALL CLOTH(N,NN,NUM,NTIME,NTR,NK,INDEX,ITHLY,KTHSL,M,R,B,G,
     1U,DELT,RA2,DECAY,MASS,CS,MS,V,KIN,A,C,LIN,LTHLY,NL,LTHSL,NSURF,Q)
      IF(NTIME - NTD)17,16,17
   16 CALL DECON(NTIME,MASS,NSURF,Q,EFFIC,DELT)
   17 IF(NTIME - NTT)19,18,18
   18 CALL PROUT(NUM,N,NTIME,M,MS,U,DELT,INDEX)
      NTT = NTN + NTIME
   19 IF(NTIME - NTOTL) 20,1,1
   20 NTIME = NTIME + 1
      GO TO 14
C
C     FORMATS FOR INPUT AND OUTPUT STATEMENTS
  100 FORMAT(2I3)
  101 FORMAT(8F10.3)
  102 FORMAT(I3,/,(I3,F10.0,F10.0))
  200 FORMAT(//,42X,'CLOTHING PARAMETERS',/,44X,'LAYER',2X,'MS',2X,'RESI
     1STANCE',2X,'CAPACITANCE',/,56X,'(MIN/CM)',6X,'(CM)',/)
  201 FORMAT(46X,I1,4X,I2,3X,F6.3,6X,F8.2)
   99 CALL EXIT
      END
VARIABLE ALLOCATIONS
     A(R )=0093-0000      B(R )=0129-0096      C(R )=01BF-012C      R(R )=0255-01C2      V(R )=02EB-0258     RT(R )=02FA-02EE
    VT(R )=0309-02FD      M(R )=039F-030C   MASS(R )=03AE-03A2  RTHIN(R )=03B1     VTHIN(R )=03B4    RAVEG(R )=03B7
 VAVEG(R )=03BA          U(R )=03BD       DECAY(R )=03C0       DELT(R )=03C3     EFFIC(R )=03C6    TOTAL(R )=03C9
    TN(R )=03CC         TD(R )=03CF          TR(R )=03D2        RA1(R )=03D5       RA2(R )=03D8        G(R )=03DB
    CS(R )=03DE          Q(R )=03E1          MS(I )=03E7-03E4 INDEX(I )=03EC-03E8      N(I )=03ED       NS(I )=03EE
     I(I )=03EF        NUM(I )=03F0       NTOTL(I )=03F1        NTN(I )=03F2       NTD(I )=03F3      NTR(I )=03F4
    NN(I )=03F5         NK(I )=03F6         NTT(I )=03F7      NTIME(I )=03F8     ITHLY(I )=03F9    KTHSL(I )=03FA
   KIN(I )=03FB        LIN(I )=03FC       LTHLY(I )=03FD         NL(I )=03FE     LTHSL(I )=03FF    NSURF(I )=0400

STATEMENT ALLOCATIONS
 100  =0409  101  =040C  102  =040F  200  =0415  201  =0448  1    =046A  2    =0475  3    =04A6  14   =0524  16   =054A
 17   =0552  18   =0558  19   =0568  20   =056E  99   =0576

FEATURES SUPPORTED
 ONE WORD INTEGERS
 EXTENDED PRECISION
 IOCS

CALLED SUBPROGRAMS
 AGENT  INDXX  CONST  CLOTH  DECON  PROUT  ELD    ESTO   CARDZ  PRNTZ  SRED   SWRT   SCOMP  SFIO   SIOFX
 SIOIX  SIOF   SIOI   SUBSC  SDFIO

INTEGER CONSTANTS
     2=0404     1=0405     4=0406     0=0407     3=0408

CORE REQUIREMENTS FOR
 COMMON      0  VARIABLES    1028  PROGRAM     372

END OF COMPILATION

// XEQ
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```
            A MATHEMATICAL MODEL FOR THE PENETRATION
                     OF CLOTHING AND SKIN

TRANSFER OF VAPOUR THROUGH CLOTHED SKIN FROM LIQUID ON AND IN CLOTHING


                SKIN TYPE - AVERAGE
                  RESISTANCE  =  4.000    (MIN/CM)
                  CAPACITANCE =  375.0    (CM)

                WINDSPEED =    6.87        (CM/SEC)
                BOUNDARY LAYER RESISTANCE     0.200  (MIN/CM)
                DECOMPOSITION RATE            0.003  (1/MIN)

                CLOTHING PARAMETERS
                  LAYER  MS  RESISTANCE  CAPACITANCE
                              (MIN/CM)       (CM)

                    1    10    0.050         500.00
                    2    10    0.050         500.00

                TIME CONSTANTS
                  TOTAL TIME         =  30.00    (HOURS)
                  TIME OF DECONTAM   =   0.00    (HOURS)
                  TIME INCREMENT     =   1.00    (HOURS)
                  DELT    = 0.100    (MINUTES)


                SATURATED VAPOR CONCENTRATION
                                SVC = 0.1500E-03  (MG/CM**3)

                       INITIAL LIQUID LOADING

                MASS IN LAYER  1          0.400  MG/CM**2
                MASS IN LAYER  2          0.400  MG/CM**2

                MASS ON SURFACE           0.400  MG/CM**2
```

MASS IN EACH LAYER IN MG/CM**2

| TIME HOURS | U MG/CM**2 | SYSTEMIC DOSE | MASS IN TRANSITIONAL LAYER | MASS IN HORNY LAYER | MASS IN FIRST CLOTH LAYER | MASS IN SECOND CLOTH LAYER |
|---|---|---|---|---|---|---|
| 1.000 | 0.04495 | 0.0000104 | 0.0105808 | 0.0550480 | 0.3051197 | 0.3865000 |
| 2.000 | 0.08991 | 0.0001746 | 0.0146571 | 0.0546033 | 0.2756698 | 0.3730001 |
| 3.000 | 0.13487 | 0.0006346 | 0.0168342 | 0.0546446 | 0.2468674 | 0.3595002 |
| 4.000 | 0.17983 | 0.0013504 | 0.0179844 | 0.0540895 | 0.2192642 | 0.3460002 |
| 5.000 | 0.22479 | 0.0022331 | 0.0185868 | 0.0535365 | 0.1919906 | 0.3325003 |
| 6.000 | 0.26975 | 0.0032130 | 0.0188659 | 0.0530523 | 0.1649487 | 0.3190004 |
| 7.000 | 0.31471 | 0.0042461 | 0.0189405 | 0.0525787 | 0.1381910 | 0.3055005 |
| 8.000 | 0.35967 | 0.0053056 | 0.0188870 | 0.0519900 | 0.1118331 | 0.2920005 |

LIQUID ALL GONE FROM SURFACE AT T= 8.89 (HOURS)

| | | | | | | |
|---|---|---|---|---|---|---|
| 9.000 | 0.40463 | 0.0063757 | 0.0187499 | 0.0512754 | 0.0859523 | 0.2738547 |

LIQUID ALL GONE IN LAYER 1 AT T= 9.56 (HOURS)

| | | | | | | |
|---|---|---|---|---|---|---|
| 10.000 | 0.44862 | 0.0074467 | 0.0185519 | 0.0504966 | 0.0707335 | 0.2062722 |
| 11.000 | 0.49015 | 0.0085124 | 0.0183080 | 0.0496954 | 0.0696731 | 0.1276530 |

LIQUID ALL GONE IN CLOTHING AT T= 11.75 (HOURS)

LAST SLICE TO CONTAIN LIQUID WAS 21

| | | | | | | |
|---|---|---|---|---|---|---|
| 12.000 | 0.52858 | 0.0095687 | 0.0179982 | 0.0477028 | 0.0636273 | 0.0596048 |
| 13.000 | 0.55445 | 0.0106116 | 0.0160290 | 0.0343954 | 0.0442316 | 0.0387056 |
| 14.000 | 0.57191 | 0.0116201 | 0.0130115 | 0.0239987 | 0.0307725 | 0.0268091 |
| 15.000 | 0.58405 | 0.0125380 | 0.0101158 | 0.0167963 | 0.0215104 | 0.0187089 |
| 16.000 | 0.59353 | 0.0133176 | 0.0076603 | 0.0117903 | 0.0150864 | 0.0131069 |
| 17.000 | 0.59849 | 0.0139451 | 0.0056993 | 0.0082952 | 0.0106074 | 0.0092078 |
| 18.000 | 0.60267 | 0.0144320 | 0.0041882 | 0.0058466 | 0.0074726 | 0.0064824 |
| 19.000 | 0.60562 | 0.0148005 | 0.0030505 | 0.0041266 | 0.0052721 | 0.0045712 |
| 20.000 | 0.60770 | 0.0150745 | 0.0022074 | 0.0029157 | 0.0037239 | 0.0032276 |
| 21.000 | 0.60917 | 0.0152759 | 0.0015897 | 0.0020619 | 0.0026328 | 0.0022812 |
| 22.000 | 0.61=21 | 0.0154225 | 0.0011406 | 0.0014590 | 0.0018627 | 0.0016135 |
| 23.000 | 0.61094 | 0.0155286 | 0.0008162 | 0.0010329 | 0.0013186 | 0.0011420 |
| 24.000 | 0.61146 | 0.0156051 | 0.0005828 | 0.0007316 | 0.0009338 | 0.0008086 |
| 25.000 | 0.61183 | 0.0156599 | 0.0004155 | 0.0005183 | 0.0006615 | 0.0005728 |
| 26.000 | 0.61209 | 0.0156991 | 0.0002959 | 0.0003673 | 0.0004687 | 0.0004058 |
| 27.000 | 0.61228 | 0.0157271 | 0.0002105 | 0.0002603 | 0.0003322 | 0.0002876 |
| 28.000 | 0.61241 | 0.0157471 | 0.0001496 | 0.0001845 | 0.0002355 | 0.0002038 |
| 29.000 | 0.61250 | 0.0157613 | 0.0001063 | 0.0001308 | 0.0001669 | 0.0001445 |

CLOTHING REPLACED AT T= 30.00 (HOURS)

| | | | | | | |
|---|---|---|---|---|---|---|
| 30.000 | 0.61257 | 0.0157714 | 0.0000755 | 0.0000870 | 0.0000057 | 0.0000000 |

// PAUS

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A mathematical model which was developed by Monaghan at DRES was extended to predict the penetration of vapour through clothed skin for an initial liquid load on or in the clothing. The model and its associated computer program along with some sample calculations are described in this report.

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Systemic Dose

Vapour Penetration

Vapour Diffusion

Protective Clothing

Liquid Contamination

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