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MODIFICATIONS TO THE VULNERABILITY MODEL

A SIMULATION SYSTEM FOR ASSESSING DAMAGE

RESULTING FROM MARINE SPILLS

FINAL REPORT

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16. Abstract

This report describes several modifications to the U. S. Coast Guard Vulnerability Model which have recently been incorporated. These modifications are in three areas:

1. Revisions of the plume and puff model for toxic damage assessment, to include remodeling of the plume model to reduce computer time and storage space, computing the dosage for the puff model by direct integration, and transferring dosage values computed in Phase I of the Vulnerability Model directly to Phase II.

2. Revision of the thermal injury and the lethality criteria in Phase II based on recent applicable experimental thermal effects data.

3. Remodeling of the flash fire for puff and plume models to compute thermal radiation during both burning and cooling phases for experimentally determined burning rates and maximum surface temperatures.

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Chapter 1

INTRODUCTION

BACKGROUND

This report describes the modification of the Vulnerability Model (VM), a computer simulation which provides quantitative measures of the consequences of maritime spills of hazardous materials. The VM is being developed for the U.S. Coast Guard under contract DOT-CG-33377-A. The first, second, and third stages of development are described in references [1], [2], and [3], respectively. This present report describes the latest modifications.

The VM is a research tool, one use for which is in the USCG Risk Management Program. It has been designed to treat virtually all of the large class of hazardous materials carried in bulk in marine transport. The simulation starts with a description of the nature of the spill, simulates the dispersion of the hazardous material, and assesses the immediate effects of the spill on surrounding vulnerable resources, namely: people, property, and the environment.

The VM requires three types of descriptive data that define: (1) the spill, (2) the physical setting in which the spill occurs, and (3) the vulnerable resources that are subject to the effects of the spill. The spill is described in terms of its location and spill rate, the physical and chemical properties of the spilled material, and the quantity of the spill. The physical setting is described in terms of the geometric configuration of the shoreline(s), hydrologic/oceanographic properties, and meteorological data. Vulnerable resources are described in terms of

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[1] Eisenberg, N. A., C. J. Lynch, and R. J. Breeding, *Vulnerability Model: A Simulation System for Assessing Damage Resulting from Marine Spills*, CG-D-136-75 (NTIS AD-A015 245), Final Report, prepared by Enviro Control, Inc., for Department of Transportation, U.S. Coast Guard, Office of Research and Development, June 1975.

[2] Rausch, A. H., N. A. Eisenberg, and C. J. Lynch, *Continuing Development of the Vulnerability Model: A Simulation System for Assessing Damage Resulting from Marine Spills*, Final Report, prepared by Enviro Control, Inc., for Department of Transportation, U.S. Coast Guard, Office of Research and Development, February 1977.

[3] Rausch, A. H., C. K. Tsao, and R. M. Rowley, *Third-Stage Development of the Vulnerability Model: A Simulation System for Assessing Damage Resulting from Marine Spills*, Final Report, prepared by Enviro Control, Inc., for Department of Transportation, U.S. Coast Guard, Office of Research and Development, June 1977.

demographic distribution, property distribution, and land/water use. The geographic area of concern may represent any user-defined location. The physical setting and the distribution of vulnerable resources are described in terms of mutually exclusive geographic cells that cover the entire area of concern.

The VM operates in two phases. Phase I simulates the spill, the physical and chemical transformations of the spilled substance, and its dissemination in space. This phase covers the time period from the initiation of the spill until a user-specified time has elapsed. Phase I consists of submodels interconnected by an executive routine, with built-in logic dictating the sequence of submodel processing as a function of the spill development. Submodels depicting spill development simulate the following phenomena: (1) cargo v' .ng, (2) surface spreading (with or without evaporation), (3) water mixing, (4) sinking and boiling, (5) air dispersion, and (6) fire and explosion. A time-history file of the spill sequence simulated during the first phase is retained in computer storage on magnetic tape and disk.

In Phase II the computer first matches this time-history file to the vulnerable resources map, and then assesses the effects of toxicity, explosion and/or fire on the vulnerable resources as a function of time. Estimates of deaths and nonlethal injuries to people and of damage to property are presented in computer-generated tables. A summary of the types of Phase II damage is given in the following table.

PHASE II DAMAGE ASSESSMENT

DAMAGE-CAUSING EVENT	VULNERABLE RESOURCE	TYPE OF INJURY OR DAMAGE	CAUSE OF INJURY OR DAMAGE
TOXICITY	People	Death Nonlethal Injury Irritation	Toxic Vapor: Concentration or cumulative dose
EXPLOSION	People	Death	Direct Blast; Impact
		Nonlethal Injury • Eardrum rupture • Bone fracture • Puncture wound • Multiple injury	Direct Blast Impact Flying Fragments Two or more of the above
	Structures	Structural Damage Glass Breakage	Direct Blast
POOL BURNING FIREBALL FLASH FIRE	People	Death First-Degree Burn	Thermal Radiation
	Structures	Ignition	

SCOPE OF WORK

The work on the Vulnerability Model described in this report is made up of three tasks.

Task 1--Modification of plume and puff models for toxic damage assessment.

- A. Remodeling of the plume model to reduce computing time and storage space.
- B. Computing the dosage for the puff model by direct integration.
- C. Transferring dosage values computed in Phase I as specified in (A) and (B) above directly to Phase II.

Task 2--Modification of the thermal injury and lethality criteria in Phase II.

- A. Rederivation of the dose equation based on applicable experimental data.
- B. Revision of the dose criteria for thermal injury and lethality.
- C. Recomputation of the coefficients in the probit equation.

Task 3--Remodeling of flash fire.

- A. Remodeling of the puff model using an adaptation of the fireball model.
- B. Remodeling of the plume model on the same basis as in (A) above.
- C. Recalculation of the mass burned in flash fire.

The results of the three tasks are presented in order in the following three chapters (Chapters 2, 3, and 4). The final chapter (5) summarizes the revisions to the VM computer program incorporating the modifications that have been developed.

CONCLUSIONS

The modifications described in this report make concrete improvements to the VM. The direct integration of toxic dose improves the accuracy of results and saves computing time and data storage. The modification of the probit equation for thermal injury and lethality makes the calculation consistent with experimental results. The modification of the flash fire model provides a more accurate simulation of the thermal radiation emitted from burning vapor clouds.

Chapter 2

MODIFICATION OF PLUME AND PUFF MODELS

INTRODUCTION

For toxic injury, the dose v depends upon both the duration of exposure and the concentration level experienced. The general form of the dose is as follows:

$$v = \int_0^\infty C^n \, dt \tag{2-1}$$

where C is the vapor concentration and n is a real number. To evaluate the dose, a finite difference model had previously been used in the Vulnerability Model (VM). It first calculated the vapor concentration in each cell at each time step and then summed the average of the nth power of concentrations over time. The drawbacks of the finite difference model are:

- Very few physical inferences can be drawn from the numerical results.
- The calculation must start from the first time step and follow the time-step sequence. There is no way to calculate the concentration at the $(j+1)$ time step without calculating the concentration of the first j time steps.
- The accuracy of the results is primarily dependent upon the size of the mesh and the fineness of the time step.
- It prolongs the computing time and burdens the storage capacity of the computer.

To improve accuracy and to reduce computing time, Equation (2-1) is now calculated by direct integration rather than time-stepped integration. This chapter describes how the direct integration is accomplished in the plume and puff models for both exterior and interior dosages.

DERIVATION OF EXTERIOR DOSAGE

In the VM the simulation of vapor dispersion is based on the diffusion equation [4,5]:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) \tag{2-2}$$

where U is the air current or wind velocity along the x-axis, and D_x and D_y and D_z are the diffusion coefficients. Consider an instantaneous point source of strength m located at the origin, with the boundary on the ground ($z = 0$), the wind velocity U and the diffusion coefficients constant; then the solution of Equation (2-2) is:

$$C_i = \frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left(-\frac{(x-Ut)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right) \tag{2-3}$$

where $\sigma_x = \sqrt{2D_x t}$ and $\sigma_y = \sqrt{2D_y t}$ and $\sigma_z = \sqrt{2D_z t}$ are the dispersion coefficients, and

$$m = \int_{-\infty}^{\infty}\int\int \frac{C}{2} dx dy dz \tag{2-3a}$$

is the total amount of material released at the origin at time ($t = 0$). Equation (2-3) is the puff solution.

For a continuous point source in a wind, let the rate of emission be $q(t')$ such that in a short interval from t' to $t' + dt'$ an amount $q\,dt'$ is emitted. Each of these 'puffs' generates its own cloud, and the total concentration field is obtained by the summation of contributions from the individual puffs. For a source maintained indefinitely, the combined concentration field of the many puffs by integration is

$$C_c = \int_0^{\infty} \frac{q\,dt'}{(2\pi)^{3/2}\sqrt{D_x D_y D_z}(t-t')^{3/2}}$$

$$\cdot \exp\left(-\frac{[x-U(t-t')]^2}{2D_x(t-t')} - \frac{y^2}{2D_y(t-t')} - \frac{z^2}{2D_z(t-t')}\right) \tag{2-4}$$

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[4] Crank, J., *The Mathematics of Diffusion*, Oxford University Press, 1956.

[5] Csandy, G. T., *Turbulent Diffusion in the Environment*, Reidel Publishing Co., Boston, 1972.

When $x^2/D_x >> y^2/D_y$ and z^2/D_z the solution is:

$$C_c = \frac{2q}{2\pi U\sigma_y\sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right) \tag{2-5}$$

Equation (2-5) is the plume solution.

The dosage for the puff model is obtained by inserting Equation (2-3) into Equation (2-1) and integrating. The resulting equation is:

$$v_i = \int_0^\infty C_i^n \, dt$$

$$= \left(\frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\right)^n \sqrt{\frac{\pi}{2n}} \frac{\sigma_x}{U} \left[1 + \text{erf}\left(\sqrt{\frac{n}{2}} \frac{x}{\sigma_x}\right)\right] \exp\left[-\frac{n}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)\right] \tag{2-6}$$

where *erf* is the error function.

The plume model does not depend on time. Hence, the dosage in a given cell is simply equal to the product of the *n*th power of concentration and the total evaporation time t_e ; that is:

$$v_c = \left(\frac{2q}{2\pi U\sigma_y\sigma_z}\right)^n t_e \exp\left[-\frac{n}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)\right] \tag{2-7}$$

DERIVATION OF INTERIOR DOSAGE

The time variation of the toxic vapor inside a building is proportional to the infiltration rate and the difference of outside and inside vapor concentration. The equation is written as:

$$V \frac{dC_I}{dt} = I(C_O - C_I) \tag{2-8}$$

where V is the total empty space of the building; I is the rate of infiltration (volume per unit time); C_O is the outside vapor concentration; and C_I is the inside vapor concentration. Equation (2-8) can also be written as:

$$\frac{dC_I}{dt} + RC_I = RC_O \tag{2-9}$$

where $R = I/V$ is the specific infiltration. The infiltration depends mainly on the tightness of the construction and on the wind velocity [6]. For high-rise buildings, the chimney effect is also important. In the case of a building with many partitions and of tight construction, air may enter on the windward side in such quantity as to build up a slight positive pressure and thereby reduce infiltration. In general, it can be assumed that the air which enters the building on the windward side is equal to that which leaves on the leeward side. Empirical equations for infiltration have been developed. In the VM, the following equation is employed [2]:

$$R = 0.25 + 0.02165\,U + 0.00833\,|\Delta T|$$

where U is the wind velocity in miles per hour, and ΔT is the temperature difference between the interior and exterior of the building in °F.

Multiplying Equation (2-9) by the integration factor

$$exp\left(\int_0^t R\,dt\right)$$

and integrating, we obtain

$$C_I = e^{-\int_0^t R\,dt} \int_0^t RC_O\, e^{\int_0^{t'} R\,dt'}\,dt' \qquad (2\text{-}10)$$

Since R is independent of time, Equation (2-10) becomes:

$$C_I = R\,e^{-Rt} \int_0^t C_O\, e^{Rt'}\,dt' \qquad (2\text{-}11)$$

For the plume, model, the outside vapor concentration does not depend upon time, so that

$$C_I = RC_O\, e^{-Rt} \int_0^t e^{Rt'}\,dt' = \frac{2q}{2\pi U\sigma_y\sigma_z}\left(1-e^{-Rt}\right) exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)\right] \qquad (2\text{-}12)$$

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[6] Jennings, B. H., *Environmental Engineering*, International Textbook Company, Scranton, Pennsylvania, 1970.

for which Equation (2-5), the continuous spill solution, has been used for C_O . Equation (2-12) shows that at $t = 0$, $C_I = 0$ and that at $t = \infty$, $C_I = C_O$. The vapor concentration inside the building is attenuated by the factor

$$\left(1 - e^{-Rt}\right).$$

For the puff model, substituting the instantaneous spill solution, Equation (2-3), into Equation (2-11) for C_O we obtain:

$$C_I = \frac{2mR}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)\right] e^{-Rt} \int_0^t \exp\left(-\frac{(x-Ut')^2}{2\sigma_x^2} + Rt'\right) dt'$$

$$= \frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \frac{R\sigma_x\sqrt{2\pi}}{2U} \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)\right] \exp\left(\frac{xR}{U} + \frac{\sigma_x^2 R^2}{2U^2}\right) e^{-Rt}$$

$$\left[erf\left(\frac{x+R\sigma_x^2/U}{\sqrt{2}\,\sigma_x}\right) + erf\left(\frac{Ut-(x+R\sigma_x^2/U)}{\sqrt{2}\,\sigma_x}\right)\right] \qquad (2\text{-}13)$$

In Equation (2-1) if $n=1$ the indoor dosage is:

$$v_I = \int_0^\infty C_I\, dt$$

$$= \int_0^\infty R\, e^{-Rt}\, dt \int_0^t C_O(t) e^{Rt'} dt$$

$$= \int_0^\infty C_O(t) dt = v_0 \qquad (2\text{-}14)$$

If $n \neq 1$, then

$$v_I = \int_0^\infty C_I^n\, dt \neq \int_0^\infty C_O^n\, dt = v_0 \qquad (2\text{-}15)$$

This means that the people inside and outside the building will inhale the same amount of toxic gas but will suffer different effects because of the time delay due to the infiltration.

The general equation of dosage for the plume model is obtained by inserting Equation (2-12) into Equation (2-1).

$$v_I = \left(\frac{2q}{2\pi U\sigma_y\sigma_z}\right)^n exp\left[-\frac{n}{2}\left(\frac{y^2}{\sigma_y^2}+\frac{z^2}{\sigma_z^2}\right)\right]\int_0^{t_e}\left(1-e^{-Rt}\right)^n dt$$

$$= \left(\frac{2q}{2\pi U\sigma_y\sigma_z}\right)^n exp\left[-\frac{n}{2}\left(\frac{y^2}{\sigma_y^2}+\frac{z^2}{\sigma_z^2}\right)\right]$$

$$\cdot\left\{ t_e - \frac{1}{R}\left[n\left(1-e^{-Rt_e}\right) - \frac{n(n-1)}{2\cdot 2!}\left(1-e^{-2Rt_e}\right)\right.\right.$$

$$+ \frac{n(n-1)(n-2)}{3\cdot 3!}\left(1-e^{-3Rt_e}\right) \ldots\ldots$$

$$\left.\left. + (-1)^{p-1}\frac{n(n-1)(n-2)\ldots(n-p-1)}{p\cdot p!}\left(1-e^{-pRt_e}\right) + \ldots\ldots\right]\right\} \qquad (2\text{-}16)$$

Here, instead of using the upper limit of integration of infinity, a finite number, t_e, the evaporation time, is used and the binomial series expansion is employed.

Substituting Equation (2-13) into Equation (2-1) gives the indoor dosage for the puff model as follows:

$$v_I = \left[\frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\frac{\sqrt{2\pi}}{2}\frac{R\sigma_x}{U}\right]^n exp\left[-\frac{n}{2}\left(\frac{y^2}{\sigma_y^2}+\frac{z^2}{\sigma_z^2}\right)\right] exp\left[\left(\frac{xR}{U}+\frac{\sigma_x^2R^2}{2U^2}\right)\right]$$

$$\int_0^\infty e^{-nRt}\left[erf\left(\frac{x+\sigma_x^2R/U}{\sqrt{2}\,\sigma_x}\right) - erf\left(\frac{x+\sigma_x^2R/U - Ut}{\sqrt{2}\,\sigma_x}\right)\right]^n dt \qquad (2\text{-}17)$$

Since n is, in general, a fractional or irrational number, no closed form of solutions of Equation (2-17) is expected. Numerical integration is used to evaluate Equation (2-17). The computing time can be reduced substantially with consideration of the property that $erf(p) \approx 1$ when $p > 5$.

DISCUSSION

The modification of the plume and puff models for toxic gas changes the calculation from the time-step method to direct integration. It improves the accuracy and saves computing time and storage space. Since there are other models that still use the time-step method for calculation, it is impossible to change the VM structure at this stage to eliminate the time-step procedure entirely.

Four test runs have been made to compare the modified VM to the original VM. Two are simulations of ammonia spills using the puff model, and the other two are simulations of chlorine spills using the plume model. For each chemical, one of the two runs is with the original VM and the other is with the modified VM. The following table compares the results between the original and modified runs.

COMPARISON OF RESULTS BETWEEN ORIGINAL AND MODIFIED VM

CHEMICAL		ORIGINAL VM		MODIFIED VM	
		Outdoors	Indoors	Outdoors	Indoors
Ammonia	Deaths	5,568	1,765	5,298	4,770
Chlorine	Deaths	8,659	8,281	7,333	7,089
	Injuries	3,670	0	5,531	6,390

For ammonia, the outdoor toxic deaths for both runs are similar, but the indoor deaths are considerably greater for the modified case. No injuries are shown because no probit equation exists in the VM for toxic injuries from ammonia. For chlorine, the indoor and outdoor toxic deaths for the original and modified cases are similar. However, for injuries, the modified VM yields a significantly greater number, particularly indoors where the old VM computed no injuries.

The input data for these test runs are given in Appendix A. Figure A-1 is a map of the geographical area showing the spill size and location, the wind direction and speed, and the location of the population cells. Figure A-2 presents the Geographic/Demographic file in the VM which shows the population and vulnerable characteristics of each population cell. (Note that cell numbers R31, R32, etc., are river cells which are not shown on the map.) Figures A-3 and A-4 give the input

data for the ammonia and chlorine spills, respectively, and Figure A-5 (extracted from reference [7]) presents the dictionary for interpreting the input field numbers. The modified program saves about 20% in computing expense including computing time and storage over the original program.

NOMENCLATURE AND UNITS

C	vapor concentration	g/cm^3
C_O	outdoor vapor concentration	g/cm^3
C_I	indoor vapor concentration	g/cm^3
D_x, D_y, D_z	diffusivity	cm^2/s
I	infiltration	cm^3/s
q	spill rate	g/s
m	total spill mass	g
R	specific infiltration	s^{-1}
t	time	s
U	wind velocity	cm/s
v	dose	
V	volume	cm^3
x, y, z	coordinates	cm
$\sigma_x, \sigma_y, \sigma_z$	dispersion coefficients	cm

[7] Rowley, R. M., and A. H. Rausch, *Vulnerability Model User's Guide*, Enviro Control, Inc., October 1977.

Chapter 3

MODIFICATION OF THERMAL INJURY AND LETHALITY CRITERIA FOR HUMANS

INTRODUCTION

In the Vulnerability Model, the fire damage to personnel is assessed by the probit equation which is defined as [1]:

$$Pr = a + b \ln v$$

where v is the thermal dosage and a and b are determined from existing experimental data. The thermal dosage, v, depends on the thermal radiation intensity, I, and the exposure time, t. In general, the thermal dosage can be written as:

$$v = tI^{\alpha}$$

where the index α is also determined from experimental data. In the VM, coefficients a and b and index α had been based on nuclear explosion data [8,9]. The thermal radiation from nuclear explosions is primarily in the ultraviolet/ visible spectra with high intensity and short duration. On the other hand, the thermal radiation from hydrocarbon combustion is in the infrared range with low intensity and longer duration. Butterfield [10] has shown that almost twice as much visible radiation is required to produce an equivalent injury caused by an infrared radiation source. Owing to these differences, data from sources other than nuclear explosions have now been used to determine the coefficients a and b, and the index α.

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[8] Glasstone, S. (ed.), *The Effects of Nuclear Weapons*, USAEC, April 1962.

[9] White, Clayton, S., *The Nature of the Problems Involved in Estimating the Immediate Casualties from Nuclear Explosions*, CEX 71.1, Lovelace Foundation of Medical Education and Research, Albuquerque, New Mexico, March 1971.

[10] Butterfield, W. J. H., E. R. Drake Seager, et al., Flash burn from atomic weapons, *Surgery, Gynecology and Obstetrics 103*(6):655-665, December 1956.

DERIVATIONS

Exponent α

In the VM, the thermal dosage is expressed by

$$v = tI^{4/3} \tag{3-1}$$

where t is in seconds and I is in joule/m^2-sec. The data from which the value of $\alpha = 4/3$ was deduced are reproduced in Table 3-1. It is obvious that Equation (3-1) is for fire deaths. However, the same expression had been used in the VM for fire injuries.

Table 3-1. RELATIONSHIP OF DEATH FROM RADIATION BURNS TO RADIATION LEVEL AND DURATION

Portion Killed (%)	Duration (s)	Radiation Intensity		Dosage $tI^{4/3}$
		(cal/cm^2-s)	(joule/m^2-s)	
1	1.43	3.50	146,000	1099×10^4
1	10.1	0.792	33,100	1073×10^4
1	45.2	0.243	10,200	1000×10^4
50	1.43	6.30	263,600	2417×10^4
50	10.1	1.385	57,950	2264×10^4
50	45.2	0.442	18,500	2210×10^4
99	1.43	14.0	586,000	7008×10^4
99	10.1	3.07	128,000	6546×10^4
99	45.2	0.952	39,800	6149×10^4

The sequence of data is for 20-KT, 1-MT, and 20-MT weapons. The dosage has been calculated for the radiation intensity in joule/m^2-s .

Figure 3-1 shows the human skin tolerance time to absorbed thermal energy. The blister-line corresponds to second-degree burns and the survival-line, to first-degree burns. The slope of the pain-line is -4/3, that of the survival-line is -1.35, and that of the blister-line is -1.375. Therefore, the thermal dosage for pain is

$$v_p = tI^{4/3}$$

and for first-degree burns is

$$v_1 = tI^{1.35}$$

and for second-degree burns is

$$v_2 = tI^{1.375}$$

There are no curves given for third-degree burns and fire deaths. In view of these values, $\alpha = 4/3$ has been retained for the thermal lethality and injury (first-degree burns) probit equations in the VM.

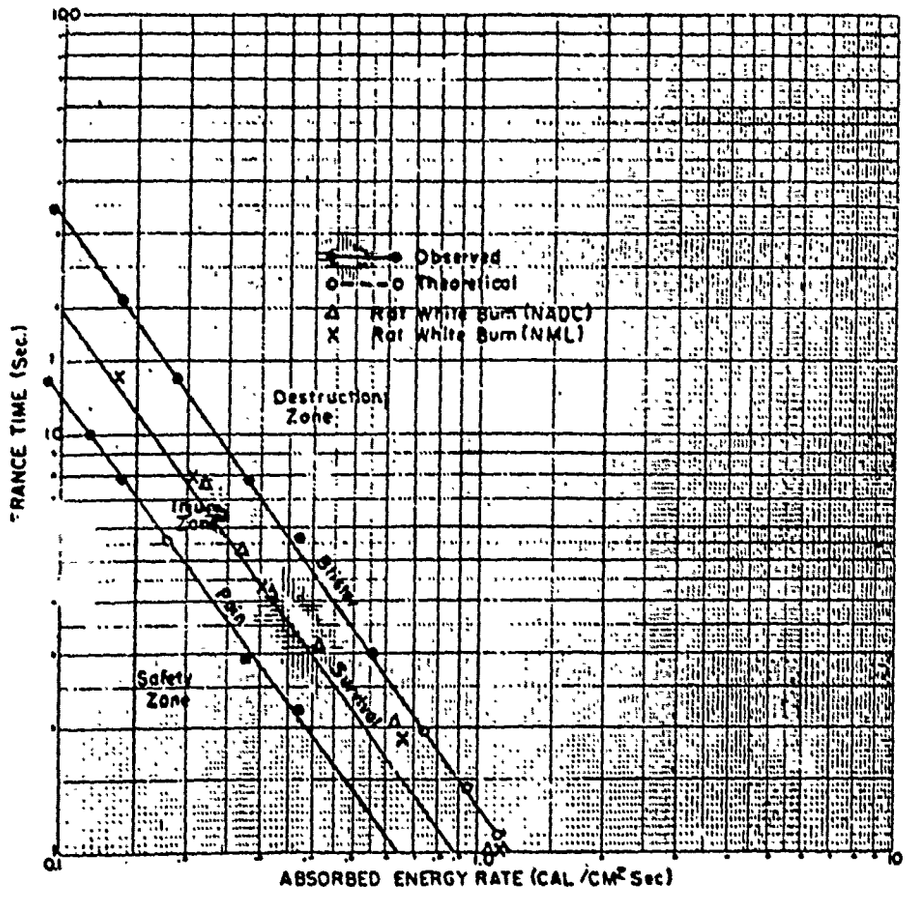

Figure 3-1. Human Skin Tolerance Time to Absorbed Thermal Energy Delivered in a Rectangular Heat Pulse

Thermal Injury Probit

In the VM, the probit equation for thermal injury was:

$$Pr = -42.25 + 3.0186 \ln (tI^{4/3}) \quad (3\text{-}2)$$

When injury is 1% ($Pr = 2.67$), the dosage is:

$$v = tI^{4/3} = 2,902,500$$

In Figure 3-1, the dosage for first-degree burns is calculated as:

$$tI^{4/3} = 1,280,000$$

In reference [10], the threshold for first-degree burns is 0.94 cal/cm^2 (3.93×10^4 joule/m^2) for a one-second duration. Thus:

$$tI^{4/3} = 1,336,100$$

In reference [11], the threshold for first-degree burns is 1.2 cal/cm^2 (5.021×10^4 joule/m^2) for a duration of 3 seconds. Thus:

$$tI^{4/3} = 1,284,300$$

The average of the last three figures is approximately 1,300,000. The value of 2,902,500 from the VM is about 2.23 times higher than this average. Using the factor of 2.23 to modify Equation (3-2), we obtain a new probit equation for thermal injury:

$$Pr = -39.83 + 3.0186 \ln (tI^{4/3}) \quad (3\text{-}3)$$

Although this adjustment factor has been derived on the basis of the 1% level of first-degree burns, it is assumed to hold for all levels, in the absence of specific data for these other levels.

Thermal Lethality Probit

The probit equation for burn deaths in the VM was:

$$Pr = -14.9 + 2.56 \ln (tI^{4/3}/10^4)$$

For burn deaths, no other data besides the nuclear explosion are available. Using the same modifying factor of 2.23, the probit equation for deaths now becomes:

$$Pr = -12.8 + 2.56 \ln (tI^{4/3}/10^4)$$

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[11] Hardy, J. D., H. G. Wolff, and H. Goodell, Studies in pain, new method for measuring pain threshold: Observations on spatial summation of pain, *Journal of Clinical Investigation 19*, 1940.

NOMENCLATURE AND UNITS

I	radiation intensity	J/m^2-s
t	time	s
Pr	probit	
v	thermal dose	
α	index	

Chapter 4

REMODELING OF FLASH FIRE

INTRODUCTION

The flash fire model had been designed using assumptions and data deemed appropriate for the first stage of development. Some of the simulated results were incompatible with experimentally observed data. Consequently, the model may underestimate injuries and deaths under certain conditions. There are three assumptions made during this first stage of development that should be modified to correct for these deficiences. First, in the flash fire model the air-fuel mixture is divided into two parts [1]. The concentration of the outer part varies from the lower flammable limit to stoichiometric. The concentration of the inner part varies from stoichiometric to upper flammable limit. It is assumed that the outer portion burns completely and that the inner portion burns incompletely from lack of sufficient oxygen content. This assumption underestimates the vapor quantity that takes part in combustion and, in turn, underestimates the total thermal radiation. For example, in Appendix C2 of the VM [1], the ratio of upper flammable limit to lower flammable limit of methane is 2.642 ([1], Table C2-1). From Figure C2-1 in reference [1], it is found that the amount of fuel consumed is about 40% of the total vapor. The real situation is that, after the fire starts, the hot gas causes a strong turbulent flow to speed up the mixing of the fuel with the ambient air. A small percent of the fuel vapor will escape to the ambient atmosphere, but the remainder will burn out.

The second assumption is that the combustion is instantaneous. Therefore, the thermal radiation from the burning fuel is neglected. Actually, the thermal radiation in the combustion period is of the same order as that in the cooling period. The total combustion time of the fuel vapor depends on the mixing process and the flame speed.

Third, in the cooling period, the hot gas is assumed to be cooled from the initial temperature T_i to a "half life" temperature T_g, which is defined as the average of the initial temperature T_i and the ambient temperature T_0, i.e., $T_g = (T_i + T_0)/2$. Based on this assumption, an expression for cooling time t is derived (Equation (4-18), reference [1]). The cooling time computed from this equation is improper. For example, the cooling time for a gas with a higher initial temperature or a larger vapor mass is shorter than that for a gas with a lower initial temperature or a smaller vapor mass. The "half life" criterion which is used in linear problems such as nuclear radiation decay and mechanical vibration damping is not suitable for a nonlinear problem such as thermal radiation.

To remedy this difficulty and to base the flash fire simulation more accurately on physical reality, a new flash fire model has been developed using a modification of the fireball model [12,13,14].

ASSUMPTIONS IN THE MODIFIED FIREBALL MODEL

The fireball model was originally designed for liquid propellant rocket explosions on a launchpad. The general assumptions for that model are as follows [13,14]:

(1) The rate of fuel addition to the fireball is constant.

(2) A stoichiometric mixture is assumed to exist at ignition.

(3) All the available fuel participates in the reaction.

(4) The fireball is an isothermal, homogeneous body which is spherical at all times.

(5) The fireball radiates as a blackbody.

(6) The fuel burnout time and the fireball liftoff time coincide.

Assumptions (1) and (6) can only be applied to a liquid fuel spilled on the ground and are inapplicable to the present problem. Assumptions (2) to (5) are applicable to the modified fireball model. One additional assumption for the present fireball model is that the flame speed is constant. A laboratory experiment [15] showed that, as a first approximation, the flame propagation took place at nearly constant velocity. Another assumption which was used but not mentioned in the original fireball model is that the fire started at the center and propagated radially outward. We will retain this assumption also.

The general assumptions in the modified flash fire model are:

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[12] Kite, F. D., and B. E. Bader, Pad-Abort Thermal Flux Model for Liquid Rocket Propellants, SC-RR-66-577, Sandia Laboratory, Albuquerque, New Mexico, November 1966.

[13] Bader, B. E., A. B. Donaldson, and H. C. Hardee, Liquid-propellant rocket abort fire model, *Journal of Spacecraft and Rockets 8*(11): 1216-1219, 1971.

[14] Hardee, H. C., and D. O. Lee, Thermal hazard from propane fireballs, *Transportation Planning and Technology 2*:121-128, 1973.

[15] Leyer, J. C., C. Guerraud, and N. Manson, Flame propagation in small spheres of unconfined and slightly confined flammable mixtures, in *Fifteenth Symposium on Combustion*, The Combustion Institute, Penn State University, 1974.

(1) Fire starts at the center and propagates with constant velocity outward.

(2) The fuel-air mixture is stoichiometric and homogeneous.

(3) The fireball is an isothermal spherical body.

(4) The fireball is a blackbody.

(5) All the fuel participates in the reaction.

DERIVATIONS

Burning Mass

Consider a fireball of radius $r(t)$. The flame front propagates outward and advances a distance δr in the time δt. The energy balance equation in the thin layer between r and $r + \delta r$ is:

$$\rho_f H 4\pi r^2 \delta r = \sum_j \rho_i C_{pi} (T - T_0) 4\pi r^2 \delta r + \varepsilon\sigma (T^4 - T_0^4) 4\pi r^2 \delta t \qquad (4\text{-}1)$$

where: ρ_f is the fuel density; H is the heat of combustion; ρ_i is the density and C_{pi} is the specific heat at constant pressure of the ith product; T_0 is the ambient temperature; σ is the Stefan-Boltzmann constant; and ε is the emissivity of the gas which is equal to unity in the present case. Let $\delta r/\delta t = S$, the flame velocity. Then Equation (4-1) becomes:

$$S\rho_f H = S \sum_i \rho_i C_{pi} (T - T_0) + \varepsilon\sigma (T^4 - T_0^4) \qquad (4\text{-}2)$$

The combustion is isobaric, so that the density ρ depends upon temperature T only, or $\rho = \rho(T)$. The specific heat C_p is also a function of temperature, or $C_p = C_p(T)$. Therefore, when the flame velocity S is known, the flame temperature T can be solved from Equation (4-2). On the other hand, if the flame temperature is measured, then the flame velocity is obtained from Equation (4-2). Usually in laboratory experiments the flame velocity is measured, and in field tests the flame temperature is measured [16,17].

Due to turbulent mixing, most of the gas in a vapor cloud will be burned once ignition takes place. As a conservative assumption, we will assume that the portion of the vapor cloud with concentration above the lower limit of inflammability, C_L, will be burned in the flash fire.

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[16] Strehlow, R. A., *Fundamentals of Combustion*, International Textbook Co., Scranton, Pennsylvania, 1968.

[17] American Gas Association, *LNG Safety Program. Interim Report on Phase II Work*, July 1974.

By rewriting Equation (2-3) as

$$C = \frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left(-\frac{(x-Ut)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right) \tag{4-3}$$

and letting $(x-Ut)/\sigma_x = x'$, $y/\sigma_y = y'$, $z/\sigma_z = z'$, we obtain:

$$C = \frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{1}{2}\left(x'^2 + y'^2 + z'^2\right)\right]$$

$$= \frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left(-\frac{1}{2}r^2\right) \tag{4-4}$$

Equation (4-4) transforms the ellipsoid into a sphere with $r^2 = x'^2 + y'^2 + z'^2$. When $C = C_L$, from Equation (4-4)

$$r_L = \left[-2\ln\left(\frac{2m}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z C_L}\right)\right]^{1/2} \tag{4-5}$$

r_L is the radius of equi-concentration surface. The total fuel consumed in the fire is the mass inside the sphere of radius r_L.

$$M_f = \frac{m}{(2\pi)^{3/2}} \iiint \frac{1}{\sigma_x\sigma_y\sigma_z} \exp\left(-\frac{x'^2 + y'^2 + z'^2}{2}\right) dx\, dy dz$$

$$= \frac{m}{(2\pi)^{3/2}} \iiint \exp\left(-\frac{x'^2 + y'^2 + z'^2}{2}\right) dx' dy' dz' \tag{4-6}$$

To carry out the integration, it is better to transform Equation (4-6) from Cartesian coordinates (x', y', z') to spherical coordinates (r, θ, ϕ) where θ is the latitude and ϕ is the azimuthal angle. Under this transform, Equation (4-6) becomes

$$M_f = \frac{m}{(2\pi)^{3/2}} \int_0^{r_L} e^{-\frac{1}{2}r^2} r^2 dr \int_0^{\pi} \sin\theta d\phi \int_0^{2\pi} d\phi$$

$$= m\left[\operatorname{erf}\left(\frac{r_L}{\sqrt{2}}\right) - \sqrt{2/\pi}\, r_L\, e^{-r_L^2/2}\right] \tag{4-7}$$

For a real spill, $erf(r_L/\sqrt{2}) \simeq 1$ and $r_L\, e^{-r_L^2/2} \simeq 0$, then $M_f \simeq m$, the total mass of fuel. For the plume model, using Equation (2-5) and following the same procedure, it will turn out that $M_f = qt_e$, where t_e is the total evaporation time. The maximum fireball radius r_b is determined from the total mass of products, $M_0 = M_f + M_a$, where M_a is the mass of air,

$$M_0 = \frac{4}{3}\pi r_b^3 \rho_p \tag{4-8}$$

where ρ_p is the average density of products at temperature T_f. For $\rho_p T_f = \rho_{p0} T_0$ where ρ_{p0} is the average density at ambient temperature T_0, then:

$$r_b = \left(\frac{3}{4}\frac{M_0 T_f}{\pi \rho_{p0} T_0}\right)^{1/3} \tag{4-9}$$

Since the fuel mass M_f is given, it is easier to estimate the radius r_b by the following relation,

$$r_b = \left[\frac{3 M_f T_f}{4 \pi \rho_{f0} T_0}\right]^{1/3} \tag{4-9a}$$

where ρ_{f0} is the fuel density at ambient temperature.

Burning Phase Thermal Dose

The probit equation for thermal damage to personnel is:

$$Pr = a + b \ln v \tag{4-10}$$

where a and b are constants and v is the thermal dosage. The thermal dosage depends upon the radiation intensity absorbed by the body and the duration. In the VM, the thermal dosage is given by the equation:

$$v = \int I^{4/3} dt \tag{4-11}$$

The radiation intensity is calculated from the equation as follows:

$$I = \alpha \varepsilon \sigma F_{12} T^4 \tag{4-12}$$

where α is the absorptivity of the body and F_{12} is the view factor. The view factor for a flat surface of unit area at a distance d from the fireball center is given by [18]:

$$F_{12} = \left(\frac{r}{d}\right)^2 \tag{4-13}$$

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[18] Love, T. J., *Radiative Heat Transfer*, Merrill Publishing Company, Columbus, Ohio, 1968.

With Equations (4-12) and (4-13), the thermal dosage becomes:

$$v = \int \left(\alpha\varepsilon\sigma T^4 \frac{r^2}{d^2}\right)^{4/3} dt \qquad (4\text{-}14)$$

For a growing fireball, the flame temperature $T = T_f$ is constant and $dt = dr/S$, Equation (3-14) can be integrated as:

$$v = \frac{1}{S}\left(\alpha\varepsilon\sigma T_f^4\right)^{4/3} \int_0^{r_b} \left(\frac{r}{d}\right)^{8/3} dr = \frac{3}{11}\frac{1}{S}\left(\alpha\varepsilon\sigma T_f^4\right)^{4/3}\left(\frac{r_b}{d}\right)^{8/3} r_b \qquad (4\text{-}15)$$

Cooling Phase Thermal Dose

After the fuel is burned out, the fireball starts to cool down through the radiation heat loss. The energy equation of the cooling process is in the form:

$$-\sum_i \rho_i C_{pi} V\, dT = A\varepsilon\sigma\left(T^4 - T_0^4\right)dt \qquad (4\text{-}16)$$

where V is the volume and A is the surface area of the fireball. From Equation (4-16) we have:

$$dt = -\frac{V\sum_i \rho_i C_{pi}}{A\varepsilon\sigma(T^4 - T_0^4)}\, dT \qquad (4\text{-}17)$$

and by substituting Equation (4-17) into Equation (4-14), we obtain:

$$v = -(\alpha^4\varepsilon\sigma)^{1/3} \int_{T_f}^{T_e} \left(T^4 \frac{r^2}{d^2}\right)^{4/3} \frac{V\sum_i \rho_i C_{pi}}{A(T^4 - T_0^4)}\, dT \qquad (4\text{-}18)$$

where the integration limit T_e is the final temperature. Since $V/A = r/3$, $r = r_b (T/T_f)^{1/3}$ and $\rho_i T = \rho_{i0} T_0$, Equation (4-18) can be transformed to:

$$v = (\alpha^4\varepsilon\sigma)^{1/3} T_0 \left(\frac{r_b}{d}\right)^{8/3} \frac{r_b}{3 T_f^{11/9}} \int_{T_e}^{T_f} \frac{T^{50/9}\sum_i \rho_{i0} C_{pi}}{T^4 - T_0^4}\, dT \qquad (4\text{-}19)$$

The specific heat C_{pi} is a function of temperature. Empirical equations are designed to fit the experimental data. However, the best-fit

equations are not always in a similar form [19]. For example, the equations for air, hydrogen, carbon dioxide, and steam are as follows:

$$\text{air:} \quad C_p = a_1 + b_1 T + c_1 T^2$$

$$H_2: \quad C_p = a_2 + b_2 T + c_2/T^{1/2}$$

$$CO_2: \quad C_p = a_3 + b_3/T + c_3/T^2$$

$$H_2O: \quad C_p = a_4 + b_4/T^{1/4} + c_4/T$$

where the a's, b's, and c's are constants. For a first approximation, we will assume that C_p is constant. Integration of Equation (4-19) yields:

$$v = 9(\alpha^4 \varepsilon \sigma)^{1/3} (\sum_i \rho_{i0} C_{pi}) T_0 \left(\frac{r_b}{d}\right)^{8/3} \frac{r_b}{T_f^{11/9}}$$

$$\cdot \left\{ T_f^{23/9} \sum_{j=0}^{\infty} \frac{1}{-13 - 36(j-1)} \left(\frac{T_0}{T_f}\right)^{4j} - T_e^{23/9} \sum_{j=0}^{\infty} \frac{1}{-13 - 36(j-1)} \left(\frac{T_0}{T_e}\right)^{4j} \right\} \tag{4-20}$$

Here the series expansion of $[1 - (T_0/T)^4]^{-1}$ has been used. In general, the final temperature T_e is the ambient temperature T_0. Here we will choose $T_e = 1.1\ T_0$. This choice will not affect the results of thermal damage, because at such a low temperature the radiation effect is negligible, but it will enhance the convergence of the series. When $T_0/T_e = 1/1.1$, the series is equal to:

$$\sum_{j=1}^{\infty} = \frac{1}{-13 - 36(j-1)} \left(\frac{1}{1.1}\right)^{4j} = -.0263656$$

and then:

$$v = 9(\alpha^4 \varepsilon \sigma)^{1/3} (\Sigma \rho_{i0} C_{pi}) T_0 \left(\frac{r_b}{d}\right)^{8/3} \frac{r_b}{T_f^{11/9}}$$

$$\cdot \left\{ T_f^{23/9} \sum_{j=0}^{\infty} \frac{1}{-13 - 36(j-1)} \left(\frac{T_0}{T_f}\right)^{4j} + .02067\ T_0^{23/9} \right\} \tag{4-21}$$

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[19] Faires, V. M., *Thermodynamics*, 5th edit., Macmillan & Company, New York, 1970.

In the VM, the assessment of fire damage to structures is based on studies of the ignition of wood [1]. Factors influencing wood ignition are: (1) radiation intensity level, (2) duration of radiation exposure, and (3) wood type. Wood type is not treated explicitly; average values are used. The criteria for ignition of structures are:

1. The radiation intensity, I_m, must exceed the value:

$$I_m = 1.34 \times 10^7 \qquad \text{erg/cm}^2\text{-s} \tag{4-22}$$

2. The effective duration of the radiation, t_{eff}, must exceed the value given by:

$$t_m = \left(\frac{1.23 \times 10^8 \ \text{erg/cm}^2\text{-s}}{I - I_m}\right)^{3/2} = \frac{1.364 \times 10^{12}}{(I - I_m)^{3/2}} \tag{4-23}$$

The criterion (4-22) can be used in the present case. However, the criterion (4-23) has to be modified because the radiation intensity I is a variable. We will define a thermal dosage for structural ignition as:

$$v = \int (I - I_m)^{3/2} dt \tag{4-24}$$

If $v > 1.364 \times 10^{12}$, then there is ignition in structures.

Figure 4-1 is a sketch of radiation intensity I vs. time t. To study the structural ignition, we have to locate the points 1 and 2 and then integrate Equation (4-24) from t_1 to t_b and from t_b to t_2. First, for the burning fireball:

$$I_m = \alpha\varepsilon\sigma \frac{r_m^2}{d^2} T_f^4$$

where r_m is the fireball radius corresponding to the radiation intensity I_m. Substituting I_m into Equation (4-24), we obtain:

$$v_1 = \left(\alpha\varepsilon\sigma \frac{T_f^4}{d^2}\right)^{3/2} \frac{1}{S} \int_{r_m}^{r_b} \left(r^2 - r_m^2\right)^{3/2} dr$$

$$= \frac{1}{4S} \left(\frac{\alpha\varepsilon\sigma T_f^4}{d^2}\right)^{3/2} \left[r_b \left(r_b^2 - r_m^2\right)^{3/2} - \frac{3 r_b r_m^2}{2} \left(r_b^2 - r_m^2\right)^{1/2} + \frac{3 r_m^4}{2} \ln \frac{r_b + \left(r_b^2 - r_m^2\right)^{1/2}}{r_m} \right] \tag{4-25}$$

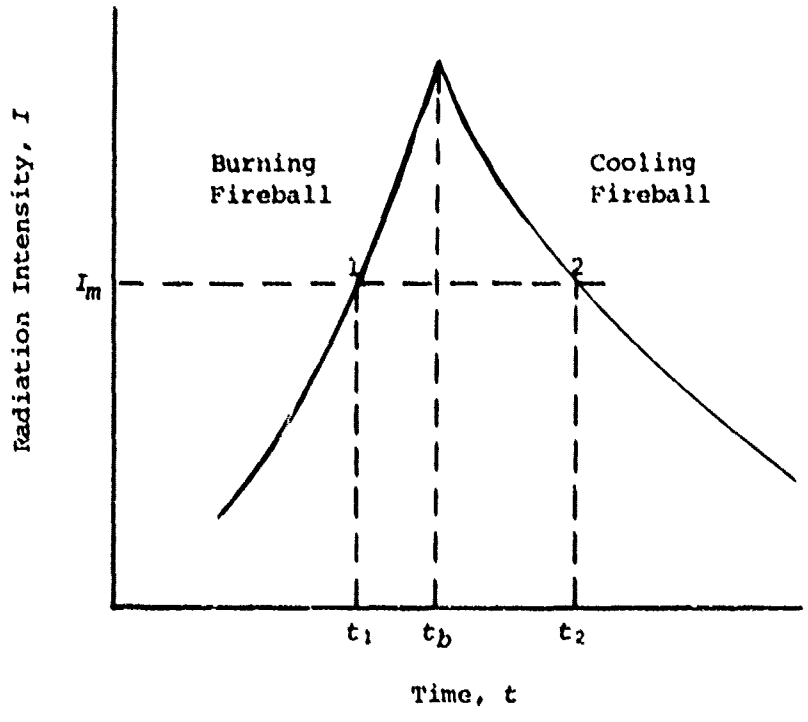

Figure 4-1. Variation of Radiation Intensity of Fireball

For a cooling fireball, the thermal radiation intensity is:

$$I = \alpha\varepsilon\sigma\left(\frac{r}{d}\right)^2 T^4 = \alpha\varepsilon\sigma\left(\frac{r_b}{d}\right)^2 \frac{T^{14/3}}{T_f^{2/3}} \qquad (4\text{-}26)$$

Here the relation $r/r_b = (T/T_f)^{1/3}$ has been used.

When $I = I_m$, the temperature at point 2 is:

$$T_2 = \left(\frac{I_m d^2 T_f^{2/3}}{\alpha\varepsilon\sigma r_b^2}\right)^{3/14}$$

The dosage v_2 is obtained as follows:

$$v_2 = \int_{T_f}^{T_2} (I - I_m)^{3/2} dt$$

$$= \left(\frac{\alpha\sigma r_b^2}{d^2}\right)^{3/2} \frac{T_0 r_b \sum_i \rho_{f0} C_{pi}}{3\varepsilon\sigma T_f^{4/3}} \cdot \left\{ 3T_f^{10/3} \left[\frac{1}{10} + \frac{3}{8}\left(\frac{T_2}{T_f}\right)^{14/3} \right.\right.$$

$$\left. - \frac{1}{48}\left(\frac{T_2}{T_f}\right)^{28/3} - \frac{1}{2}\left(\frac{T_0}{T_f}\right)^4 - \frac{3}{32}\left(\frac{T_2}{T_f}\right)^{14/3}\left(\frac{T_0}{T_f}\right)^4 \right]$$

$$\left. - 3T_2^{10/3}\left[.4556 - .4188\left(\frac{T_0}{T_2}\right)^4 - .0536\left(\frac{T_0}{T_2}\right)^8\right]\right\} \qquad (4\text{-}27)$$

In deriving this equation, the binomial expansion and Equations (4-17) and (4-26) are used. $v = v_1 + v_2$ is the total radiation dose. If v is greater than or equal to v_m ($v_m = 1.364 \times 10^{12}$), the structure will be ignited.

DISCUSSION

The modification of flash fire is based on the fireball model. For both the puff and the plume, it has been shown that the fuel consumed in the fire is very close to the total evaporated mass. The equivalent fireball diameter is determined from the total evaporated mass (Equation (4-8)). For the case of vapor clouds arising from instantaneous spills, the spherical fireball model is a good approximation to the ellipsoidal puff cloud. However, for continous spills which form a plume, the shape of a plume is an elongated truncated ellipsoid. When the ignition cell is not far from the spill center, the spherical fireball is a reasonable approximation for the plume fire, as has been assumed in references [13] and [14]. But when the ignition cell is far downwind, the fireball model is not suitable for the plume because of the significant geometrical difference. This difference affects both the area covered by the vapor cloud and the view factor calculation. In this case, either an ellipsoidal or a cylindrical fireball model should be used. Neither of these has been developed at this time. Consequently, for a continuous spill, the flash fire computation is presently limited to situations in which ignition occurs fairly close to the spill site and the ratio of the major to minor axis for the truncated ellipsoid is less than three.

In the energy balance equation (4-1), the conduction and convective heat transfer are not included. The conduction heat transfer is smaller than the radiation heat transfer. In reference [13] the authors mention that, for a flat plate, the convective heat transfer is about 1/32 of the radiation heat transfer. For a fireball, there is no solid boundary, and it is by no means clear that the convective heat transfer can be neglected. Consequently, further investigation of the role of convective heat transfer in the fireball model is needed.

In the derivation of Equation (4-1), it is assumed that the fireball is an isothermal, homogeneous body. In reality, the temperature at the fireball center is the highest and then decreases toward the boundary. The temperature obtained from Equation (4-1) for a given flame speed is an average value between the maximum and the surface temperature. But in the damage assessment, the thermal radiation is from the fireball surface. In Equation (4-15) the thermal dose depends upon the flame speed and fireball surface temperature. Therefore if the average temperature obtained from Equation (4-1) is used in the dose calculation, an overestimated damage will result.

Take methane as an example. The following table is obtained from Equation (4-1)

Flame temperature, °K	2000	1900	1800	1400
Flame speed, m/s	4.44	3.12	2.20	0.74

From laboratory and field measurements, the flame speed is in the range of 3 to 5 m/s [20,21]. The field measurements of LNG fires indicate that the surface temperature lies between 1000 and 1400°K [22]. If we use a value of 4.44 m/s for the flame speed, then we obtain from Equation (4-1) a flame temperature of 2000°K and, in turn, a very high thermal dose from Equation (4-15). Similarly, if we use a value of 1400°K for flame temperature, then we obtain a lower than usual flame speed of 0.74 m/s from Equation (4-1) and, in turn, from Equation (4-15) we obtain a very high thermal dose. No matter which measured value, temperature or flame speed, is used in Equation (4-1), an unusually high thermal damage will result. To resolve this difficulty at the present time, we will not use Equation (4-1); instead, we will use measured values for both flame temperature and flame speed in Equation (4-15).

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[20] Lewis, B., and Von Elbe, *Combustion, Flames and Explosions of Gases*, Academic Press, 1951.

[21] Pangor, E., *Flame Photometry*, Van Nostrand, 1967.

[22] Kanury, A. Murty, *Introduction to Combustion Phenomena*, Golden and Breach, 1975.

The original fireball model was designed for rocket fuel and oxidizer. Since there is no nitrogen in the fuel-oxidizer mixture, the flame speed is higher than in a fuel-air mixture. Because of this difference, a comparison of the results of the original fireball model with those of the modified flash fire model would be meaningless.

The modified flash fire model is divided into two phases: the burning phase and the cooling phase. The duration of each phase depends on the flame velocity and the vapor quantity. The burning time may take several minutes for large vapor clouds, and the cooling time much longer. In an actual situation, as soon as the fire starts the exposed people will attempt to evade the radiation by running to a shielded location. Those who survive or are not seriously injured during the time it takes to reach a sheltered position will most likely not be killed or injured during the remainder of the radiant period. Because of this evasive action, the casualty assessment for flash fire should be made for a radiation intensity integration time corresponding to the time required for the people to reach shielded positions. In a normal residential or urban area, 30 seconds would be a reasonable time for most people to attain shelter. However, for people located on a beach or in a stadium, a much longer integration time would be required. Consequently, the user must select the integration time to suit the particular situation being studied. For the case of structural ignition, the integration time would be for the entire time period that the radiation intensity exceeds the threshold value.

Four test runs have been made with the modified flash fire model. These are made for an instantaneous LNG spill of 25,000 m^3 at the same location and for the same wind conditions as shown in Figure A-1 (Appendix A). Thus, the geographic/demographic file of Figure A-2 applies. The four runs correpond to integration times of 30 seconds, 60 seconds, entire burning time (109 seconds), and infinity (entire burning and cooling time). The table below presents the casualties for these four cases. Figure A-6 in Appendix A is a listing of the inputs for these test runs.

Integration Time	*Injuries*	*Deaths*	*Buildings Destroyed*
30 s	55	30	NA
60 s	1,969	1,554	NA
109 s (burning time)	5,808	5,622	NA
Infinity	10,374	47,362	5,648

These results show the strong dependency of tne casualties on the integration times. Thus, it is important in assessing casualties from flash fire to use realistic estimates of time required for evasive action.

NOMENCLATURE AND UNITS

A	area	cm^2
C_p	specific heat	erg/g
d	distance	cm
H	heat of combustion	erg/g
I	radiation intensity	erg/cm^2-s
n	index	
v	dosage	
r	radius	
S	flame velocity	cm/s
t	time	s
T	temperature	°K
V	volume	cm^3
α	absorptivity	
ε	emissivity	
ρ	density	g/cm^3
σ	Stefan-Boltzmann constant	erg/cm^2-s-$°K^4$

Chapter 5

SUMMARY OF REVISIONS TO VULNERABILITY MODEL COMPUTER PROGRAM

INTRODUCTION

Major programming revisions to modify the puff and plume models for toxic chemicals and the flash fire model for flammable gases have been made to the VM. A general overview of each modification, changes to the user input, and flowcharts of major programs and subroutines are given in this chapter.

PHASE I

Executive Program, VMEXEC (Figure 5-1)

The main program of the Vulnerability Model (VM), called VMEXEC, initializes the data files and controls the execution of the various simulation submodels over each time step for each geographic cell. VMEXEC is now modified to call a subroutine DOSAGE at the end of the program. The subroutine DOSAGE integrates the dose for the puff and plume models for each geographic cell. The time step call in VMEXEC operates as usual because models such a pool burning still use the time step calculation.

New Subroutine, DOSAGE (Figure 5-2)

Subroutine DOSAGE computes the outdoor dose and indoor dose for each cell for plume and puff models. This subroutine recalls some variables from the State file. The dispersion coefficients for the plume model are from subroutine CSSIGS and those for the puff model are from subroutine ISSIGS. If the outdoor dose is less than the threshold value, the outdoor and indoor doses are set equal to zero. The indoor dose is set equal to zero when it is less than the threshold value. This will save some computing time. Both outdoor and indoor doses are written on a tape which is transferred to Phase II for processing.

Subroutine, FLFIRE (Figure 5-3)

The subroutine FLFIRE computes the thermal dose for the burning and cooling periods for personnel fire casualties for each cell. It also computes the accumulated thermal radiation for structural ignition at each cell. Both thermal dose and accumulated radiation for ignition are written on tape for Phase II processing. In addition, for the secondary fire model the subroutine computes the distance from the flash fire to each secondary fire source and the radiation flux from the flash fire received at the secondary source location.

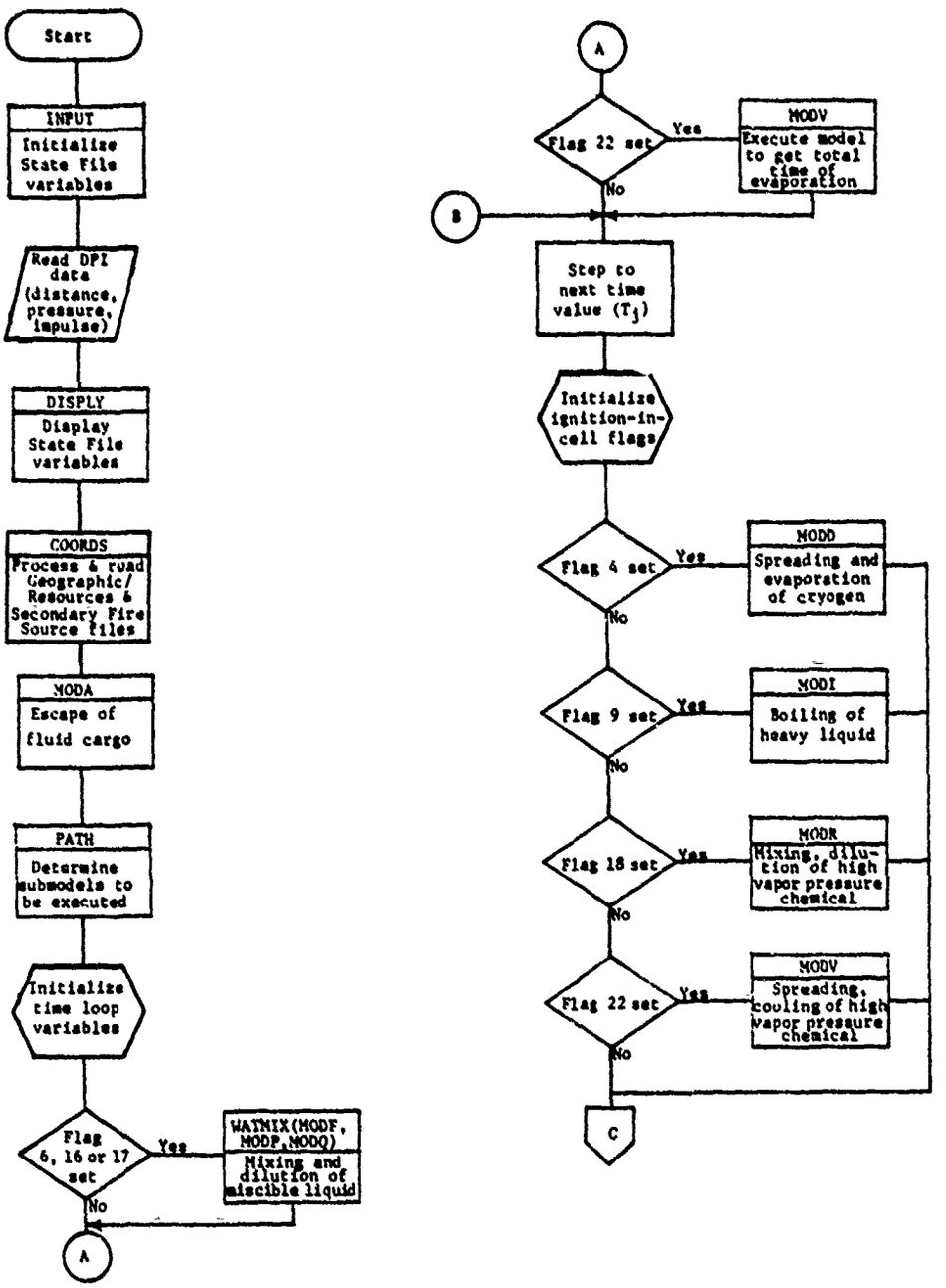


Figure 5-1. Flow Chart of Executive Program, VMEXEC

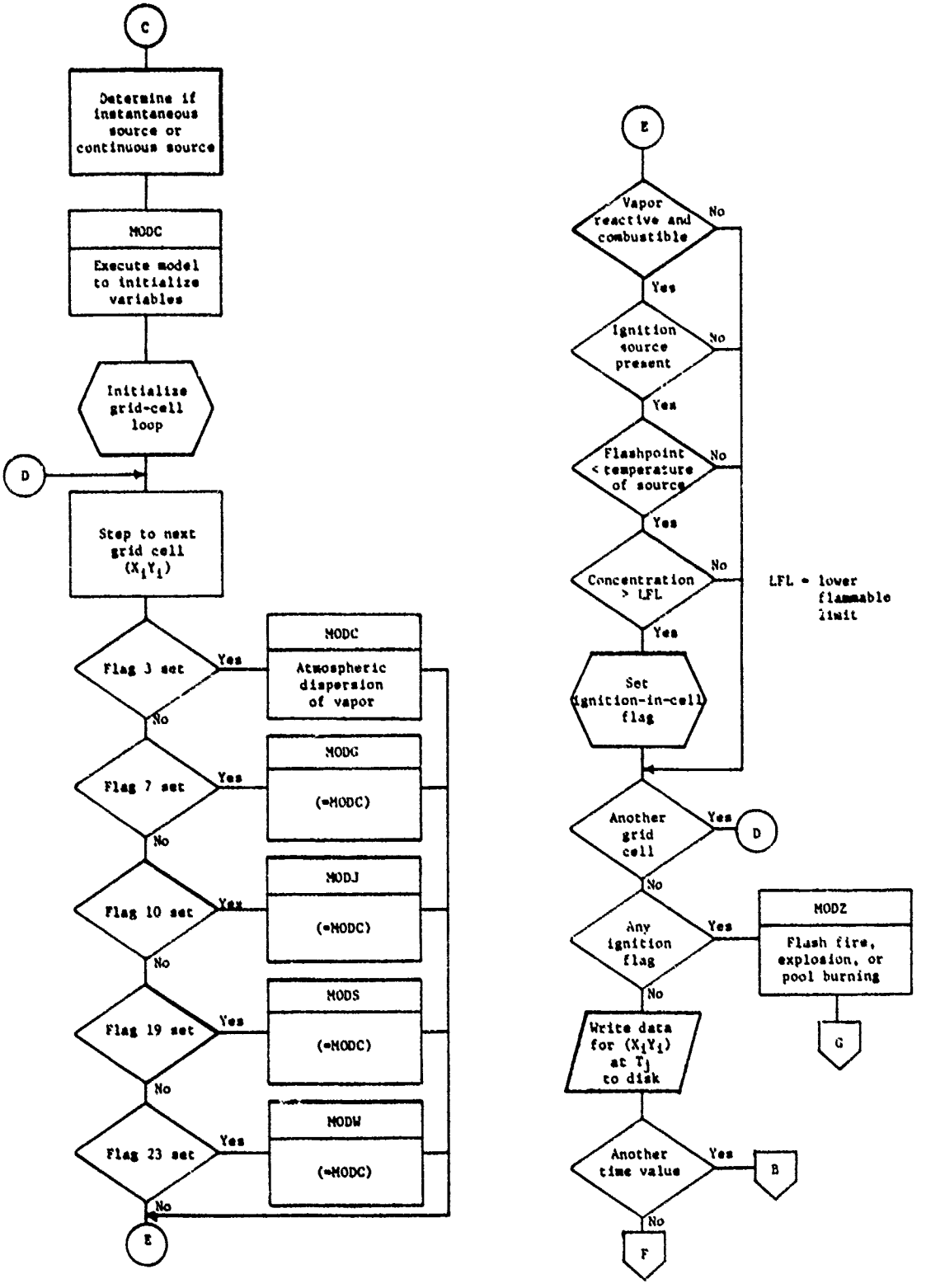


Figure 5-1 (continued)

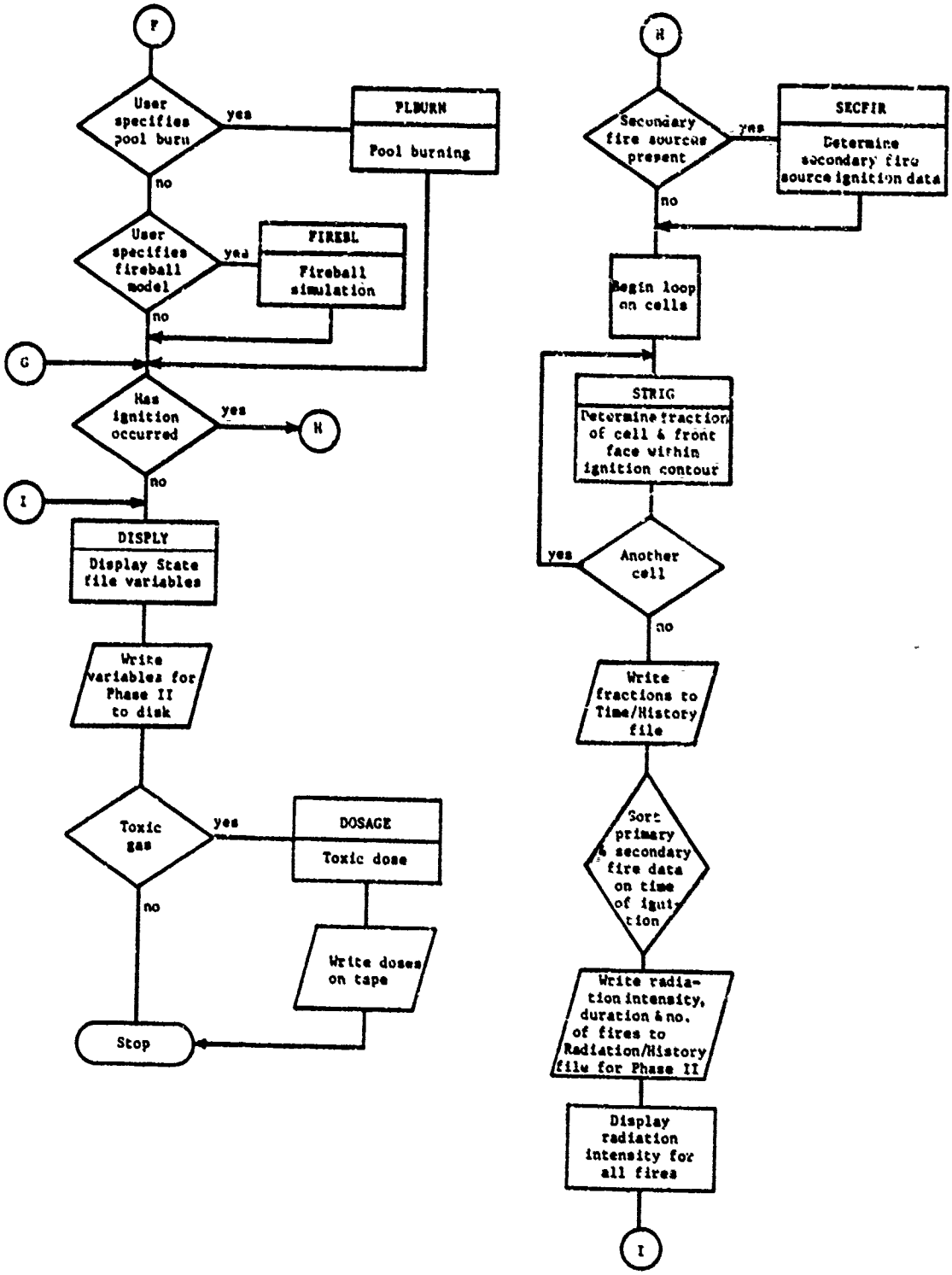


Figure 5-1 (continued)

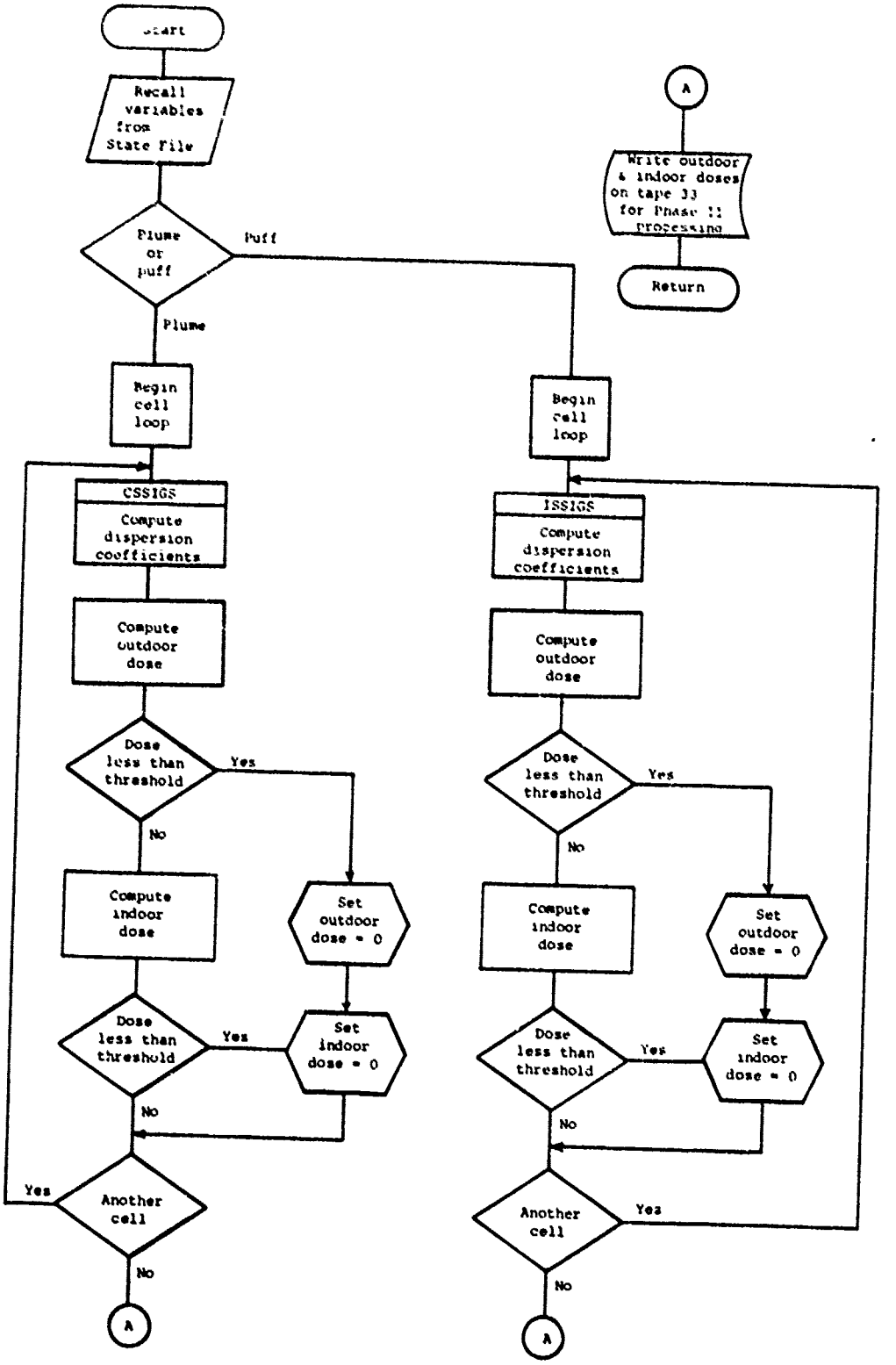


Figure 5-2. Flow Chart of Subroutine DOSAGE

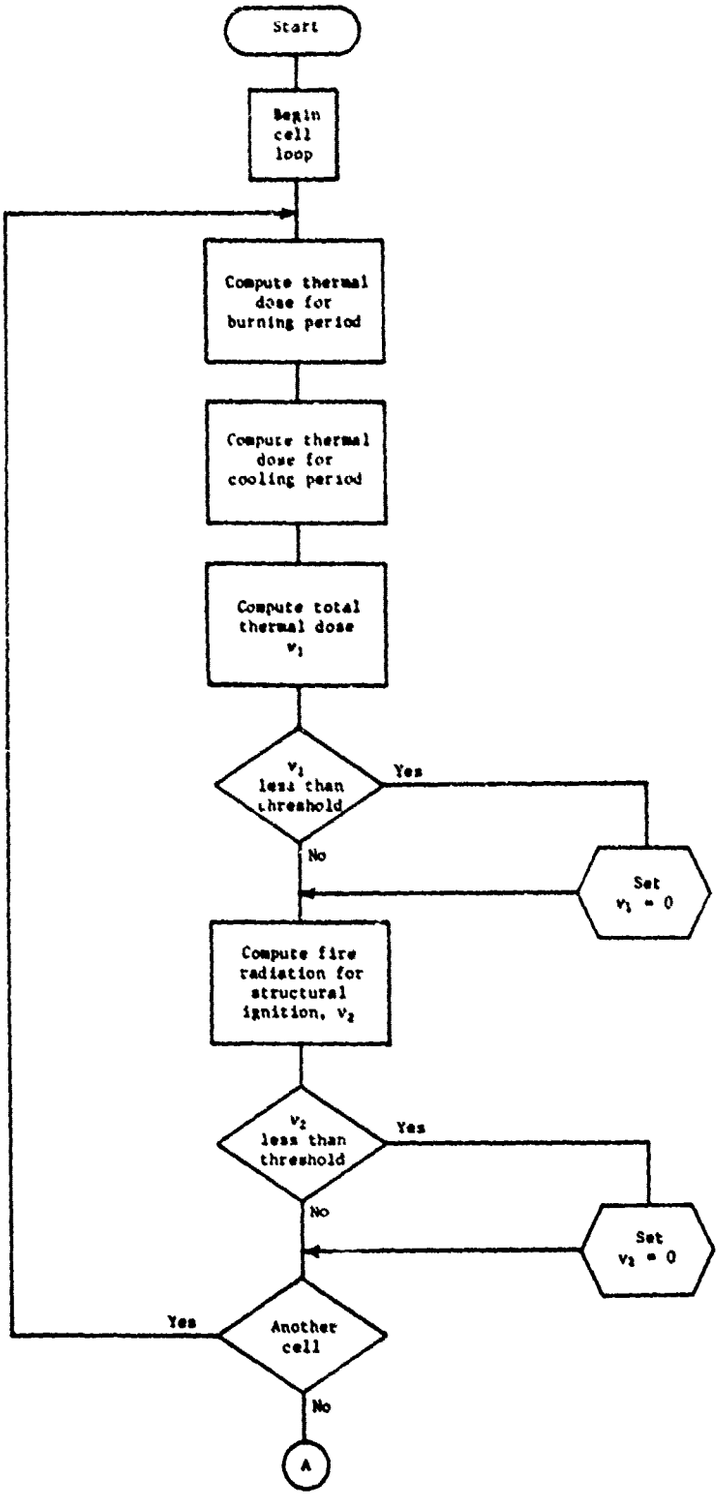


Figure 5-3. Flow Chart of Subroutine FLFIRE

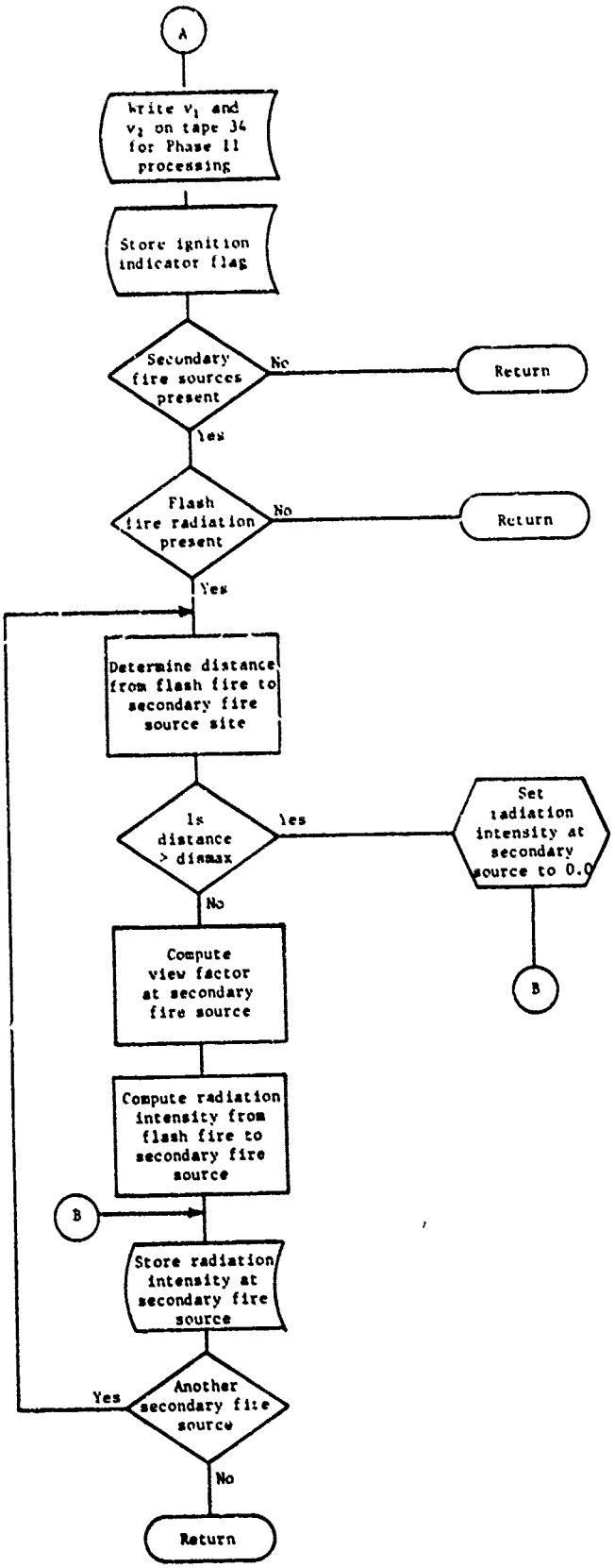


Figure 5-3 (continued)

PHASE II

For Phase II, no programming changes have been made. Changes to numerical values only have been made to incorporate alterations in thermal criteria and probit equations. The flow charts for Phase II are the same as those reported in reference [7].

USER INPUT

Several additional user input variables are necessary in modifying the VM. These are given in Table 5-1.

Table 5-1. ADDITIONAL USER INPUT VARIABLES

Field Number	Default Value	Unit	Variable Name	Comment
2011	36000.	erg/cm^3-C	HEAT	Summation of density and heat capacity
2026	600.	g/cm^3	RHOT	Average density of product
2033	100.0	cm/s	FLMSPD	Flame speed
1019	800.0	°C	TFLAM	Flame temperature

UPDATE PROGRAMS

Two update programs are given in Appendix B. The program MODVMA modifies Phase I of the VM, and the program MODVMB modifies Phase II of the VM. The magnetic tape, number S13346, contains this updated version of the VM.

Appendix A

INPUT DATA FOR TEST RUNS

Figure A-1. SPILL SCENARIOS FOR TEST RUNS

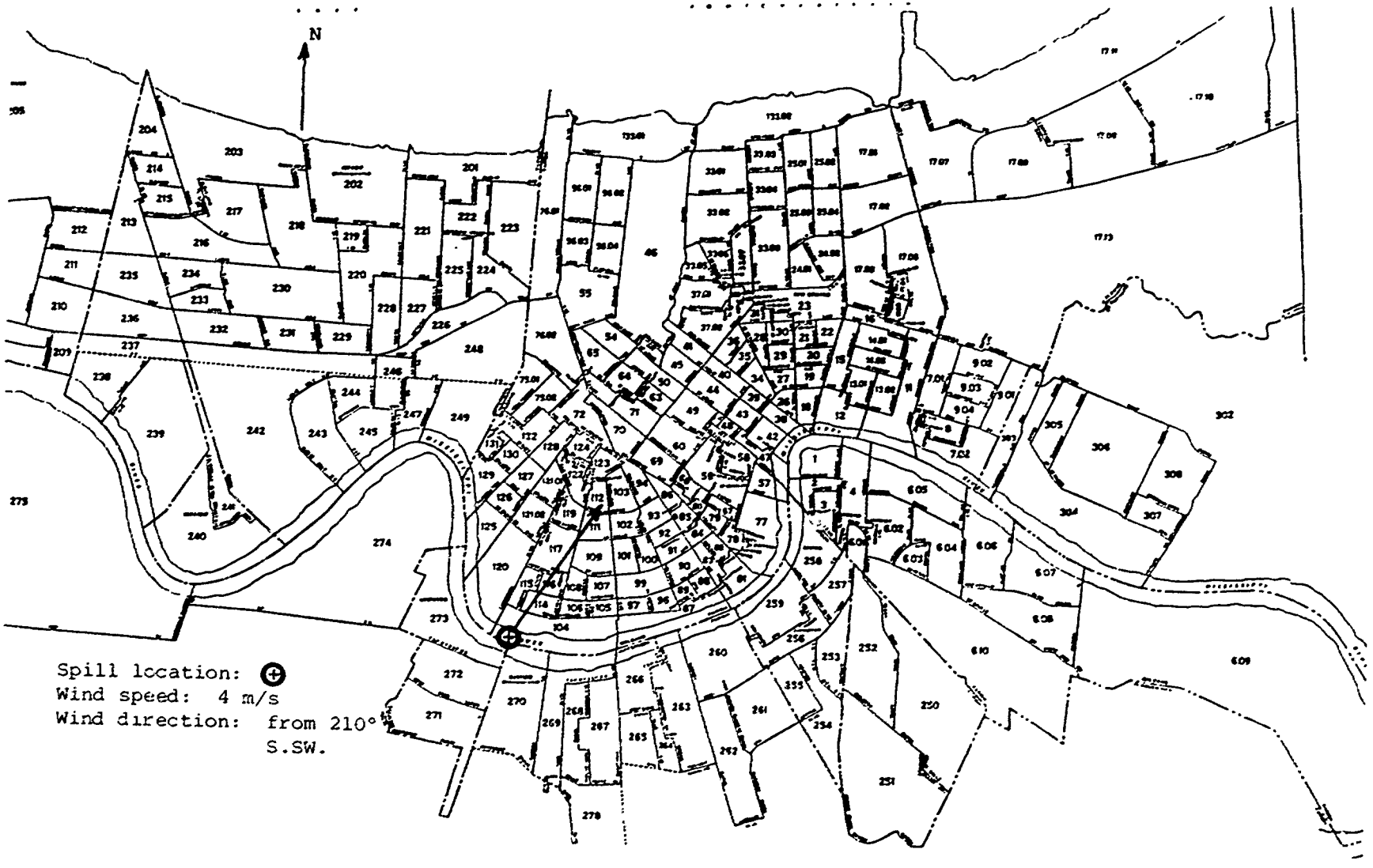
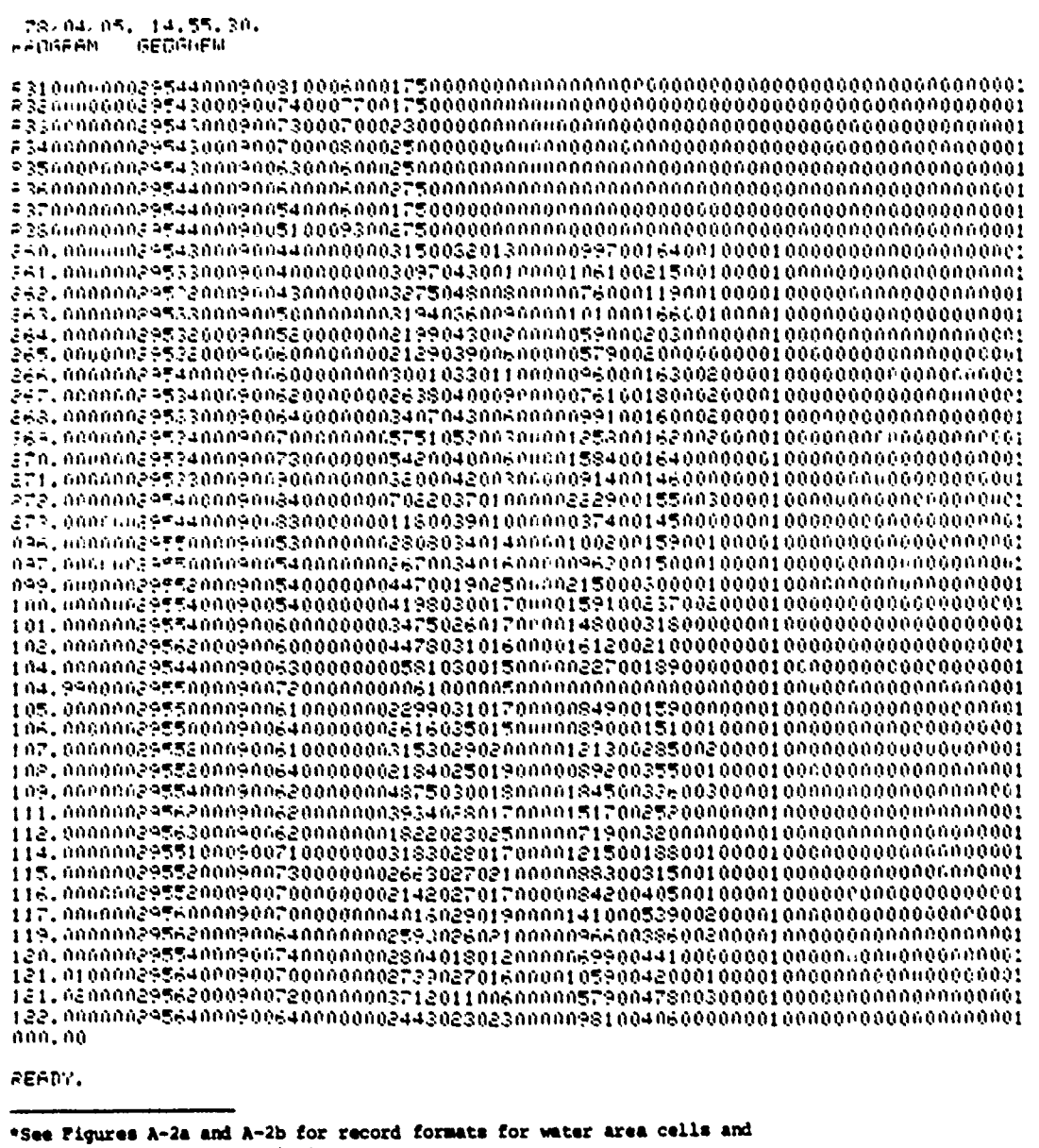


Figure A-2. GEOGRAPHIC/DEMOGRAPHIC FILE



*See Figures A-2a and A-2b for record formats for water area cells and land area cells, respectively.

Figure A-2a

RECORD FORMAT FOR WATER AREA CELLS

Columns	Format	Field
1-8	(A8)	*Cell identification
9-16	(I8)	*Latitude, north
17-24	(I8)	*Longitude, west
25-28	(I4)	*Depth in feet
29-34	(I6)	*Length in feet
35-57	(23X)	--not used--
58-60	(A3)	Direction of current
61-78	(18X)	--not used--
79-80	(I2)	*Ignition source

*Data used by Vulnerability Model for this study.

Figure A-2b

RECORD FORMAT FOR LAND AREA CELLS

Columns	Format	Field
1-8	(A8)	*Cell identification
9-16	(I8)	*Latitude, north
17-24	(I8)	*Longitude, west
25-28	(I4)	*Depth (blank or zero)
29-34	(I6)	*Total population
35-37	(I3)	Percent under 18 yr
38-40	(I3)	Percent over 62 yr
41-43	(I3)	*Percent sheltered
44-48	(I5)	*Total housing units
49-53	(I5)	*Average value (in $100)
54	(A1)	Housing material
55-57	(I2,A1)	Number of schools
58-60	(A3)	Land use
61	(I1)	Land uniformity
62-78	(17X)	--not used--
79-80	(I2)	*Ignition source

*Data used by Vulnerability Model for this study.

Figure A-3. INPUTS FOR AMMONIA SPILL

```
AMONIA SPILL

1001AMA
2001 .6000E+09
1002 17.03
1004 .6821
2044 2000.
2047 100.
2045 100000.0
2002   500.0
2003  0.0
2004  21.0
2005 .333VE+07
2006  0.0
2007 .31 00E+05
2008  15.24
2016  400.0
2013 2.0
2017  4.000
2019 5000.0
2021 0.2 3E-05
2023  15.00
2027 2400.
2029 1.0
2036  21.0
2033 8318.0
2054 -9.0
2053  20.00
3004  0.
3006  3.0
3002  0.0
3009  1.000
3007  0.0
4001 .2120E+05
4004 2400.0
5001  0.0
5002  0.0
5003  1.000
5004  1.000
5010  0.0
5011  1.000
5012  -101.0
5021  1.4000
5022 .10132+07
5030  8.750
5031  -30.57
5032  1.385
5033  0.
5034  0.
5035  100.
5037  0.0
5038  0.5000
6004  1.000
6005  4.00
6006  1.000
6010  25543.
6011  30073.
   0  000
```

Figure A-4. INPUTS FOR CHLORINE SPILL

```
CHLORINE SPILL

1001CL X
2001 .2000E+03
2044 2000.
2047 100.
2048 100000.0
2002   500.0
2003  100.0
2004  -33.9
2005 1.013E+06
2006  0.0
2007 2.330E+05
2008  15.24
2016  400.0
2017  4.000
2018 2.0
2019 5000.0
2020 6000.0
2021 2.380E-05
2023  15.00
2036  -33.9
2053  -30.0
3004  0.
3006  3.0
3008  0.0
3012  1.000
3007  0.0
4001 .1000E+03
4014  1.0
4016 35000.0
4028  660.
4031  .10+0E-3
5004  1.000
5010  1.0
5018  -101.0
5023 .1013E+07
5030  2.750
5031  -17.10
5032  1.430
5033  -3.400
5034  5.300
5035  3.000
5036 1.000E-07
5037  0.0
5038  0.5000
5050 100.0
5004  3.0
5005  4.0
5006  2.0
5010  402343.
5011  741553.
   0  006
```

Figure A-5. LIST OF STATE FILE VARIABLES WITH CURRENT DEFAULT VALUES

Field Number	Default Value	Unit Code	Display Name	Comment
1001*	OTW	01	CHEM NAME	Name of cargo
1002	200.0	23	MOLEC WEIGHT	Molecular weight of cargo
1003	282.	06	BOIL TEM LIQ	Boiling temperature of liquid cargo
1004	0.87	04	DENS LIQ AMB	Density of liquid at ambient temperature
1005	0.261846	22	VISCOSITY-BP	Viscosity of liquid at boiling point
1006	1.9739	22	VISCOSITY-AM	Viscosity of liquid at ambient temperature
1007	0.60	09	HEAT CAPC LQ	Heat capacity of cargo in liquid phase
1008	20.0	18	SURF TENSION	Surface tension of cargo
1009	0.001	04	DEN FUEL VPR	Density of fuel vapor at boiling point
1010	7.8	01	VPE COEFF A	
1011	1443.	01	VPE COEFF B	Coefficients (A,B,C) of the vapor pressure equation
1012	273.	01	VPE COEFF C	
1013	0.1	09	HEAT CAPC VP	Heat capacity of cargo in vapor phase
1014	136.	10	HEAT OF VPR	Heat of vaporization
1015	4.	15	BURNING RATE	(Equivalent to #5018)
1016	800.	06	AD FLME TEMP	(Equivalent to #5017)
1017	0.5	01	MOLEC RATIO	Not used in VM
1018	2.5	01	STO AIR/FUEL	(Equivalent to #5015)
1019	800.	06	FLAME TEMP	Flame temperature
1020	.01	01	MOLE FRACTN	Water concentration below which evaporation is negligible
1021	.87	04	LIQ DENS BP	Density of liquid at boiling point
2001	10000.	03	TANK VOLUME	Volume of tank
2002	1000.	02	TANK HEIGHT	Height of tank
2003	0.0	02	HOLE HEIGHT	Height of bottom of hole above bottom of tank
2004	20.0	06	TEMP START	Temperature in tank before discharge
2005	0.0	05	TANK PRESS	Pressure in tank before discharge
2006*	1	01	ISO=0, ADB=1	Indicator specifying isothermal or adiabatic tank conditions
2007	5000.	08	INITIAL MASS	Initial mass of cargo
2008	50.	02	HOLE DIAM	Average diameter of hole in tank
2009*	200	01	NUM MASS INC	Number of increments used for venting integration (MODA)
2010	100000.	02	OBSVR DIST	Distance from burning pool at which flux is computed
2011	36000.	27	HEAT	Summation of density x heat capacity
2012	100000.	02	COORD X **	Distance in downwind direction
2013	0.	02	COORD Y **	Distance in crosswind direction
2014	100.	02	COORD Z **	Height above ground surface
2015	0.	02	HT OVER SURF	Height of centerline of hole in tank above water surface
2016	200.	15	WIND SPEED	Wind speed
2017	6	01	ATMOS COND	Atmospheric stability flag
2018	2	01	CHL=1, RAD=2	Flag for channel spill or radial spill
2019	5000.	02	CUR DIM POOL	Current dimension of liquid pool
2020	50000.	02	CHAN'L WIDTH	Channel width
2021	0.0001	16	HAZARD CONC	Not used in VM
2022*	0	01	FLUX, CN1, LM2	Flag specifying conditions of heat transfer (for MODD)
2023	15.0	06	WATER TEMP	Water temperature
2024	2.0	14	HEAT FLUX	Heat flux between water and chemical

* Denotes integer variable.
** Coordinates of point at which the concentration in air is being calculated.

Figure A-5 (continued)

Field Number	Default Value	Unit Code	Display Name	Comment
2025*	1	01	CRIT FLAG	Flag for calculation of critical values (MODD)
2026	600.	04	RHOT	Average density of product
2027	600.	11	EVAP TIME	Not used in VM
2028*	1	01	SPILL INDC	Flag indicating spill environment
2029*	0	01	SPL DUR INDC	Indicator for duration of discharge
2030	0.0	02	EMMIS POWER	Emissivity power
2031	1000000.	02	MAX DIST HFM	Not used in VM
2032	36000	11	MX TIME CONC	Not used in VM
2033	100.0	15	FLMSPD	Flame speed
2034	0.0	02	MIN HAZ ZONE	Not used in VM
2035	1000000.	02	MAX HAZ ZONE	Not used in VM
2036	15.0	06	TEMP LIQUID	Temperature of liquid discharged
2037	36000.	11	MAX TIME CONC	Not used in VM
2038	100000.	12	AVG ESC RATE	Average escape or discharge rate
2039	100000.	02	CONC PT X **	Downstream coordinate
2040	100000.	02	CONC PT Y **	Cross-stream coordinate
2041	0.	02	CONC PT Z **	Depth coordinate
2042	600.0	11	TIME CONC PT	Not used in VM
2043	50.	19	DIF COEF H20	Diffusion coefficient of liquid
2044	10000.	02	RIVER DEPTH	Mean depth of flowing water
2045	50000.	02	RIVER WIDTH	Mean width of flowing water
2046	0.0	02	OFF DIST	Cross-stream position of discharge
2047	100.0	15	STREAM VEL	Velocity of flowing water
2048	50.0	15	TIDAL VEL	Maximum amplitude of tidal current
2049	518400.	11	TIDAL PERIOD	Tidal period
2050	0.	11	PHASE LAG	Time to next highwater slack tide
2051	0.0	01	DECAY COEFF	Decay coefficient
2052	0.03	03	MANNING FACT	Manning roughness factor
2053	0.1	19	DIF COEF V-A	Diffusion coefficient of vapor in air
2054	15.0	06	AIR TEMP	Air temperature
2055	36000.	11	TIME LIQ SPR	Not used in VM
2056	36000.	11	LIQ SPR TIME	Not used in VM
2057	36000.	11	TIME SPL COND	Not used in VM
2058	90.	21	WIND TOWARD	Degrees from north toward which wind blows
3001*	3	01	PROB TYPE	Not used in VM
3002*	0	01	PRINT FILE	Logical unit for output file
3003*	0	01	PLOT RAD FIX	Not used in VM
3004*	0	01	NSF	Secondary fire source indicator
3005*	0	01	ISF	Number of secondary fire sources
3006*	0	01	ISHLD	Shielding situation
3007*	0	01	NSFIGN	Number of secondary fire ignitions
3008*	0	01	PLOT CONC LQ	Not used in VM
3009*	0	01	PLOT SPREAD	Not used in VM
3010*	0	01	PLOT HVP LQ	Not used in VM

* Denotes integer variable.
** Coordinates of point at which the concentration in water is being calculated.

Figure A-5 (continued)

Field Number	Default Value	Unit Code	Display Name	Comment
3011*	0	01	OPPER FILE	Logical unit for output file
4001	0.0	08	TOT MASS GAS	Total mass of gas which escapes
4002	0.0	08	TOT MASS LIQ	Total massof liquid which escapes
4003	0.0	03	TOT VOL LIQ	Total volume of liquid which escapes
4004	0.0	11	TIME OF RFL	Elapsed time of release from tank
4005	0.0	06	MX TEMP TANK	Maximum temperature in tank during release
4006	0.0	02	FLAME LENGTH	Length of flame
4007	0.0	02	DIAM FLAME	Diameter of flame
4008	0.0	13	FLAME ANGLE	Angle of flame from vertical
4009	0.0	14	RAD FLUX	Thermal radiation flux (pool burn)
4010	0.0	04	VAP CONC	Vapor concentration
4011	0.0	02	1/2 HAZ ZONE	Not used in VM
4012	0.0	11	DUR HAZ CLD	Not used in VM
4013	0.0	11	ARRL TME HAZ	Not used in VM
4014*	0	01	IN OR OUT	Not used in VM
4015	0.0	02	SPILL SIZE	Not used in VM
4016	0.0	11	TIME LQ EVAP	Elapsed time for chemical to evaporate
4017	0.0	12	DISSOL RATE	Dissolution rate of chemical on riverbed
4018	0.0	02	POOL FLM HGT	Height of flame
4019	0.0	03	VOL LIQ POOL	Volume of liquid remaining in pool
4020	0.0	12	TOT EVP RATE	Average evaporation rate of total liquid pool
4021	0.0	11	DISSOL TIME	Time for all chemical to dissolve on riverbed
4022	0.0	04	LIQ-H2O CONC	Concentration of chemical in water
4023	0.0	08	MASS VAP LIB	Mass of vapor liberated from pool
4024	0.0	02	SAFE DIST	Distance at which concentration is less than limiting value
4025	0.0	02	MAX DIM POOL	Maximum dimension of liquid pool
4026	0.0	07	POOL SIZE	Area of liquid pool on riverbed
4027	0.0	02	POOL LENGTH	Length of pool on riverbed
4028	0.0	06	TCRIT	Critical temperature of cargo
4029	0.0	18	SURT	Interfacial surface tension
4030	0.0	26	CSAT	Solubility of substance
4031	0.0	19	DIFW	Diffusion coefficient of chemical in water, cm^2/sec
4032	0.0	11	SINK TIME	Time of chemical to sink to bed
4033	0.0	02	DIST TRAV	Distance traveled by chemical to reach bed
5001*	0	01	MESSAGE FLAG	Flag which controls output messages
5002*	0	01	MISCIBLE IND	Miscibility indicator
5003*	0	01	REACTIVE IND	Reactivity indicator
5004*	0	01	TOX,ASPH IND	Toxicity and asphyxiation indicator
5005*	0	01	LIQ CONC IND	Liquid toxicity indicator
5006*	0	01	IGNITION IND	Flag which indicates type of ignition
5007*	0	01	IGNITN CELL	Cell in which ignition first occurred
5008*	0	01	IGNITN CODE	Ignition code of the ignition cell
5009*	0	01	SPILL CELL	Cell in which discharge occurred
5010*	0	01	FLAG,ISO,CS1	Flag for use of puff or plume equation

*Denotes integer variable.

Figure A-5 (continued)

Field Number	Default Value	Unit Code	Display Name	Comment
5011	1.0	04	DENS WATER	Density of water
5012	-40.	06	FREEZING PT	Freezing point of chemical
5013	0.0	01	CONC, LO LIM	Lower flammability limit, percent
5014	0.0	01	CONC, UP LIM	Upper flammability limit, percent
5015	0.0	01	AIR/FUEL RAT	Stoichiometric air/fuel ratio
5016	0.0	10	HEAT COMBUST	Heat of combustion
5017	0.0	06	ADFLAME TEMP	Adiabatic flame temperature
5018	0.0	15	BURNING RATE	Burning rate of chemical
5019	0.0	01	MOLES OXYGEN	Moles of oxygen per mole of fuel
5020	282.	06	FLASHPOINT	Flashpoint of chemical
5021	1.4	01	SPC HEAT RAT	Ratio of specific heats
5022	1013250.	05	PRESSURE AMB	Ambient atmospheric pressure
5023	0.0	04	CONC, LO LIM	Lower limit, flammable vapor concentration
5024	0.0	04	CONC, UP LIM	Upper limit, flammable vapor concentration
5025	0.0	04	CONC, STOICH	Stoichiometric vapor concentration
5026	0.0	05	VP PR TANK	Vapor pressure in the tank
5027	0.0	08	LIQ REM TANK	Total mass of liquid remaining in tank
5028	0.0	02	SIGY,DISPERS	Horizontal dispersion coefficient (MODC)
5029	0.0	02	SIGZ,DISPERS	Vertical dispersion coefficient
5030	2.75	01	EXP, TOX SUM	Exponent in weighted sum for toxicity
5031	0.0	01	T1, COEFF A	Coefficients of probit equation T1
5032	0.0	01	T1, COEFF B	
5033	0.0	01	T2, COEFF A	Coefficients of probit equation T2
5034	0.0	01	T2, COEFF B	
5035	0.0	01	T3,CONC PPM	Irritation threshold for T3
5036	100.0	01	T4, COEFF ING	Coefficient of ingestion T4
5037	0.0	01	QUAL STD AIR	Not used in VM
5038	0.0	01	FRAC POP SHL	Fraction of population sheltered
5039	0.0	02	FFDIA	Flash fire diameter
5040	0.0	11	TIME AT IGN	Time at which ignition occurred
5041	0.0	02	PUFF CENTER	Downwind location at center of vapor puff
5042	0.0	14	FL FIRE RADN	Intensity of flash fire radiation
5043	0.0	11	FL FIRE TIME	Effective duration of flash fire
5044	0.0	08	MASS VAP EXP	Mass of cargo vapor which exploded
5045	0.0	01	PCT VAP EXP	Mass exploded given as percent of total mass
5046	0.0	20	EXPL YIELD	Yield of the explosion
5047	0.0	25	TNT EQUIV	Yield equivalent in short tons of TNT
5048	0.0	11	PL BURN TIME	Effective duration of pool burn
5049	0.0	01	RAD' COORD	Radius of vapor cloud
5050	0.0	11	CURRENT TIME	Current value, elapsed time
6001*	0	01	TIME,SEC,BEG	Time in seconds, begin loop 1
6002*	0	01	TIME,SEC,END	Time in seconds, end loop 1
6003*	0	01	TIME,SEC,INC	Time in seconds, increment value for loop 1

*Denotes integer variable.

Figure A-5 (continued)

Field Number	Default Value	Unit Code	Display Name	Comment
6004*	0	01	TIME,MIN,BEG	Time in minutes, begin loop 2
6005*	0	01	TIME,MIN,END	Time in minutes, end loop 2
6006*	0	01	TIME,MIN,INC	Time in minutes, increment value for loop 2
6007*	0	01	TIME,MIN,BEG	Time in minutes, begin loop 3
6008*	0	01	TIME,MIN,END	Time in minutes, end loop 3
6009*	0	01	TIME,MIN,INC	Time in minutes, increment value for loop 3
6010*	0	01	SPILL LAT	Latitude, north, of spill site
6011*	0	01	SPILL LONG	Longitude, west, of spill site

*Denotes integer variable.

Figure A-6

INPUT DATA FOR LNG SPILL
(FLASH FIRE TEST RUNS)

```
1001LNG
1002   16.04
2011   .1372E+05
2026   .1234E-02
2001   .3000E+11
2002   1500.
2003   100.0
2004   -151.0
2005   .2027E+07
2006   1.000
2007   .1250E+11
2008   100.0
2014   100.0
2015   0.
2016   400.0
2017   4.000
2018   2.000
2020   .6096E+05
2021   .1246E-03
2022   1.000
2023   20.00
2025   1.000
2027   180.0
2033   500.0
2054   15.00
2058   30.00
3004   1.000
3006   2.000
5001   0.
5002   0.
5003   1.000
5004   0.
5010   1.000
5011   1.000
5012   -182.0
5013   5.400
5014   14.00
5016   -.1300E+05
5017   1100.
5018   .2083E-01
5019   2.000
5020   -161.0
5021   1.400
5022   .1013E+07
5036   0.
5037   0.
5038   .5000
6001   0.
6002   0.
6003   0.
6004   2.000
6005   10.00
6006   2.000
6007   0.
6008   0.
6009   0.
6010   .2954E+06
6011   .9007E+06
   0   0.
```

Appendix B

UPDATE PROGRAMS MODVMA AND MODVMB

UPDATE PROGRAM, MODVMA

```
*IDENT VMEXED
*DELETE,VMEX1.2
     1TAPE9,TAPE10,TAPE12,TAPE13,TAPE14,TAPE15,TAPE24,TAPE33,
     1TAPE34,TAPE30=SECFRE)
*INSERT,VMEXEC.16
      COMMON/RADOS/G1(400),G2(400)
*INSERT,VMEXEC.144
      IF(ITOX .EQ. 1)GO TO 901
*INSERT,VMEX1.48
      WRITE(6,704)
  704 FORMAT(1H1,10X,7HCELL NO,8X,11HPEOPLE DOSE,10X,10HHOUSE DOSE)
      DO 70 I=1,NCELL
      IF(G1(I) .EQ. 0.0 .AND. G2(I) .EQ. 0.0)GO TO 70
      WRITE(6,702)I,G1(I),G2(I)
   70 CONTINUE
  702 FORMAT(10X,I5,5X,1E16.4,5X,1E16.4)
*DELETE,VMEX5.36
C     WRITE(6,9194)
*DELETE,VMEX1.144
C     WRITE(6,9195)LC,((IP,TINC(IP),THRI(IP,LC)),IP=1,NINC
*DELETE,VMEX1.148,VMEX1.152
C9194 FORMAT(*1 TIME INCREMENTED RADIATION FLUX AT EACH CELL*,//,
C    1       *  CELL  INCREMENT   EFFECTIVE DURATION   RADIATION*,/,
C    2       *   NO.      NO.            (SEC)         FLUX(J/M2/S)*)
C9195 FORMAT((2X,I3,5X,I3,11X,F8.2,7X,E12.4,21(/,10X,I3,11X,F8.2,
C    1         7X,E12.4))
*INSERT,VMEXEC.231
      CALL FRCL(4016,TEVAP,IS,IR)
      CALL FRCL(4023,TMVAP,IS,IR)
      CALL FRCL(2016,UWIND,IS,IR)
      CALL FRCL(4030,TMEND,IS,IR)
      CALL IRCL(5004,ITOX,IS,IR)
      IF(ITOX .EQ. 1   )CALL DOSAGE
*IDENT ERFFA
*DELETE,ERF.22
       IF(Y .GT. 6.0 .OR. Y .EQ. 6.0)EX=0.0
      IF(Y .LT. 6.0)EX=EXP(-Y*Y)
*IDENT DOSAA
*INSERT DMSDEG.11
      SUBROUTINE DOSAGE
      COMMON/CELL/IXLAT(400),IYLON(400),CDEP(400),CLEN(400),IGCODE(400),
     1X(400),Y(400),IGCELL(400),NCELL,ISPLAT,ISPLON,WINDEG
      DIMENSION CX(500),DX(500),EX(500)
      DIMENSION  DOS(400),DOSIN(400)
C     DOS = OUTDOOR DOSAGE
C     DOSIN = INDOOR DOSAGE
      CALL FRCL(1002,WTMOL,IS,IR)
```

```
      CALL FRCL(2014,Z,IS,IR)
      CALL FRCL(2016,UWIND,IS,IR)
      CALL FRCL(2019,SIZE,IS,IR)
      CALL FRCL(2020,CHNLW,IS,IR)
      CALL FRCL(4001,TMG,IS,IR)
      CALL FRCL(4016,TEVAP,IS,IR)
      CALL IRCL(2017,IAC,IS,IR)
      CALL IRCL(2018,IDIM,IS,IR)
      CALL FRCL(2054,AIRTEM,IS,IR)
      CALL IRCL(5010, SCS,IS,IR)
      CALL FRCL(5030,CPOW,IS,IR)
      CALL FRCL(5031,T1A,IS,IR)
      CALL FRCL(4023,TMVAP,IS,IR)
      CALL FRCL(5032,T1B,IS,IR)
      CALL FRCL(5033,T2A,IS,IR)
      CALL FRCL(5034,T2B,IS,IR)
      CALL FRCL(5035,T3A,IS,IR)
      DATA PI/3.14159/
      THRS = 3.0
      KCOD = 1
      RAD = SIZE
C     THRS = THRESHOLD FOR IRRITATION, PPM
      SQ2 = SQRT(2.0)
      ALF = 28.966*1.E6/(.001225*WMOL)
C     ALF IS A CONVERSION FACTOR CHANGING G/CC TO PPM IN VOLUME
C     28.966 IS AIR MOL WT, .001225 IS AIR DENSITY AT SAME CONDITION
C     AS THE CHEMICAL
      VWIND=UWIND*.022369
C      VWIND IN MPH
      TEMD=ABS(25.0-AIRTEM)
      R=(.25+.02165*VWIND+.00833*TEMD)/60.0
C     R IS THE INFILTRATION PER MINUTE
      IF (TMG .EQ. 0.0)TMG=TMVAP
      IF(IDIM .EQ. 1 )RAD=SQRT(SIZE*CHNLW/PI)
      IF(ISCS .EQ. 0)GO TO 101
C     PLUME MODEL
      QB = TMG/(PI*TEVAP*UWIND)
C     DOS IS IN PPM AND MINUTE
      DO 5 I=1,NCELL
      DOS(I)=0.
      DOSIN(I)=DOS(I)
      IF(X(I) .LT. 0.)GO TO 5
      XA = X(I) + 10.0*RAD
      CALL CSSIGS(XA,IAC,SIGY,SIGZ)
      IF(SIGZ .GT. 100000.)SIGZ=100000.
C      CC IS THE MAXIMUM VAPOR CONCENTRATION
      CC = ALF*QB/(SIGY*SIGZ)
      CE=0.5*((Y(I)/SIGY)**2+(Z/SIGZ)**2)
      CAX=CC**CPOW
      CAY=CPOW*CE
```

```
      CG=0.
      IF(CAY .LT. 23.0) CG=CAX/EXP(CAY)
      DOS(I)=CG*TEVAP/60.0
      IF(T3A .NE. 0.0 .AND. CC .LE. T3A)DOS(I)=0.0
      IF(T3A .EQ. 0.0 .AND. CC .LE. THRS)DOS(I)=0.0
C     CALCULATE PLUME INDOOR DOSAGE
      DOSIN(I) = DOS(I)
      IF(DOS(I) .EQ. 0.0)GO TO 5
      CX(1) =CPOW
      DX(1) = 1.0
      CRT = .0001*CPOW
      YE = EXP(-R*TEVAP)
      AXA = CPOW*(1.0 - YE)
      DO 91 J=1,100
      XI = J
      DX(J+1)=(XI+1.0)*(XI+1.0)*DX(J)
      CX(J+1)=CX(J)*(CPOW-XI)
      AXB=(-1)**J*(CX(J+1)/DX(J+1))*(1.-YE**(J+1))
      AXA=AXA+AXB
      IF(AXB .LT. CRT)GO TO 93
   91 CONTINUE
   93 CONTINUE
      DOSIN(I)=CG*(TEVAP-AXA/R)/60.0
    5 CONTINUE
      GO TO 900
  101 CONTINUE
C     CALCULATE PUFF DOSAGE
      BA=2.0*TMG*ALF/(2.0*PI)**1.5
C     BC IS THE MAXIMUM CONCENTRATION IN THE CELL
      BB = (2.0/CPOW)**0.5
      DO 15 I=1,NCELL
      DOS(I)=0.
      DOSIN(I)=0.
      IF(X(I) .LT. 0.)GO TO 15
      XA=X(I)+10.0*RAD
      CALL ISSIGS(XA,IAC,SIGY,SIGZ)
      SIGX = SIGY
      BC=(BA/(SIGX*SIGY*SIGZ))
      BD=BC**CPOW*BB*SIGX/UWIND
      BE=CPOW*((Y(I)/SIGY)**2+(Z/SIGZ)**2)/2.0
      IF(BE .GT. 23.)GO TO 15
      IF(BE .LT. 23.0 .AND. BE .GT. 1.E-25)BF=BD/EXP(BE)
      IF(BE .LT. 1.0E-25)BF=BD
      BG=(CPOW/2.0)**0.5*X(I)
      BH=(PI**0.5/2.0)*(1.0+ERF(BG/SIGX))
      DOS(I)=BF*BH/60.0
      IF(T3A .NE. 0.0 .AND. BC .LE. T3A)DOS(I)=0.0
      IF(T3A .EQ. 0.0 .AND. BC .LE. 3.0)DOS(I)=0.0
C     TO CALCULATE INDOOR DOSAGE
      IF(DOS(I) .EQ. 0.0)GO TO 15
```

```
      EA=(SQRT(2.*PI)*SIGX*R/(2.*60.*UWIND))**CPOW
      EB=CPOW*(X(I)*R/(60.*UWIND)+(SIGX*R/(60.*UWIND))**2/2.)
      EX=EB-BE
      IF(ABS(EX) .LE. 1.E-25)EC=BC**CPOW*EA
      IF(ABS(EX) .GT. 1.E-25)EC=BC**CPOW*EA*EXP(EX)
      ED=(X(I)+(R*SIGX**2)/(60.*UWIND))/(SQ2*SIGX)
      IF(ED .LT. 5.0)EF=ERF(ED)
      IF(ED .GE. 5.0)EF=1.0
      FA=(X(I)+(SIGX**2)*R/(60.*UWIND))/UWIND
      IT2=FA
      FB=FA-5.0*SQ2*SIGX/UWIND
      IT1=FB
      FC=FA+5.0*SQ2*SIGX/UWIND
      IT3=FC
      XT=IT1
      SUM=0.
      DO 20 K=IT1,IT3
       EI=EXP(-CPOW*R*XT/60.0)
      EM=EXP(-CPOW*R*(XT+1.)/60.0)
      IF(XT .GE. IT2)GO TO 25
      EG=ED-UWIND*XT/(SQ2*SIGX)
      IF(EG .LT. 5.)EH=ERF(EG)
      IF(EG .GE. 5.)EH=1.
      EJ=EI*(EF-EH)**CPOW
      XT=XT+1.
      EK=ED-UWIND*XT/(SQ2*SIGX)
      IF(EK .LT. 5.)EL=ERF(EK)
      IF(EK .GE. 5.)EL=1.
      EN=EM*(EF-EL)**CPOW
      SUM=SUM+(EJ+EN)*1./2.
      GO TO 20
   25 CONTINUE
      EG=UWIND*XT/(SQ2*SIGX) - ED
      IF(EG .LT. 5.)EH=ERF(EG)
      IF(EG .GE. 5.)EH=1.
      EJ=EI*(EF+EH)**CPOW
      XT=XT+1.
      EK=UWIND*XT/(SQ2*SIGX) -ED
      IF(EK .LT. 5.)EL=ERF(EK)
      IF(EK .GE. 5.)EL=1.
      EN=EM*(EF+EL)**CPOW
      SUM=SUM+(EJ+EN)*1./2.
   20 CONTINUE
      EP=CPOW*R*(FA+5.0*SQ2*SIGX/UWIND)/60.0
      EQ=2.0**CPOW*EP*60.0/(CPOW*R)
      DOSIN(I)=EC*(SUM+EQ)
   15 CONTINUE
  900 CONTINUE
      REWIND 33
      WRITE(6,743)
```

```
  743 FORMAT(1H1,10X,4HCELL,8X,12HDOSE OUTSIDE,6X,11HDOSE INSIDE/)
      DO 752 I=1,NCELL
      WRITE(33,741)DOS(I),DOSIN(I)
  752 CONTINUE
      DO 757 I=1,NCELL
      IF(DOS(I) .EQ. 0.)GO TO 757
      WRITE(6,742)I,DOS(I),DOSIN(I)
  757 CONTINUE
  742 FORMAT(10X,I4,8X,E12.4,5X,E12.4)
  741 FORMAT(2E16.6)
      RETURN
      END
*IDENT MODZA
*INSERT,MODZ2.1
      COMMON/RADOS/Q1(400),Q2(400)
*IDENT FLABA
*INSERT,FLFIR1.4
      COMMON/RADOS/Q1(400),Q2(400)
*DELETE,FLFIR1.5,FLFIRE.11
      DATA PI/3.141592567/
*DELETE,FLFIR1.6,FLFIR1.30
      DATA SIGMA/5.6697E-5/,ALF/0.9/,RAM/1.34E+7/
C     RAM IS THE CRITERION FOR WOOD BRUN, ERG/CM2-S
      CALL FRCL(2011,HEAT,IS,IR)
      CALL FRCL(2026,RHOT,IS,IR)
      CALL FRCL(1019,TFLAM,IS,IR)
      CALL FRCL(5023,CONCLO,IS,IR)
      CALL FRCL(5025,ROF,IS,IR)
      CALL FRCL(2033,FLMSPD,IS,IR)
C     HEAT IS THE SUM OF DENSITY X CP
      TF=TFLAM
C     RHOT IS THE SUM OF PRODUCT DENSITY
      ABA=TMV/((2.0*PI)**1.5*SIGX*SIGY*SIGZ*KL)
C     KL IS THE LOWER FLAMMABLE LIMIT
      RL=(3.0*TMV/(4.0*PI*ROF))**(1./3.)
C     ROF IS THE FUEL DENSITY
      QIR=SIGMA*(TF**4 - TA**4)*TF
C     SIGMA IS STEFAN-BOLTZMANN CONSTANT
C     CHANGE HCOMB FROM CAL/G TO ERG/G
      HBURN=HCOMB*4.184E+07
      ACB=-ROF*TA*HBURN-(TF-TA)*HEAT*TA
C     HCOMB IS IN NEGATIVE VALUE
C     SV=QIR/ACB
C     SV IS THE FLAME VELOCITY
C     FLMSPD IS THE INPUT FLAME SPEED
C     TOTMA IS THE AIR/FUEL MASS
      TOTMA=TMV*18.1869
      RB=(3.0*TMV*TF/(4.0*PI*ROF*TA))**(1./3.)
C     RB IS THE MAX FIREBALL RADIUS
      SV=FLMSPD
```

```
      TFDUR=RB.SV
      CALL FSV(5043,TFDUR,4)
      X=XC(IGNID)
      Y=YC(IGNID)
C     IGNID IS THE NUMBER OF IGNITED CELL
      TR=TA/TF
C     HERE TA AND TF ARE IN KELVIN, SEE MODZ SUBROUTINE
      CD=.020666*TA**(23./9.)
      CE=9.0*(ALF**4*SIGMA)**(1./3.)*HEAT*TA
      CF=CE*RB/(TF**(11./9.))
      BC=ALF*SIGMA*TF**4
      BA=BC**(4./3.)
      EA=TA*RB*HEAT/(3.*SIGMA*TF**(4./3.))
        DO 5 I=1,NCELL
      Q1(I)=0.
      Q2(I)=0.
      CONC=QDATA(I)
      DIS=((XC(I)-X)**2+YC(I)**2)**0.5
      IF(I .NE. IGNID)GO TO 150
      WRITE(6,91)I,CONC
   91 FORMAT(*0   CELL*,I4,* IN FLASH FIRE, CONC= *,E12.3)
  150 CONTINUE
      BB=(RB/DIS)**(8./3.)
      IF(RB .GE. DIS)BB=1.0
      QA=3.0*BA*BB*RB/(11.*FLMSPD)
C     CHANGE I TO JOULE/M2, SEE ORIGINAL EQUATION
      CA=1./23.-TR**4/13.-TR**8/49.-TR**12/85.
      QB=CF*BB*(CA+CD)
      Q1(I)=QA
C     Q IS THE TOTAL RADIATION IN CELL I
      IF(Q1(I) .LT. 1.E+3)GO TO 5
C     CALCULATE STRUCTURE RADIATION HEAT
      IF(I .NE. IGNID)GO TO 66
      Q2(I)=2.0E+13
      GO TO 5
   66 CONTINUE
      RIM=(RAM*DIS**2/BC)**0.5
C     RIM IS THE CRITICAL RADIUS FOR WOOD BURN
      QC=0.
      DA=(BC/DIS**2)**1.5/(4.*SV)
      DB=RB**2-RIM**2
      IF(DB .LT. 0.)GO TO 56
      DC=RB*DB**1.5-1.5*RIM**2*RB*DB**0.5
      DE=DC+1.5*RIM**4*ALOG((RB+DB**.5)/RIM)
      QC=DA*DE
   56 CONTINUE
      QD=0.
      E1=RAM*DIS**2*TF**(2./3.)
      T2=(E1/(ALF*SIGMA*RB**2))**(3./14.)
      EJ=T2/TF
```

```
      IF(EJ .GT. 1.0)GO TO 5
      EK=TA/T2
      EL=0.1+3.*EJ**(14./3.)/8. -EJ**(28./3.)/48.
      EM=EL-0.5*EK**4+3.*EJ**(14./3.)*EK**4
      EN=.4556-.4188*EK**4-.05358*EK**8
      EP=3.*(TF**(10./3.)*EM-T2**(10./3.)*EN)
      EQ=ALF*SIGMA*RB**2/(DIS**2)
      QD=EQ*EA*EP
      Q2(I)=QC+QD
C     Q2 IS THE STRUCTURE EIDIATION
    5 CONTINUE
      REWIND 34
      DO 10 I=1,NCELL
      WRITE(34,701)Q1(I),Q2(I)
   10 CONTINUE
  701 FORMAT(2E16.5)
*DELETE,FLFIR4.2
      IF(Q2(LC) .GT. 0.0)NPFLAG=1
*DELETE,FLFIR5.15,FLFIR5.25
      IF(DIST .GE. RL)GO TO 51
      QSR(IF)=QIR
      GO TO 55
   51 CONTINUE
      QSR(IF)=(RL**2/(2.*DIST**2))*QIR
*IDENT STRUC
*INSERT,FLFIR1.44
      COMMON/RADOS/Q1(400),Q2(400)
*INSERT,FLFIR1.57
      CALL IRCL(5006,IIGN,IS,IR)
      IF(IIGN .GT. 1)GO TO 941
      F=0.
      FLIT=0.
      IF(Q2(LC) .LT. 1.364E+12)RETURN
      F=1.0
      FLIT=1.0
      RETURN
  941 CONTINUE
```

```
*IDENT PHASIA
*DELETE,PH2.1
     1TAPE23,TAPE24,TAPE25,TAPE26,TAPE33,TAPE34,TAPE6=OUTPUT)
*INSERT,PHASEII.9
      COMMON/TOX/DOS(400),DOSIN(400)
      COMMON/RADOS/Q1(400),Q2(400)
*INSERT,PHASEII.60
      IF(ITOX .NE. 1)GO TO 778
      REWIND 33
      DO 1 I=1,NCELL
      READ(33,777) DOS(I),DOSIN(I)
      IF(EOF(33))965,1
    1 CONTINUE
  777 FORMAT(2E16.6)
  778 CONTINUE
      REWIND 34
      DO 5 I=1,NCELL
      READ(34,740)Q1(I),Q2(I)
      IF(EOF(34))965,5
    5 CONTINUE
  965 CONTINUE
  740 FORMAT(2E16.5)
*DELETE,PHASEII.74
  130 IF(ITOX .NE. 1)CALL PRCONC(WTMOL,COPW)
*DELETE,PHASEII.96
     *         10HFIREBALL ,7X,12HPOOL BURNING)
*INSERT,PHASEII.141
      IF(ITOX .EQ. 1)GO TO 275
*IDENT SADTOX
*DELETE SADTA1.5,SADTA1.35
      COMMON/TOX/DOS(400),DOSIN(400)
      PCT1=0.
      PCT2=0.
      PCT3=0.
      IF(DOS(I).LT.0.0.OR.DOSIN(I).LT.0.)WRITE(6,431)I,DOS(I),DOSIN(I)
      IF(DOS(I).LT.0.0.OR.DOSIN(I).LT.0.)GO TO 900
  431 FORMAT(I10,2E16.4)
      IF(DOS(I) .EQ. 0.)GO TO 40
      PRT1=T1A+T1B*ALOG(DOS(I))
      PCT1=XNORMA(PRT1-5.)
      PRT2=T2A+T2B*ALOG(DOS(I))
      PCT2=XNORMA(PRT2-5.)
      PCT2=PCT2-PCT1
      IF(PCT2 .LT. 0.)PCT2=0.
      IF(DOS(I) .LE. T3A)GO TO 40
      PCT3=1. -PCT1-PCT2
   40 PARR(1,KOUT)=PCT1
```

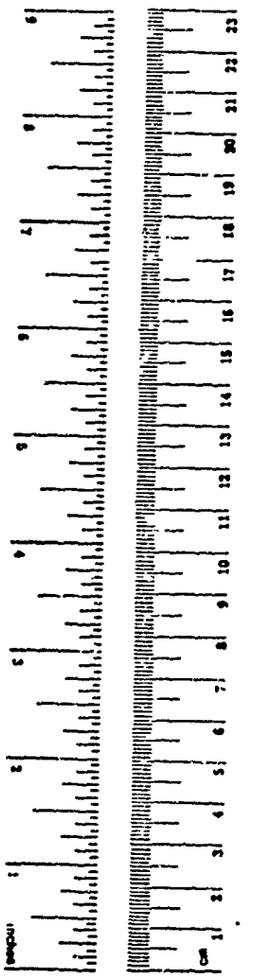
```
      PARR(2,KOUT)=PCT2
      PARR(3,KOUT)=PCT3
C     EVALUATE INDOOR DEATHS
      PCT18=0.
      PCT19=0.
      PCT20=0.
      IF(DOSIN(I) .EQ. 0.)GO TO 75
      PRT18=0.
      PRT19=0.
      PRT20=0.
      PRT18=T1A+T1B*ALOG(DOSIN(I))
      PCT18=XNORMA(PRT18-5.)
      PRT19=T2A+T2B*ALOG(DOSIN(I))
      PCT19=XNORMA(PRT19-5.)
      PCT19=PCT19-PCT18
      IF(PCT19 .LT. 0.)PCT19=0.
      IF(DOSIN(I) .LE. T3A)GO TO 75
      PCT20=1.-PCT18-PCT19
   75 PARR(18,KOUT)=PCT18
      PARR(19,KOUT)=PCT19
      PARR(20,KOUT)=PCT20
  900 CONTINUE
*IDENT SADFA
*INSERT,SADF2.5
      COMMON/RADOS/Q1(400),Q2(400)
*DELETE,SADF2.8,SADF2.13
      PCF1=0.
      PCF2=0.
      Q=Q1(I)/1.0E+08
      IF(Q .EQ. 0.)GO TO 200
*DELETE,SADF2.14
      PRF1=-12.8+2.56*ALOG(Q)
*DELETE,SADF4.4
      PRF2=-39.83+3.0186*ALOG(Q*1.0E+4)
*INSERT,SADF4.7
  200 CONTINUE
*IDENT SADSS
*INSERT,SADS2.6
      COMMON/RADOS/Q1(400),Q2(400)
```

METRIC CONVERSION FACTORS

Approximate Conversions to Metric Measures

Symbol	When You Know	Multiply by	To Find	Symbol
		LENGTH		
in	inches	*2.5	centimeters	cm
ft	feet	30	centimeters	cm
yd	yards	0.9	meters	m
mi	miles	1.6	kilometers	km
		AREA		
in^2	square inches	6.5	square centimeters	cm^2
ft^2	square feet	0.09	square meters	m^2
yd^2	square yards	0.8	square meters	m^2
mi^2	square miles	2.6	square kilometers	km^2
	acres	0.4	hectares	ha
		MASS (weight)		
oz	ounces	28	grams	g
lb	pounds	0.45	kilograms	kg
	short tons (2000 lb)	0.9	tonnes	t
		VOLUME		
tsp	teaspoons	5	milliliters	ml
tbsp	tablespoons	15	milliliters	ml
fl oz	fluid ounces	30	milliliters	ml
c	cups	0.24	liters	l
pt	pints	0.47	liters	l
qt	quarts	0.95	liters	l
gal	gallons	3.8	liters	l
ft^3	cubic feet	0.03	cubic meters	m^3
yd^3	cubic yards	0.76	cubic meters	m^3
		TEMPERATURE (exact)		
°F	Fahrenheit temperature	5/9 (after subtracting 32)	Celsius temperature	°C

*1 in = 2.54 (exactly). For other exact conversions and more detailed tables, see NBS Misc. Publ. 286, Units of Weights and Measures, Price $2.25, SD Catalog No. C13.10:286.



Approximate Conversions from Metric Measures

Symbol	When You Know	Multiply by	To Find	Symbol
		LENGTH		
mm	millimeters	0.04	inches	in
cm	centimeters	0.4	inches	in
m	meters	3.3	feet	ft
m	meters	1.1	yards	yd
km	kilometers	0.6	miles	mi
		AREA		
cm^2	square centimeters	0.16	square inches	in^2
m^2	square meters	1.2	square yards	yd^2
km^2	square kilometers	0.4	square miles	mi^2
ha	hectares (10,000 m^2)	2.5	acres	
		MASS (weight)		
g	grams	0.035	ounces	oz
kg	kilograms	2.2	pounds	lb
t	tonnes (1000 kg)	1.1	short tons	
		VOLUME		
ml	milliliters	0.03	fluid ounces	fl oz
l	liters	2.1	pints	pt
l	liters	1.06	quarts	qt
l	liters	0.26	gallons	gal
m^3	cubic meters	35	cubic feet	ft^3
m^3	cubic meters	1.3	cubic yards	yd^3
		TEMPERATURE (exact)		
°C	Celsius temperature	9/5 (then add 32)	Fahrenheit temperature	°F