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Turbulent Chemistry Modeling Program
Volume 2—Nuclear Dust Cloud Radioactive Microphysics Sensitivity Studies

Philip A. Hookham, et al.
Titan Corporation
California Research & Technology Div.
20943 Devonshire St.
Chatsworth, CA 91311

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Philip A. Hookham, Douglas W. Hatfield, Richard J. Schlamp,
Paul J. Hassig and Martin Rosenblatt

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A two-or three-dimensional compressible, Reynolds-averaged, Navier-Stokes hydrocode using adaptive zoning and finite-volume TVD differencing (called MAZ for Multiphase Adaptive Zoning) was used to simulate the formation of radioactive nuclear dust clouds. A series of sensitivity studies examining the effect of changes in particle agglomeration and radioactive vapor condensation models on the activity particle size distribution (APSD) were performed. In addition, a model which accounts for the effect of turbulent fluctuations on the radioactive vapor condensation process was implemented and tested. Accounting for agglomeration of wet particles was found to have the single largest effect on APSD.

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PREFACE

Work reported herein was performed by the California Research and Technology Division of the Titan Corporation during the period August 1991 through December 1992 for the Defense Nuclear Agency (DNA) under contract DNA001-91-C-0099.

The authors would like to acknowledge the contributions of the following individuals to this work. Assistance in preparation of the manuscript was provided by Ms. Jean Lierman. The work was supported and monitored by A. Anton Frederickson and Major John Kyme of DNA/SPWE.

CONVERSION TABLE

Conversion factors for U.S. Customary to metric (SI) units of measurement

MULTIPLY ⟶ BY ⟶ TO GET

TO GET ⟵ BY ⟵ DIVIDE

angstrom	1.000 000 X E -10	meters (m)
atmosphere (normal)	1.013 25 X E +2	kilo pascal (kPa)
bar	1.000 000 X E +2	kilo pascal (kPa)
barn	1.000 000 X E -28	meter^2 (m^2)
british thermal unit (thermochemical)	1.054 350 X E +3	joule (J)
calorie (thermochemical)	4.184 000	joule (J)
cal (thermochemical)/cm^2	4.184 000 X E -2	mega joule/m^2(MJ/m^2)
curie	3.700 000 X E +1	*giga becquerel (GBq)
degree (angle)	1.745 329 X E -2	radian (rad)
degree Fahrenheit	t_k = t°f + 459.67)/1.8	degree kelvin (k)
electron volt	1.602 19 X E -19	joule (J)
erg	1.000 000 X E -7	joule (J)
erg/second	1.000 000 X E -7	watt (W)
foot	3.0048 000 X E -1	meter (m)
fout-pound-force	1.355 818	joule (J)
gallon (U.S. liquid)	3.785 412 X E -3	meter^3 (m^3)
inch	2.540 000 X E -2	meter (m)
jerk	1.000 000 X E +9	joule (J)
joule/kilogram (J/kg) (radiation dose absorbed)	1.000 000	Gray (gy)
kilotons	4.183	terajoules
kip (1000 lbf)	4.448 222 X E +3	newton
kip/inch^2 (ksi)	6.894 757 X E +3	kilo pascal (kPa)
ktap	1.000 000 X E +2	newton-second/m^2 (N-s/m^2)
micron	1.000 000 X E -6	meter (m)
mil	2.540 000 X E -5	meter (m)
mile (international)	1.609 344 X E +3	meter (m)
ounce	2.834 952 X E -2	kilogram (kg)
pound-force (lbs avoirdupois)	4.448 222	newton (N)
pound-force inch	1.129 848 X E -1	newton-meter (N-m)
pound-force/inch	1.751 268 X E +2	newton-meter (N/m)
pound-force/foot^2	4.788 026 X E -2	kilo pascal (kPa)
pound-force/inch^2 (psi)	6.894 747	kilo pascal (kPa)
pound-mass (1bm avoirdupois)	4.535 924 X E -1	kilogram (kg)
pound-mass-foot^2 (moment of inertia)	4.214 011 X E -2	kilogram-meter^2 (kg-m^2)
pound-mass/foot^3	1.601 846 X E +1	kilogram/meter^3 (kg-m^3)
rad (radiation dose absorbed	1.000 000 x E -2	**Gray (Gy)
roentgen	2.579 760 X E -4	coulomb/kilogram (*C/Kg)
shake	1.000 000 X E -8	seconds (s)
slug	1.459 390 X E +1	kilogram (kg)
torr (mm Hg, 0°C)	1.333 22 X E -1	kilo pascal (kPa)

* The becquerel (Bq) is the SI of unit of radioactivity; 1 Bq = 1 event/s.

** The gray (GY) is the SI unit of absorbed radition.

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Figures

SECTION 1

INTRODUCTION

1.1 BACKGROUND.

Currentlv, DELFIC is the standard code for prediction of radioactive cloud dispersion and fallout. It is sophisticated in the treatment of processes which were well studied at the time of its development (the 1960s), such as radioactive decay. Its treatment of hydrodynamics and microphysics is more crude, however. Research in hydrodynamics and microphysics in the DNA and other communities since DELFIC was developed has advanced the state-of-the-art considerably, particularly in the field of turbulence. It was therefore recognized that first-principles hydrodynamics codes developed under DNA sponsorship, such as MAZ (Hatfield et al. 1991), could be upgraded to give more accurate predictions of radioactive nuclear clouds. In particular, microphysics models for condensation of radioactive species and agglomeration of radioactive particles were recognized as areas where improvement was needed.

The modeling of turbulence in the simulation of nuclear airblast and cloud rise has advanced considerably under DNA sponsorship (see Hassig et al. 1991, 1992; Hookham et al. 1991, e.g.). Further, the phenomenon of turbulent unmixedness (Walitt et al. 1991) has been shown to be potentially important when computing source terms for non-linear processes such as chemical reactions. The conventional approach of using cell-averaged values of turbulently fluctuating quantities to compute these source terms can give erroneous results. Turbulent fluctuations in such quantities as radioactive vapor concentration, particle velocity, and temperature could have a significant effect upon microphysics processes such as condensation, agglomeration, and ablation. The effect of turbulence and turbulent unmixedness upon microphysics processes was therefore identified as an area which warranted further investigation.

1.2 OBJECTIVES.

The primary objectives of this study are listed below.

- Determine the sensitivity of the distribution of radioactivity within a nuclear cloud to agglomeration and condensation models and their parameters.
- Determine which physical processes are important to model and which are not.
- Perform sensitivity studies on parameters which are not well characterized.
- Develop improved condensation and agglomeration models for radioactive species.
- Investigate the effects of turbulence upon condensation and agglomeration.

1.3 APPROACH.

The sensitivity of the calculated distribution (spatial and temporal) of radioactivity in a nuclear cloud to agglomeration and condensation models was studied by performing parametric variations on a test case, described below.

Test Case
- 300 kt at 50 sft
- Production zoning (10,000 zones max.)
- 6 particle size groups: mean diameter = 4.5, 32, 112, and 500 μm, and 0.2 and 0.89 cm for groups 1-6
- One composite radioactive species based on curve ,f McGahan (1990)
- Current standard nuclear dust cloud physical sub-models
- Moscow July atmosphere (relatively humid)

The test case was re-run as changes in the agglomeration and condensation models were made. The calculations were performed with the MAZ hydrocode (Hatfield et al. 1991).

SECTION 2

RADIOACTIVE DUST CLOUD MICROPHYSICS MODELS

The microphysics model improvements will be separated into "basic" model improvements and turbulent unmixedness model improvements. The effect of the model changes will be illustrated by comparing results from the test case as each change was made. The matrix of test cases and model changes is shown in Table 1.

2.1 BASIC MODEL IMPROVEMENTS.

The "baseline" model for condensation of radioactive vapor and subsequent agglomeration of radioactive particles was adopted to give a preliminary estimate of the distribution of radioactivity in a nuclear cloud. The model considered agglomeration between pure radioactive particles and non-radioactive dust only, and neglected radioactive dust-dust agglomeration and pure-pure agglomeration. In an attempt to study the effect of agglomeration, the radioactive vapors were forced to condense preferentially upon the pure radioactive particles relative to dust particles in a 90/10 ratio (if this were not so, most of the vapor would condense upon the dust, which was not allowed to agglomerate). A 1 μm size was assumed for the pure condensed radioactive particles (conrads). Case TM01 used these baseline models.

The first model improvement was to allow radioactive dust-dust agglomeration and to not force the radioactive vapors to condense preferentially upon the pure particles. Agglomeration was allowed to occur as a result of relative mean velocities between particles of different sizes, and thus since all particles of a given size have the same velocity, particles of the same size could not agglomerate. The agglomeration model for this "differential scavenging" process is described in Figure 2-1.

Calculation TM02A included dust-dust agglomeration and removed the restriction on where radioactive vapors could condense. Calculation TM02B investigated the effect of lowering the particle collision efficiency to 1 from the previous value of 2 (2 was used previously to account for the effects of turbulence upon agglomeration in a very crude way). Calculation TM02C then investigated the effect of changing the "sticking efficiency" from the nominal value of 1 (an upper bound, since presumably all particles that collide will not stick) to 1 if the particle surface temperature was greater than the melting point of dust, and 0 if it was not. The latter condition is probably closer to a lower bound on sticking efficiency. TM03 then added a simple turbulent agglomeration model, described in Figure 2-1, which accounted only for agglomeration of similar-size particles which were smaller than the small turbulent eddies in the flow (there is no such simple model for larger particles which do not follow the flow, although we can address this issue with our unmixedness model).

The distribution of radioactivity within a dust cloud can be effectively summarized by the cumulative activity particle size distribution (APSD) for the cloud, which is shown in Figure 2-2 for

Table 1

TABLE OF AGGLOMERATION/CONDENSATION SENSITIVITY STUDIES.

CASE NUMBER	END TIME (MIN)	WATER MICRO-PHYSICS ON?	AGGLOMERATION MODEL				CONDEN-SATION MODEL
			DUST-PURE AGGLOM.?	DUST-DUST AGGLOM.?	COLLISION EFFICIENCY	ST'CKING EFFICIENCY	
TM01	1	no	yes	no	2	1	90% on pure, 10% on dust
TM02A	1	no	yes, relative velocity	yes, relative velocity	2	1	if dust exists, condense on dust, if not, form pure
TM02B	1	no	"	"	1	1	"
TM02C	1	no	"	"	1	1 if melted, 0 if not	"
TM03	1	no	yes, relative velocity and Saffman-Turner turbulent	yes, relative velocity and Saffman-Turner turbulent	1	"	"
TM03A	10	yes	"	"	1	1 if particle is melted or condensed water is present, 0 if not	"
TM04	1	no	"	"	1	1 if melted, 0 if not	turbulent model

Collection rate of particles size i by particles size j : $d\rho_{ij}/dt$

Differential Scavenging (due to relative mean velocities)

$$d\rho_{ij}/dt = \pi (R_i+R_j)^2 (V_i-V_j) (\rho_i/M_i) (\rho_j/M_j) CE_{ij} SE_{ij} M_i \quad ,$$

where:		
	ρ_i	is the "continuum" (not grain) mass density of particles i,
	R_i	is the radius of particle i,
	V_i-V_j	is the relative mean velocity between particles i and j,
	M_i	is the mass of individual particle i,
	CE_{ij}	is the collision efficiency, and
	SE_{ij}	is the sticking efficiency. For nuclear case: = 1 if $T_{surface} > T_{melt}$ 0 otherwise.

Turbulent Agglomeration (Saffman-Turner, 1956)

$$d\rho_{ij}/dt = 1.3 (R_i+R_j)^3 (\varepsilon/v)^{1/2} (\rho_i/M_i) (\rho_j/M_j) SE_{ij} M_i$$

where:		
	ε	is the turbulent kinetic energy dissipation, and
	v	is the kinematic viscosity (μ/ρ).

Assume valid for R_i < Kolmogorov turbulence length scale $= (v^3/\varepsilon)^{1/4} =\sim 100\ \mu m$

For SOCTM: $\varepsilon = \grave{o}\, q^3 / \Lambda$ $\sim 10^4 - 10^5\ cm^2/s^3$

Figure 2-1. Agglomeration model description.

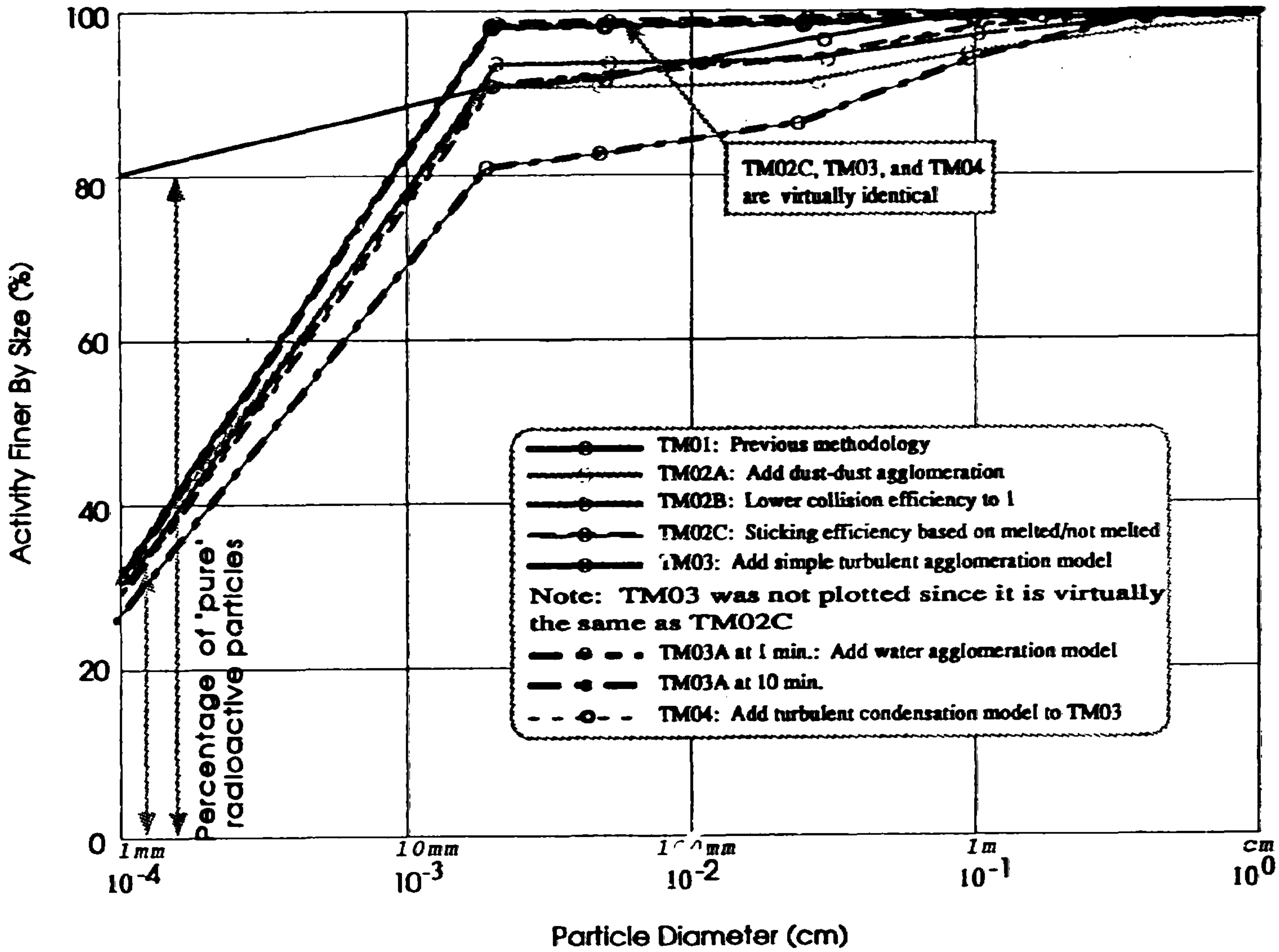


Figure 2-2. Cumulative activity particle size distribution comparison.

the cases listed in Table 1 (all curves are for 1 minute, except TM03A, which is shown at 1 and 10 minutes). Case TM01 shows a large amount of pure radioactive particles, which agglomerate relatively rapidly due to their small size. (Agglomeration rate due to particle relative mean velocity is inversely proportional to particle radius, neglecting the effect of lower collision efficiencies for small particles, which can flow around larger particles instead of colliding.) This calculation is shown for comparison only, as it does not represent a realistic condensation/agglomeration model. Proceeding to Case TM02A, allowing dust-dust agglomeration and not forcing the bulk of the radioactivity to condense on the conrad (pure radioactive) particles resulted in a reduction in conrad concentration from ~80 to ~30% of total activity. The amount of activity on the larger dust particles increased also. Lowering the collision efficiency to 1 in Case TM02B resulted in somewhat less agglomeration, and hence less activity on the larger particles.

Assuming a sticking efficiency of 1 for hard dust particles seemed intuitively to be an overestimate. Thus, the sticking efficiency was made a function of the presence of physical forces that would act to hold the particles together. Making the sticking efficiency a function of whether liquid is present on particle surfaces (Case TM02C) resulted in a substantial decrease in agglomeration rate, and only ~2% of the activity resides on larger particle sizes. Allowing agglomeration when there was condensed water present (Case TM03A) increased agglomeration substantially, particularly if the calculation was continued to 10 minutes. The effect of wet agglomeration is further illustrated in Figure 2-3, which shows vertical distributions of cumulative attached activity and agglomerated activity (pure radioactive particle to dust agglomeration only is shown) for all dust groups together and individually. Wet agglomeration clearly makes a substantial difference in the amount of agglomeration, at least for the relatively humid atmosphere used for these calculations.

Adding the simple turbulent agglomeration model in Case TM03 resulted in essentially no change in the APSD. We must remember, however, that this model only considers small particles moving with the turbulent eddies, and neglects entirely larger particles moving relative to the turbulent eddies.

In addition to the effect of agglomeration on the radioactive APSD, adding agglomeration of non-radioactive dust caused significant changes in the non-radioactive dust cloud. Figure 2-4 shows a comparison of Case TM01, which had no dust-dust agglomeration, to Case TM03, which agglomerated if particles were melted, and TM03A, which agglomerated if particles were melted or wet. Case TM03 gave similar results to Case TM01, but Case TM03A, while having a similar amount of total dust lofted, lofted a substantially larger amount of the larger size particles (group 6, e.g.). (Note that in the lower figures the numbered contours correspond to size group number, while in the upper figures they refer to concentration.)

As an indication of how the APSD varied with location in the dust cloud, Figure 2-5 shows APSDs computed for horizontal "fly-throughs" at several locations for Case TM03A. The fly-through calculations simulate an aircraft flying a straight horizontal path through the cloud and

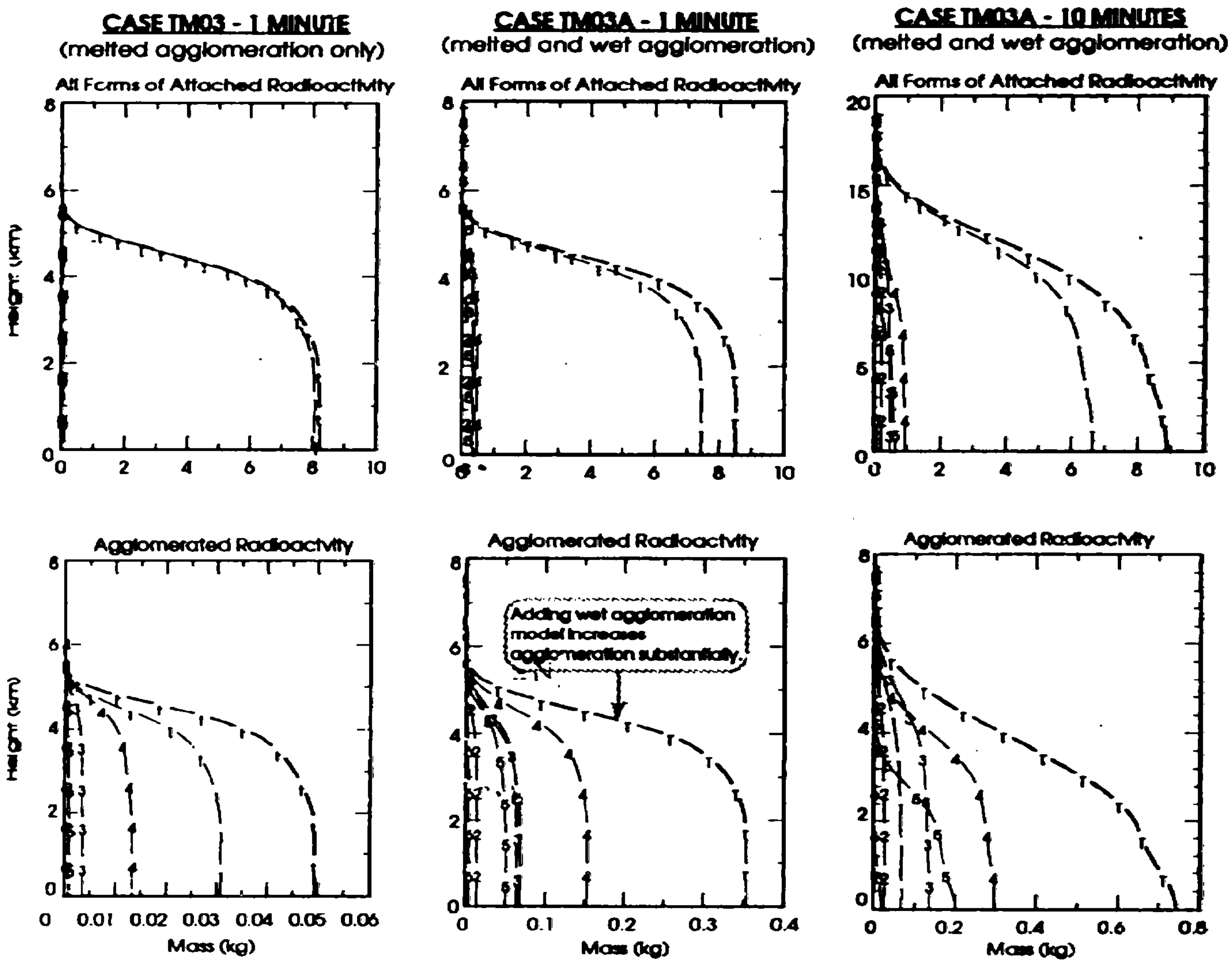


Figure 2-3. Effect of wet agglomeration model.

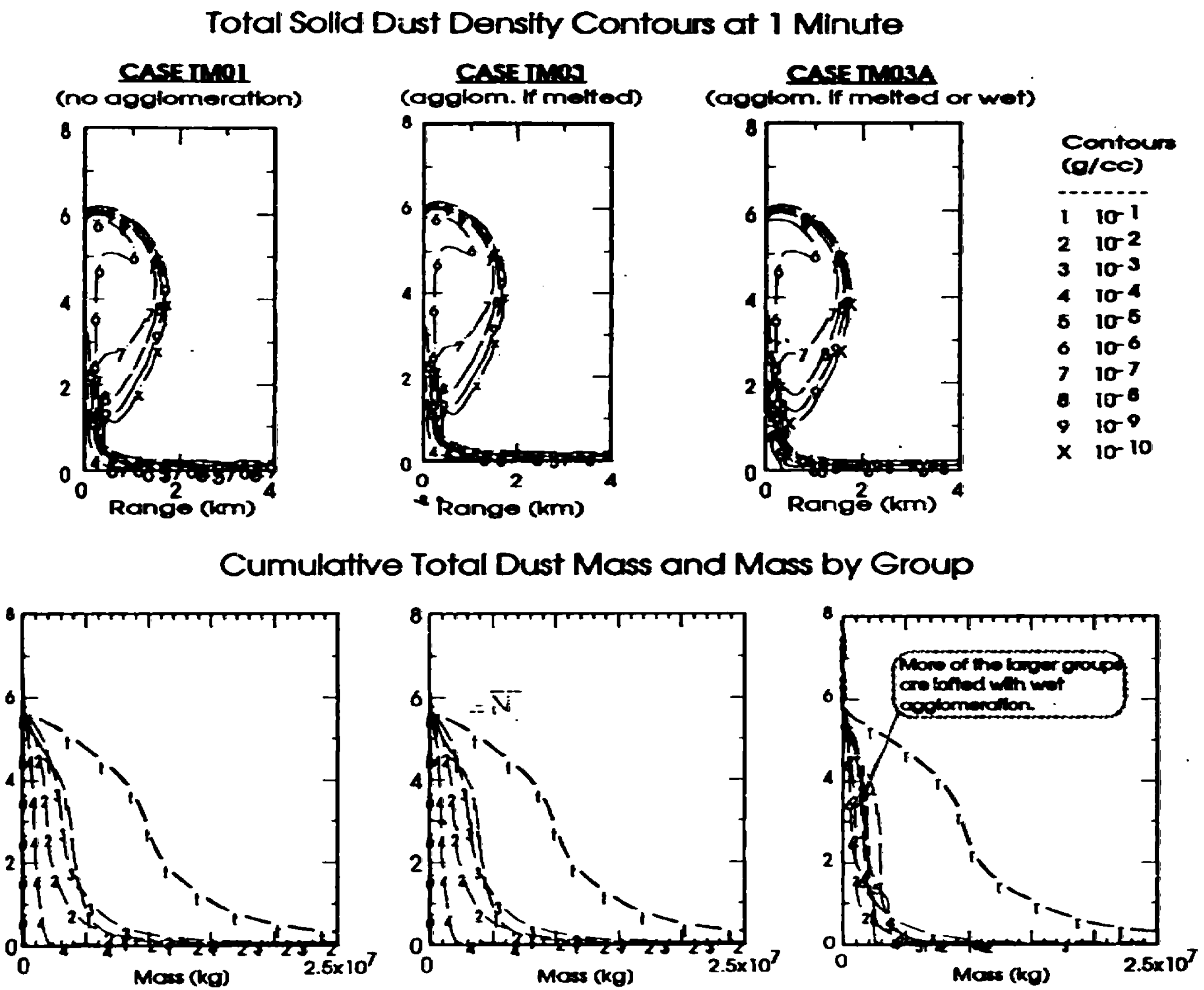


Figure 2-4. Effect of agglomeration on non-radioactive dust cloud.

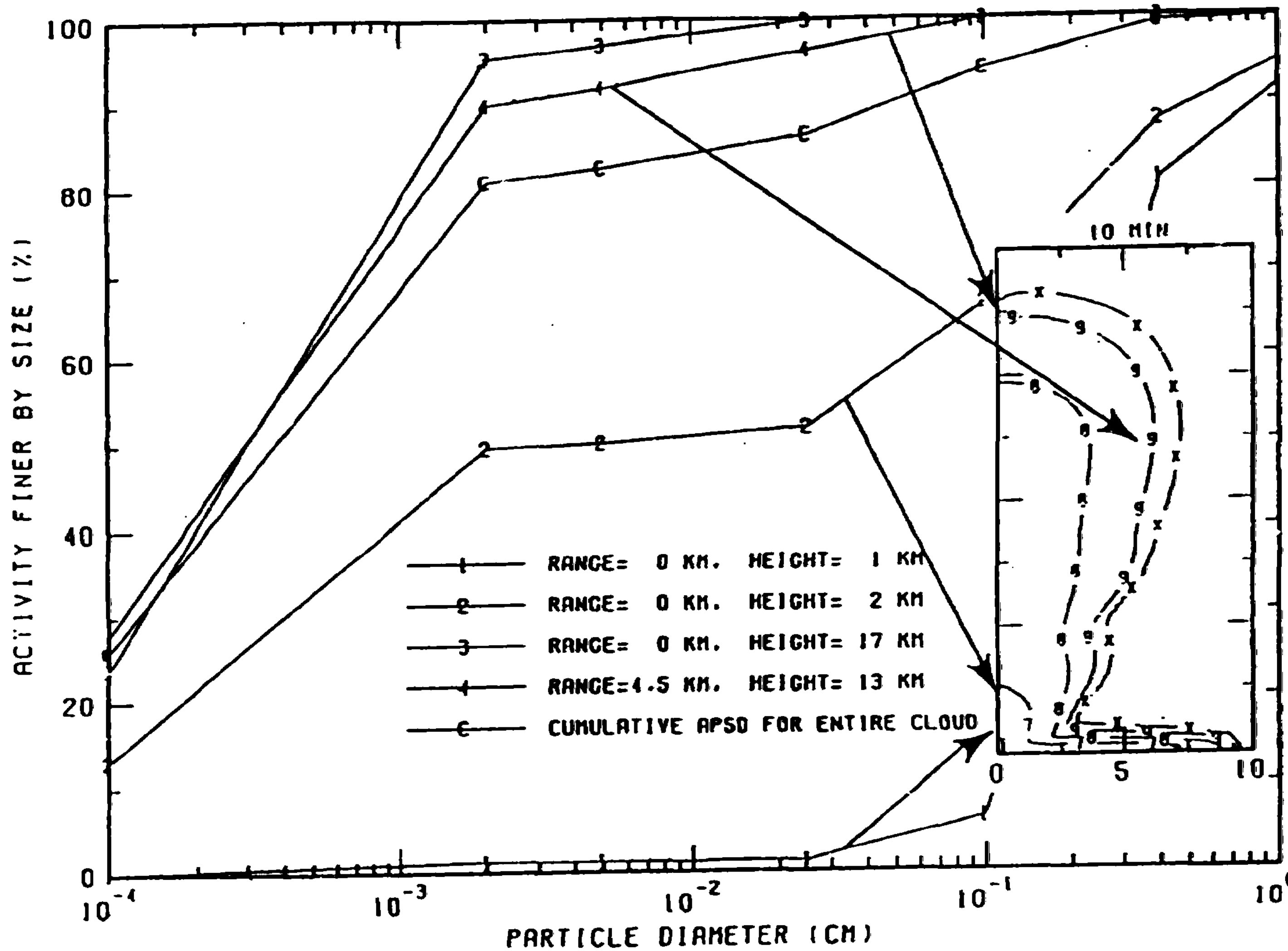


Figure 2-5. Case TM03A (300 kt at 50 sft) activity psds for cloud fly-throughs at 10 min.

collecting mass. It is evident that the cloud stem contains many more large particles than the cloud as a whole, while the top of the cloud contains more small particles.

2.2 TURBULENT UNMIXEDNESS CONDENSATION MODEL.

The condensation model was chosen as a first test of turbulent unmixedness modeling. The model is described in some detail below.

Consider condensation of a trace quantity of radioactive vapor species, with mass fraction c_s, on solid particles with number density N_ℓ. In order to evaluate the time rate of change of mean vapor concentration, we need to know the mean condensation rate. Figure 2-6 expresses the instantaneous rate as a function of local gas and particle properties. The relationship is non-linear in the vapor and particle concentrations, temperature, and velocities. Hence, the mean condensation rate, say averaged over a timestep, cannot, in general, be evaluated by using only mean cell properties (see Figure 2-6). If we perform a Taylor series expansion on the rate expression, we obtain equation 2-4 in Fig. 2-7, indicating a second-order concentration correlation. (The dots in the equation refer to additional correlations in the expansion.) This correlation can be positive or negative. When for example, at interfaces where intermixing of vapor and solid particles (condensation sites) occurs, the correlation is negative, indicating a condensation rate less than that predicted using conventional (mean-value) models. This phenomenon is referred to as unmixedness in turbulent combustion.

To proceed, we require the second-order concentration correlation. Following standard turbulent closure model practices, we develop a continuity equation for the correlation by mathematically manipulating the individual vapor and particle continuity equations and taking an ensemble average of the result. Sparing the details, Figure 2-8 shows the final equation, in which triple correlations have been replaced by modeled diffusion and dissipation terms. These modeled terms are analogous to similar terms in the air closure equations. For small particles, which follow local air eddies, we set the empirical coefficients in the modeled terms to the air values, which have been calibrated to experiment. For larger particles which slip relative to the gas phase, the coefficients may need adjustment. The research of Rizk and Elghobashi (1989), which indicates particle size dependency on turbulent diffusion velocities, will be of value here. Ultimately, the validity of models is established by matching calculations with controlled experiments.

The last term in equation 2-5 represents the high-order moments of the condensation rate in the vapor continuity equation. Conventional closure methods do not permit its evaluation. Instead, we apply the turbulent chemistry pdf approach. Figure 2-8 shows 2-D slices of the pdf for vapor and particle concentrations. (The pdf is actually a surface in c_s-N space.) The pdf can be approximated with a finite number of Dirac functions with as-yet undetermined strengths ε_j. Constraints include the values of mean concentrations and double correlation. (In an explicit numerical scheme, we take values from the previous timestep as known quantities in order to advance these quantities to the next cycle.) The locations of the Dirac functions are specified, discrete events; they are chosen to represent the physics of the problem.

RADIOACTIVE VAPOR CONDENSATION ON SOLID/LIQUID PARTICLES

$$\dot{\rho}_{s\ell} = K_{s\ell}(T_s, T_\ell, \Delta u_{s\ell}) A_\ell N_\ell (c_s - c_i) \quad (2.1)$$

where $\dot{\rho}_{s\ell}$ = condensation rate (g / cc - sec) of vapor species "s" on particle group "ℓ"

$K_{s\ell}$ = rate constant as function of vapor and particle temperatures, T_s, T_ℓ, slip velocity, $\Delta u_{s\ell}$, between phases, and particle diameter, d_ℓ.

A_ℓ = surface area of a particle

N_ℓ = number density of particles (#/cc)

c_s = mass fraction of vapor species $(\rho_s / \rho_{gas,\ total})$

c_i = equilibrium mass fraction of vapor at gas/ particle interface (depends on interface temperature)

Figure 2-6. Radioactive vapor condensation on solid/liquid particles.

Why Turbulence Affects the Radioactive Vapor Condensation Rate

Instantaneous rate:

$$\dot{\rho}_{s\ell} = K_{s\ell} A_\ell N_\ell (c_s - c_i) \quad (2.2)$$

Time-averaged rate:

$$\overline{\dot{\rho}_{s\ell}} = \overline{K_{s\ell} A_\ell N_\ell (c_s - c_i)} \neq \overline{K_{s\ell}} A_\ell \overline{N_\ell} (\bar{c}_s - \bar{c}_i) \quad (2.3)$$

If we consider concentration flucuations:

$$\overline{\dot{\rho}_{s\ell}} = \overline{K_{s\ell}} A_\ell \left[\overline{N_\ell} (\bar{c}_s - \bar{c}_i) + \overline{N_\ell' c_s'} \right] + \cdots \quad (2.4)$$

The correlation $\overline{N_\ell' c_s'}$ can be either positive or negative. It tends to be negative when the vapor and particle phases are intermixing as in a fireball. Hence, if turbulent fluctuations are large, using mean properties to evaluate the condensation rate can overestimate the effect. This is analogous to unmixedness effects on gaseous chemical reactions in turbulent flows.

Figure 2-7. Why turbulence affects the radioactive vapor condensation rate.

Mean transport equations of $\overline{c_s}$ and $\overline{N_\ell}$ require source term $\overline{\dot{\rho}_{s\ell}} = K_{s\ell} A_\ell \left[\overline{N_\ell}(\overline{c}_s - c_i) + \overline{N_\ell' c_s'} \right]$
Hence we need a transport differential equation for the $\overline{N_\ell' c_s'}$ correlation.

Following Donaldson's method for turbulent chemistry:

$$\frac{D}{Dt}\bar{\rho}\overline{c_s' N_\ell'} = -\bar{\rho}\overline{u_j' c_s'}\frac{\partial \overline{N_\ell}}{\partial x_j} - \bar{\rho}\overline{u_{\ell j}' N_\ell'}\frac{\partial \bar{c}_s}{\partial x_j} \quad \longrightarrow \text{production term (exact)} \qquad (2.5)$$

$$+\frac{\partial}{\partial x_j}\left\{ v_c q \Lambda \frac{\partial}{\partial x_j}\bar{\rho}\overline{c_s' N_\ell'} \right\} \quad \longrightarrow \text{diffusion term (modeled)}$$

$$-b_{s\ell}\frac{q}{\Lambda}\bar{\rho}\overline{c_s' N_\ell'} \quad \longrightarrow \text{dissipation term (modeled)}$$

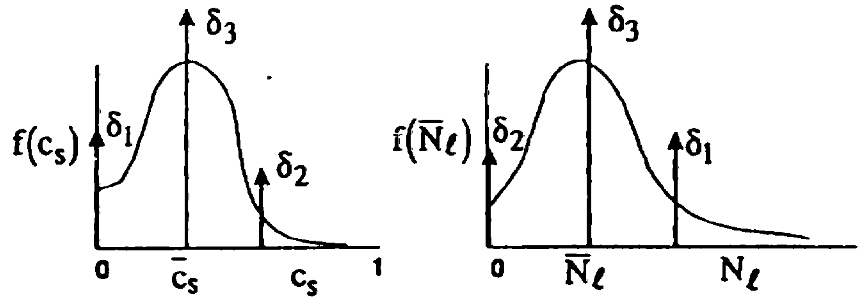
$$+\left[\overline{N_\ell}\overline{\dot{\rho}_{s\ell}} - \overline{N_\ell \dot{\rho}_{s\ell}} \right] \quad \longrightarrow \text{source term due to condensation}$$

where $\bar{\rho}$ is the mean total gas density, $0.5q^2$ is the turbulent kinetic energy, Λ is a length scale, and v_c and $b_{s\ell}$ are empirical constants.

The last term involves a triple correlation in concentrations, e.g., $\overline{N_\ell'^2 c_s'}$, hence additional modeling is required.

Figure 2-8. Method of solution: radioactive vapor condensation.

Probability Density Function (PDF) for concentrations.



Continuous PDF functions for vapor and particle concentrations are approximated with a finite number (M) of delta functions, δ_i, with strengths, ε_i.

Constraints:

$$\sum_{i=1}^{M} \varepsilon_i c_{si} = \overline{c_s} \qquad c_{si} \text{ are } c_s \text{ at specified events} \tag{2.6}$$

$$\sum_{i=1}^{M} \varepsilon_i N_{\ell i} = \overline{N_\ell} \tag{2.7}$$

$$\sum_{i=1}^{M} \varepsilon_i c_{si} N_{\ell i} = \overline{c_s N_\ell} = \bar{c}_s \overline{N}_\ell + \overline{c_s' N_\ell'} \tag{2.8}$$

Notes: (1) A minimum of three events (delta functions) must be specified, and for exactly three events, the strengths (or probabilities), ε_i, can be computed analytically.

(2) For more than three events, there are more unknowns than equations, so minimization of an entropy function, $\sum \varepsilon_i \ell n \varepsilon_i$, can determine appropriate values for the strengths.

Figure 2-8. Method of solution: radioactive vapor condensation (Continued).

Suitable events should include states at the mean (i.e., when turbulence levels are low) as well as states where one or both concentrations disappear (intermittency).

If $\overline{{}_s{}' N_\ell{}'} < 0$, we may choose

State 1: $c_{s_1} = 0$, $N_{\ell_1} = 2\overline{N_\ell}$

State 2: $c_{s_2} = 2\overline{c_s}$, $N_{\ell_2} = 0$

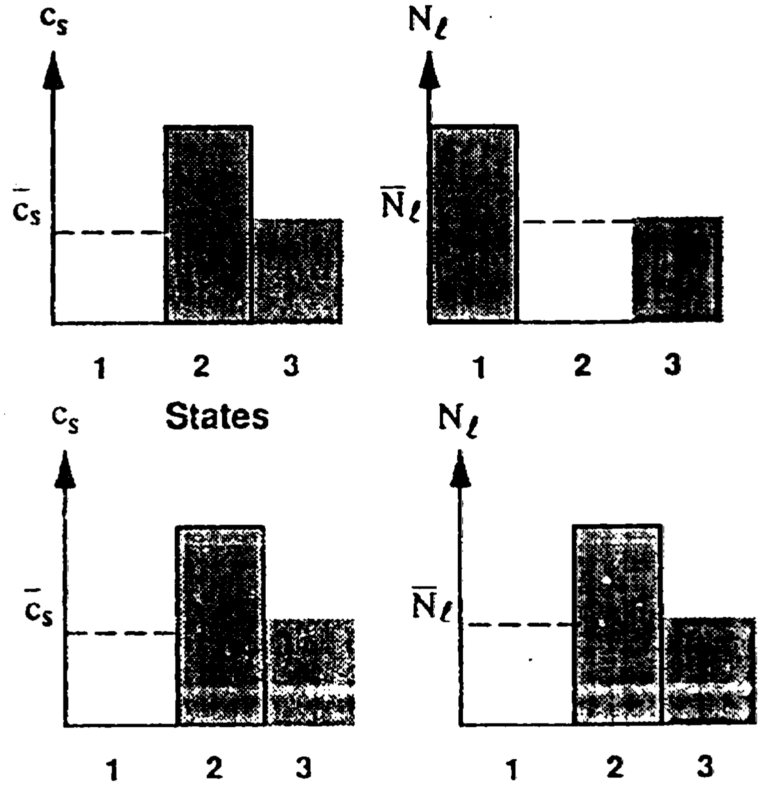
State 3: $c_{s_3} = \overline{c_s}$, $N_{\ell_3} = \overline{N_\ell}$

Or if $\overline{c_s{}' N_\ell{}'} > 0$,

State 1: $c_{s_1} = 0$, $N_{\ell_1} = 0$

State 2: $c_{s_2} = 2\overline{c_s}$, $N_{\ell_2} = 2\overline{N_\ell}$

State 3: $c_{s_3} = \overline{c_s}$, $N_{\ell_3} = \overline{N_\ell}$



The choice of event states can be prescribed locally for each computational zone depending on known sign and magnitude of $\overline{c_s{}' N_\ell{}'}$. **The factor "2" in the above states is a nominal value and can be closer to unity if** $\left|\overline{c_s{}' N_\ell{}'}\right| << \bar{c}_s \overline{N}_\ell$.

Figure 2-8. Method of solution: radioactive vapor condensation (Continued).

For example, if $\overline{c_s' N_\ell'} < 0$, the strengths ε_i (which satisfy $\varepsilon_1 + \varepsilon_2 + \varepsilon_3 = 1$) are computed from the constraint equations. There follows

$$\varepsilon_1 = \varepsilon_2 = -\frac{1}{2}\frac{\overline{c_s' N_\ell'}}{\bar{c}_s \overline{N}_\ell}, \quad \varepsilon_3 = 1 + \frac{\overline{c_s' N_\ell'}}{\bar{c}_s \overline{N}_\ell} \tag{2.9}$$

Once the event states are specified and the strengths are determined, any correlation involving concentrations can be computed.

For example:

$$\overline{N_\ell^2 c_s} = \sum \varepsilon_i N_{\ell i}{}^2 c_{si} = \varepsilon_1 N_{\ell 1}{}^2 c_{s1} + \varepsilon_2 N_{\ell 2}{}^2 c_{s2} + \varepsilon_3 N_{\ell 3}{}^2 c_{s3} \tag{2.10}$$

$$= \varepsilon_3 \overline{N}_\ell^2 \bar{c}_s \qquad \text{if } \overline{c_s' N_\ell'} < 0$$

$$= (4\varepsilon_2 + \varepsilon_3) \overline{N}_\ell^2 \bar{c}_s \qquad \text{if } \overline{c_s' N_\ell'} > 0$$

Figure 2-8. Method of solution: radioactive vapor condensation (Continued).

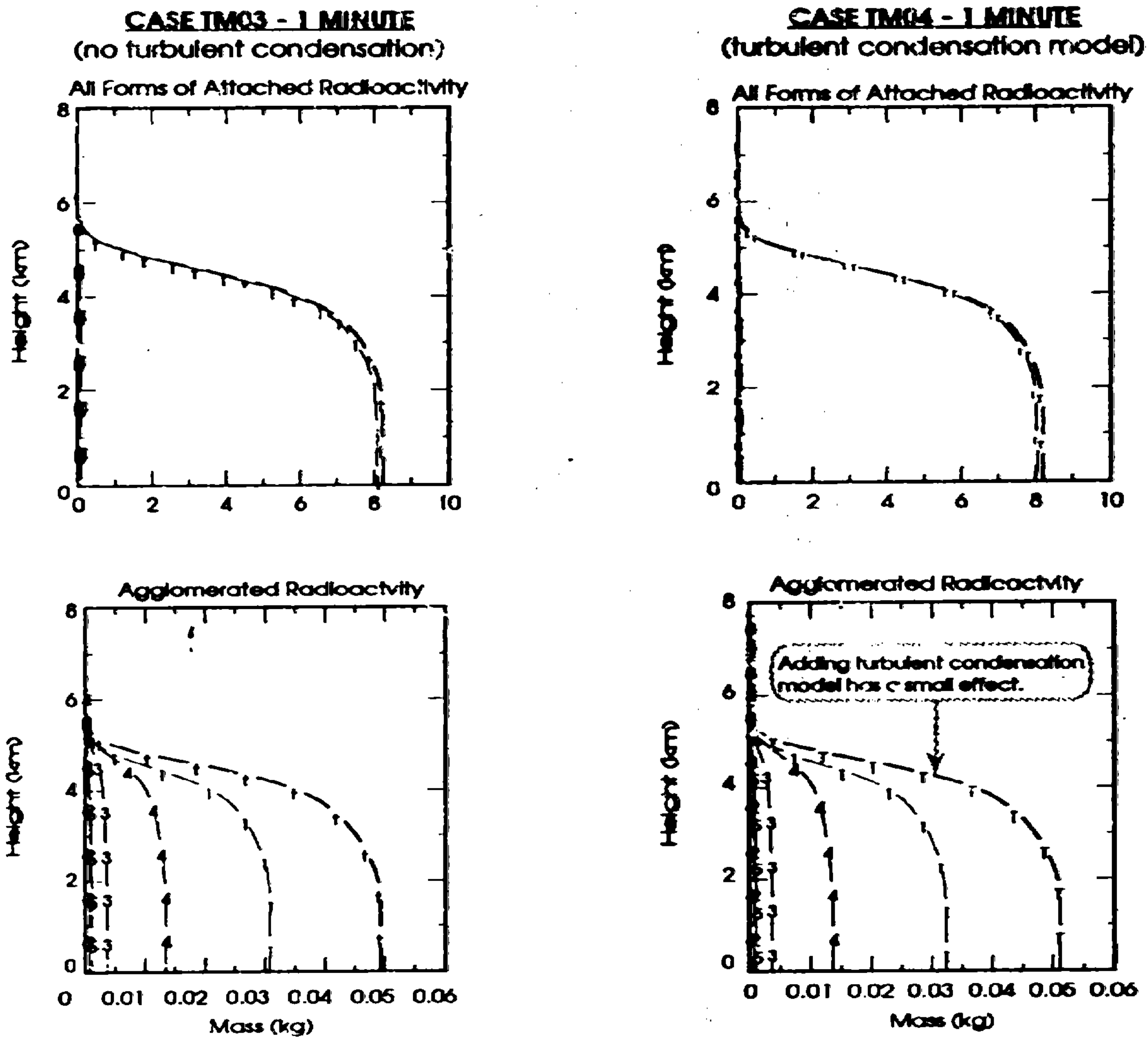


Figure 2-9. Effect of turbulent condensation model.

For this application, we choose three events as indicated in Figure 2-8. One state is naturally chosen at the mean concentrations to get a reasonable state description when turbulence levels are low. Local fluctuations can force concentrations of one or both species to zero (intermittency), hence, Dirac functions are introduced at these states. Instantaneous concentrations greater than the mean are accommodated with Dirac functions placed at a multiple of the mean concentration. Constraint equations 2-6 through 2-8 allow the exact computation of Dirac function strengths for 3 states. More states may be desirable, however. In this case, there are more unknown quantities than constraints, so minimization of an "entropy" function "F", can be employed. Note that for the test calculation described below, the turbulent correlation $\overline{c_g' N_\ell'}$ was calculated using a mixing-length approximation to determine if turbulent unmixedness was important to the condensation process before the full second-order closure correlation was calculated.

Once discrete states have been chosen (in each computational cell based on local physics), and the Dirac function strengths are determined (see equation 2-9, which follows from equations 2-6 to 2-8 and states indicated in Figure 2-8), any high order moment involving vapor and/or particle concentrations can be computed. Equation 2-10 in Figure 2-8 shows an example for a triple correlation which is needed to close the double concentration correlation, equation 2-5.

Figure 2-9 shows a comparison of Case TM04, which used the turbulent condensation model described above, to Case TM03, which did not (the calculations were otherwise the same). It can be seen that adding the turbulent unmixedness model had only a small effect upon the amount of condensation. Examination of the solution revealed that although the unmixedness model did change the instantaneous condensation rate substantially, the overall rate of condensation was limited by the rate of cooling of a given computational cell, so that increasing the instantaneous rate had a small effect.

SECTION 3

CONCLUSIONS AND RECOMMENDATIONS

3.1 CONCLUSIONS.

The conclusions from this study are summarized as follows.

- Adding agglomeration of wet particles (mud) produced a substantial amount of agglomeration which continued to about 10 minutes. **This phenomenon had the single biggest effect on agglomeration**.
- Basing the agglomeration model only on whether the particle surface was melted resulted in a relatively small amount of agglomeration. If a sticking efficiency of 1 was assumed even when a particle was not melted, significant agglomeration occurred.

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- Adding agglomeration of wet particles (mud) produced a substantial amount of agglomeration which continued to about 10 minutes. **This phenomenon had the single biggest effect on agglomeration.**
- Basing the agglomeration model only on whether the particle surface was melted resulted in a relatively small amount of agglomeration. If a sticking efficiency of 1 was assumed even when a particle was not melted, significant agglomeration occurred.
- The simple Saffman-Turner agglomeration model did not cause a substantial amount of agglomeration in addition to that caused by relative mean particle velocity (differential scavenging).
- The addition of a turbulent condensation model produced only a small change in the radioactive cloud, since condensation was generally limited by the rate of cooling in the cloud, rather than local radioactive vapor and particle concentrations fluctuations.
- Agglomeration of non-radioactive dust had a small effect on the total dust mass in the cloud, but increased significantly the amount of larger particles, assuming particle sticking based on melted/not melted or wet. If a sticking efficiency of 1 is assumed for all conditions, total mass in the cloud at 1 minute drops by about a factor of three and the amount of larger particles increases further.

3.2 RECOMMENDATIONS.

It is recommended that the full turbulent unmixedness model for agglomeration be tested. Although the simple turbulent agglomeration model did not show an effect, that does not necessarily mean that the full model will not, since the simple model was limited in scope (the simple model only considered small particles moving with the turbulent eddies, whereas in the real case there will be substantial numbers of larger particles which do not follow the flow).

SECTION 4

REFERENCES

Hassig, P.J., et al. (1991), "Numerical Simulations of Dust/Ice Clouds from Nuclear Bursts,"(U) DNA-TR-90-91. (UNCLASSIFIED)

Hassig, P.J., et al. (1992), "Advances in Nuclear Cloud Modeling,"(U) DNA-TR-92-23. (UNCLASSIFIED)

Hatfield, D., Hookham, P., and Rosenblatt, M. (1991), "MAZ: An Advanced 2-D/3-D Research Code for Solving Complex Multiphase CFD Problems with Adaptive Zoning,"(U) CRT Technical Report. (UNCLASSIFIED)

Hookham, P.A., Rosenblatt, M., and Hatfield, D.W. (1991), "Non-Ideal Surface Airblast and Vehicle Loads Predictions in Support of Rail Garrison,"(U) DNA-TR-90-197. (SECRET)

McGahan, J. (1990), Private communication. (UNCLASSIFIED)

Rizk, M.A., and Elghobashi, S.E. (1989), "Two-Equation Turbulence Model for Dispersed Dilute Confined Two-Phase Flows,"(U) *Int. J. Multiphase Flow* 15:119-133. (UNCLASSIFIED)

Saffman P. G., and Turner, J. S. (1956), "On the Collision of Drops in Turbulent Clouds,"(U) *J. Fluid Mech.* 1,16-30. (UNCLASSIFIED)

Walitt, L., Rosenblatt, M., and Sullivan, R. (1991), "Direct Solution of Turbulence (DST) for Scientific and Engineering Applications. Volume II: Turbulent Combustion Modeling Including Unmixedness and Temperature Spottiness,"(U) CRT Report 91-3288FR. (UNCLASSIFIED)

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