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Report

MATADOR: A COMPUTER CODE FOR THE ANALYSIS OF RADIONUCLIDE BEHAVIOR DURING DEGRADED CORE ACCIDENTS IN LIGHT WATER REACTORS

by

P. Baybutt, S. Raghuram and H. I. Avci

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NOTICE

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ABSTRACT

A new computer code called MATADOR (Methods for the Analysis of Transport And Deposition Of Radionuclides) has been developed to replace the CORRAL computer code which was written for the Reactor Safety Study (WASH-1400). This report contains a detailed description of the models used in MATADOR. A companion report provides a User's Manual for the code.

MATADOR is intended for use in system risk studies to analyze radionuclide transport and deposition in reactor containments. The principal output of the code is information on the timing and magnitude of radionuclide releases to the environment as a result of severely degraded core accidents. MATADOR considers the transport of radionuclides through the containment and their removal by natural deposition and the operation of engineered safety systems such as sprays. The code requires input data on the source term from the primary system, the geometry of the containment, and thermal-hydraulic conditions in the containment.

MATADOR was written with the principal purpose of correcting three deficiencies identified in the CORRAL-2 code. First, it improves upon several transport and deposition models used in CORRAL and includes models for potentially important processes not present in that code at this time. Second, it incorporates a source term in the transport and deposition equations, thereby providing much needed flexibility in the description of the time dependence of the source term; this improvement also implies that releases of structural materials can be modeled using MATADOR. Third, it improves upon the CORRAL treatment of particle size by allowing particles of up to ten sizes to coexist and explictly models aerosol agglomeration.

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SUMMARY

The analysis of the transport and deposition of radioactive material in containment buildings is important in determining the consequences of degraded core accidents in light-water reactors. The first attempt at constructing a detailed model to perform this analysis was made at the time of the Reactor Safety Study [1] when the codes CORRAL-PWR and CORRAL-BWR were written. They were subsequently combined into one code, CORRAL-2, which has been in prominent use since that time but has received no significant modeling or structural improvements.

It was, therefore, considered appropriate that a thorough review of CORRAL-2 be undertaken to identify its major shortcomings. The review revealed several areas where improvements were possible, and it was decided that a new code should be written to replace CORRAL-2. This new code, MATADOR (Methods for the Analysis of Transport And Deposition Of Radionuclides), incorporates both structural and modeling changes. It includes the radionuclide source term in the transport and deposition equations, thereby providing much needed flexibility in the description of the time dependence of the release. Additionally, the release groups are input by the user, whereas in CORRAL they were fixed within the code. This allows for an explicit analysis of the behavior of structural materials which may be released to the containment during a degraded core accident.

MATADOR allows for the existence of particles of up to ten sizes, whereas CORRAL assumed that all particles were of the same size. MATADOR also models vapor and particle deposition processes not currently included in CORRAL and provides for the use of improved correlations for existing processes. Specifically, MATADOR models iodine transport by both natural and forced convection and treats deposition on both dry and wet surfaces. Particle deposition by gravitational settling and diffusional, thermophoretic, and diffusiophoretic deposition is modeled. Removal of airborne radionuclides by such engineered safeguards as sprays, filters, suppression pools, and ice condensers is also included in the code. MATADOR takes into account the possible degradation of filters. It also treats the attenuation of radionuclides during passage through leak pathways in the containment. The new

code has been written in a modular fashion to facilitate future modifications and improvements. Designed interfaces with other codes have also been included in MATADOR. The intent of these modifications was not to develop a mechanistic, first-principles code but rather to write a code that would execute quickly while producing reasonably accurate results so that it would be useful in system risk studies where many runs of the code are required.

1.0 INTRODUCTION

The computer codes CORRAL-PWR and CORRAL-BWR were written at the time of the Reactor Safety Study [1]. They were subsequently combined into one code called CORRAL-2. This code models radionuclide transport and deposition in light-water-reactor containment buildings during loss-of-coolant (LOCA) and meltdown accidents, and it calculates the resulting releases of radioactivity to the environment. No significant changes in the modeling of radionuclide transport and deposition by CORRAL have been made since the time of the Reactor Safety Study. Those changes which have been made relate to improving the flexibility of the code to treat a wider spectrum of accidents and reactor designs.

In the past few years, it has become apparent that several potentially important radionuclide transport and deposition processes are not modeled in CORRAL. Examples of processes not modeled but which can be important are removal of radionuclide vapors by steam condensing on the containment walls and thermophoretic particle deposition. Additionally, a number of the models presently used in CORRAL can now be replaced by newer and improved ones. Furthermore, there is a need for a more flexible description of the radionuclide source term to the containment and in improved treatment of particle size by CORRAL. Presently, CORRAL employs a rather rigid four-component source term (see Chapter 3) and does not consider inert materials which may be released to the containment in a meltdown accident. These can have a significant effect on radionuclide behavior in the containment. Particle size is a key variable in controlling aerosol removal rates, and CORRAL utilizes only a very simple description. Owing to the lack of a formal subroutine structure, modifications which have been made to the code have caused it to become unwieldy and difficult to develop further. For all these reasons, it was decided that a new code should be written. In this report, we provide details of the results of the review of CORRAL-2 and identify the major improvements that were considered necessary. A description of the new containment radionuclide transport and deposition code that was written incorporating these improvements is also included.

In Chapter 2, the existing CORRAL code is reviewed and discussed. Chapter 3 examines the radionuclide source term in detail. An overview of the way the MATADOR code classifies the radionuclide states and handles transfers between these states in light-water-reactor (LWR) containments is given in Chapter 4. The vapor and aerosol behavior models presently used in CORRAL are reviewed in Chapters 5 and 6, respectively. In these chapters, we also discuss the models used in the new code. Chapter 7 outlines the aerosol coagulation and gravitational settling models used in MATADOR. The need for providing designed interfaces with other computer codes used in reactor accident analysis is discussed in Chapter 8. Some of the codes, such as MARCH and TRAP, provide input data to codes such as CORRAL, while codes such as CRAC use the output from CORRAL.

After the list of the references cited in the report, two appendices have been included. The first appendix outlines the solution method used in solving the matrix rate equations employed in the code, and the second appendix lists major assumptions made in putting the code together.

The description of the code with its major subroutines, input and output is provided in a companion report [2].

2.0 THE CORRAL CODE

The CORRAL computer code models radionuclide transport and deposition in the LWR containments during loss-of-coolant and meltdown accidents. Both vapor and particulate radionuclide forms are considered in the code. The radionuclides that could be released during an accident are classified into eight groups, based on their volatility and chemical nature. A detailed description of this classification scheme and the time dependence of the radionuclide source term is provided in the next chapter.

The LWR containment is modeled in CORRAL as a series of interconnected compartments. The nature of the accident defines the path of fluid flow between these compartments. The radionuclides released to the containment from the primary system are assumed to transport in phase with the fluid flow, and the fluid in each compartment is assumed to be well mixed. This latter assumption implies that all radionuclide concentrations as well as thermal-hydraulic conditions such as temperature, pressure, and moisture fraction are uniform within each compartment. The subdivision of the reactor containment into a sufficiently large number of compartments helps to validate this assumption. However, the division of the containment into a series of well-mixed compartments is not always possible. One known instance where the well-mixed assumption can be expected to break down is in the boiling-water reactor (BWR) dry-well annular airspace. The CORRAL code models this region of the reactor containment as a cylindrical annulus with a gradient of radionuclide concentration along its length rather than as a well-mixed volume. The model assumes, however, that all thermal hydraulic conditions remain uniform even in this volume.

Input data to CORRAL can be classified into several groups. First, information is needed on the radionuclide source terms from the primary system. Second, the geometry of the containment and the flow path of the radionuclides from their point of origin to their point of release to the environment is required. Third, thermal-hydraulic data for the containment need to be specified; these include the temperature, pressure, surface temperature, and fluid composition in each compartment used to describe the containment, as well as the flow rates and compositions of the fluid flows between compartments. Finally, information on the operation of the engineered safety features in the containment is needed.

CORRAL uses these input data and the transport and deposition models within it to calculate the release rates of the various radionuclides to the environment. This is its principal output. The airborne concentrations of the radionuclides in the various compartments used to model the containment are also output, and one can compute, by difference, the quantities of radioactivity removed by the natural processes and engineered safeguards. The calculated environmental release rates can be used in a code such as CRAC to estimate the health effects of the accident. Figure 2.1 summarizes the relationship between the various codes that can now be used to model the consequences of severe core damage accidents in light-water reactors.

Several radionuclide deposition and depletion processes are modeled in the CORRAL code. These could either be natural or be the result of the operation of the engineered safety features. Vapors are assumed to deposit on the containment surfaces due to natural convection, and particulate radionuclides are removed from the containment atmosphere due to gravitational settling. In addition to these natural processes, several engineered safety features are also modeled in the code. These include absorption by the spray systems, filters, and the BWR suppression pool water.

For a particular radionuclide and release type, the transport and deposition equations in CORRAL-2 take the following form:

$$\frac{dC}{dt} = AC \qquad (2\text{-}1)$$

where C is a column vector of airborne release fractions in the various compartments, A is a matrix of rate constants for the several removal, deposition, and leak processes acting to deplete the radionuclide concentration, and t is time. A more detailed description of the system equations, including their development, may be found in Appendix VII of Reference [1]. The set of equations is solved using a numerical technique, and the solution yields the magnitudes of the radionuclide releases to the environment from the breach in the containment building as a function of time.

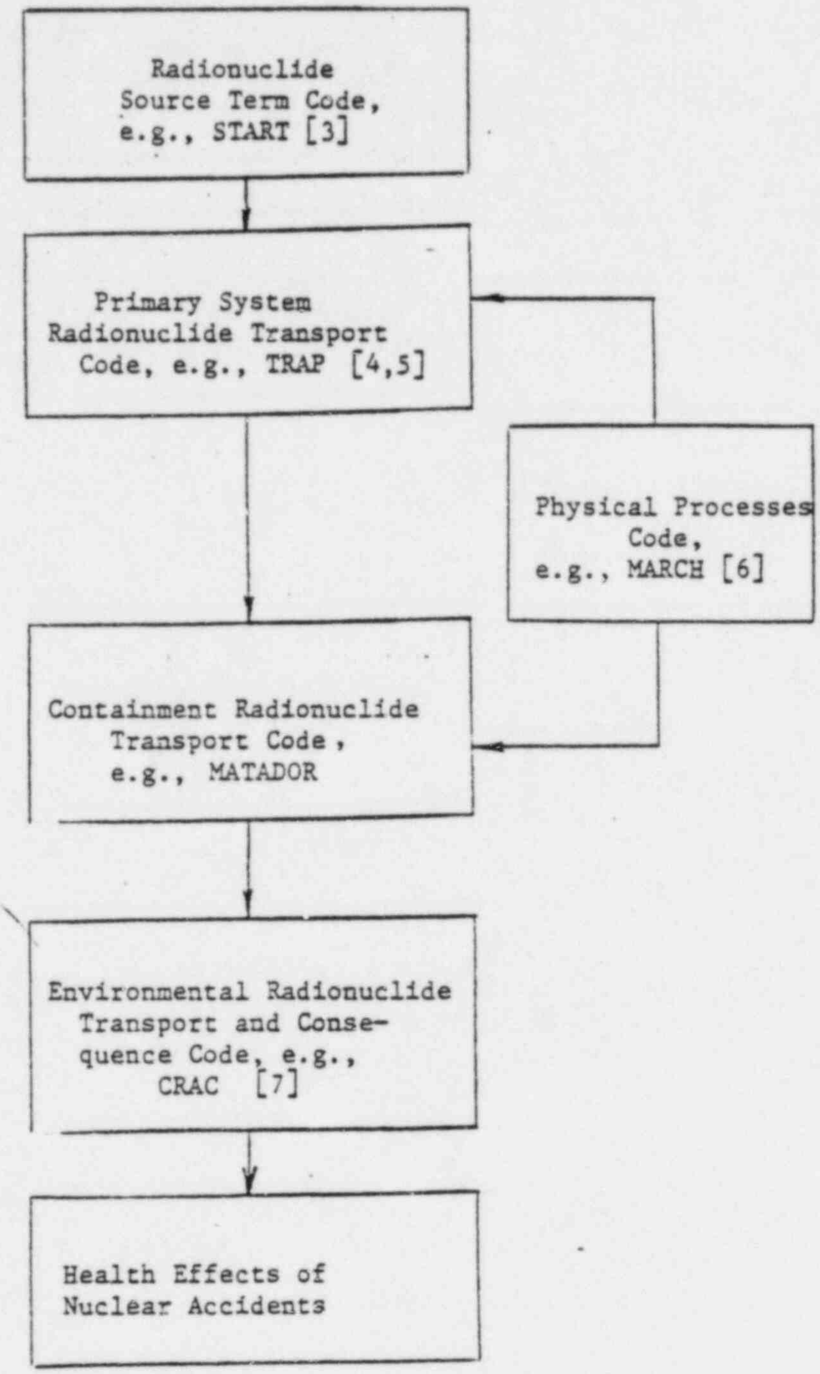

FIGURE 2.1. RELATIONSHIP BETWEEN VARIOUS REACTOR ACCIDENT ANALYSIS CODES

- In its present form, the CORRAL computer code lacks a subroutine structure. In addition, the manner in which changes have been made to it over the last several years has resulted in a code that is not easily amenable to further modifications and/or improvements.

3.0 RADIONUCLIDE SOURCE TERMS FROM THE FUEL

The Reactor Safety Study estimated radionuclide source terms from the reactor core during LWR terminated LOCAs and meltdown accidents using simple models and limited experimental data available at the time. For the majority of the accident sequences considered, it was assumed that the quantities of radionuclides entering the containment were the same as those released from the core. This simplification was used because of a lack of information about the extent of radionuclide deposition on primary system surfaces.

There are many materials present in the reactor core that could be released as a result of an accident. These include fission products such as iodine and actinides such as plutonium, as well as fuel and core structural and control component materials such as zirconium and iron. For containment transport and deposition analyses using CORRAL, the Reactor Safety Study suggested the classification of the radionuclides into several groups. Since species of similar chemical nature and volatility can be expected to behave in similar ways during transport and deposition in the reactor containment, these properties were used as a basis for the classification of the radionuclides into the eight groups listed in Table 3.1.

The noble gases (Xe, Kr) constitute one group. In CORRAL, these are assumed to transport through the containment with no deposition. Members of the iodine family constitute another group. It was assumed, in the Reactor Safety Study, that a fraction of the airborne iodine was converted to an organic form, probably methyl iodide. The fractional conversion was estimated using available information summarized by Postma and Zavadoski [8]. The remaining iodine was assumed to transport in molecular form, i.e., as I_2. Vapor deposition and removal mechanisms were assumed to attenuate iodine during transport through the reactor containment. All the other radionuclides released from the fuel were assumed to transport and deposit as particles. The particulates were separated into the six other groups shown in Table 3.1 since they were estimated to have different source rates.

TABLE 3-1. RADIONUCLIDE CLASSIFICATION SCHEME USED IN WASH-1400

Xe (Kr)
I (Br)
Cs (Rb)
Te (Se, Sb)
Ba (Sr)
Ru (Rh, Pd, Mo, Tc)
Y (La, Ce, Pr, Nd, Pm, Sm, Eu, Np, Pu)
Zr (Nb)

During a reactor accident, radionuclides are probably released from the core in a continuous fashion. This release was broken down in the Reactor Safety Study into four components for use in the CORRAL-2 code. These components quantify releases due to four different physical processes that occur during the course of a core meltdown. The first component is the gap release that occurs as a result of the fuel clad being breached following accident initiation. The breach results in the release of radionuclides that have collected in the void spaces of the fuel rods. The gap component is a very small fraction of the total meltdown source term. As the accident progresses, fuel melting occurs as a result of uncovering the core. Radionuclides released during this period of the accident constitute the second component, called the melt release, of the source term. Later in the meltdown accident, the molten mixture of fuel and structural material penetrates the reactor pressure vessel and falls into the reactor cavity. In the event that water is contained in the cavity, a steam explosion could occur and material be dispersed in the containment in finely divided form. Owing to the presence of oxygen in the containment atmosphere and the large surface area of the material produced as a result of the explosion, a release of radionuclides due to an oxidation process is associated with this event. This is the third component of the Reactor Safety Study source term and is called the oxidation release. The fourth and last component of the Reactor Safety Study source term is associated with the interaction between the molten core and the concrete of the reactor basemat. The resulting decomposition of concrete produces gases that bubble through the molten core material and help release radionuclides.

The Reactor Safety Study provided estimates of these four source term components for the radionuclide groups listed in Table 3.1. It also specified the time-dependence of these releases for use in the CORRAL calculations. The gap release was assumed to take place instantaneously at the beginning of the accident. The melt release was assumed to take place uniformly over the meltdown period. However, CORRAL-2 models this release as ten equally spaced spikes with each spike quantifying one tenth of the total melt release. An exponentially decaying rate expression was found adequate to describe radionuclide releases due to vaporization. As in the case of the melt release, the vaporization release is modeled as a series of 20 spikes. The sizes of the spikes are such that one half of the total vaporization release takes place in the first half hour and the other half over the next one and a half hours. The oxidation release was assumed to be instantaneous. At the time that the analyses for the Reactor Safety Study were performed, few data were available on the mechanisms and magnitudes of radionuclide releases during reactor accidents. Consequently, estimates of the four components of the source term have large associated uncertainties.

The four-component source term developed during the Reactor Safety Study has consistently been used in reactor meltdown accident analyses using the CORRAL code. Nevertheless, this method of treating the releases of radionuclides has been recognized to have its limitations. It has been shown, since the publication of the Reactor Safety Study, that other mechanisms for radionuclide release exist under accident conditions. For example, a delayed diffusional release for radionuclides has been postulated by researchers at Oak Ridge National Laboratory [9]. This sustained release takes place immediately following the burst release associated with clad rupture but prior to meltdown.

Other mechanisms affecting the magnitude of the radionuclide source term from the core can also be postulated. For example, the high fluid flow rates that occur during certain periods of time for some accident sequences could cause physical carryover of radionuclide particles that are only loosely attached to the fuel. Additionally, for radionuclides that are released from the central region of the core, the outer fuel could act as an effective filter, trapping a fraction of them and decreasing the magnitude of the source term. On the other hand, the trapped radionuclides could be revaporized at some later time. These phenomena were not addressed at the time of the Reactor Safety Study. As a result, the radionuclide source term that has been in use since that time needs major modifications.

Additionally, except for the organic form of iodine, no chemical interactions were taken into account in the formulation of the radionuclide source term. For example, the assumption that, except for a small amount of methyl iodide, all of the iodine is released in elemental form does not appear to be substantiated. It has been postulated that under reducing conditions the iodine will be released principally as cesium iodide (CsI). Similarly, the chemical forms of the other released radionuclides were not considered in the Reactor Safety Study. Also, the release of structural and control component material was not considered in the Reactor Safety Study. These releases can be expected to have a significant impact on the consequences of meltdown accidents by changing the number concentration of particulates in the containment building and thereby affecting their deposition rates. Additionally, CORRAL imposes severe restrictions on the time dependence of the radionuclide source to the containment. Many of these shortcomings have been overcome in the radionuclide source term developed for use in the MATADOR code.

A time-dependent source term is used in MATADOR as part of the transport equations modeling the behavior of the released radionuclide in the reactor containment. The set of differential equations formulated and solved by CORRAL (see Chapter 2 of this report) has been modified to include this source term. The transport equations can thus be represented in the following compact form:

$$\frac{dC}{dt} = AC + S \quad . \qquad (3\text{-}1)$$

Equation (3-1) is similar to Equation (2-1) except for the S term. The elements of the C vector are the masses of a particular radionuclide in various radionuclide states in the different compartments used to describe the LWR containment, and the elements of the A matrix are obtained from radionuclide deposition, removal and leak rate models (see discussion in Chapter 4). The incorporation of the source vector S into the set of equations describing radionuclide transport provides much needed flexibility in the time-dependence of the radionuclide releases into the containment. Equation (3-1) is solved numerically using an algorithm described in detail in Appendix A.

In CORRAL, the radionuclide release groups were fixed within the code itself. This means that analyses using CORRAL can be performed only for the eight specific release groups given in the Reactor Safety Study. This is no longer true in MATADOR, where the release groups are user-specified. This facilitates the analysis of the behavior of structural material that could be released to the containment in some degraded core accidents for it need only be treated as an additional species.

4.0 THE MATADOR CODE TREATMENT OF RADIONUCLIDES

In the MATADOR code treatment, each radionuclide can exist either as vapor or aerosol. If it exists as aerosol, it can be in up to 10 particle size classes. Whether the radionuclide exists as vapor or as particles, it is considered to reside in 4 different states within each containment control volume: (1) it can be suspended in the atmosphere; (2) it may be deposited on the containment walls; (3) it may be picked up by spray water droplets if sprays are operational; (4) it may reside in the bulk water in the sump or on the containment floor. Radionuclides can also be picked up and collected by engineered safety systems other than sprays such as filters, ice condensers, and pressure suppression pools. The transfer and removal of radionuclides through these systems, called adhoc transfers, are affected by the use of decontamination factors and do not enter into the rate equations to be discussed below.

If one considers a containment system consisting of 3 control volumes, the chemical species molecular iodine could exist in the vapor form in 12 different states, 4 in each control volume. A chemical species that exists as particle, cesium for example, can have up to 10 particle forms. Particles in each form belong to a different size class and can exist in 4 states within each volume. Thus, assuming 10 particle size classes and 3 control volumes, cesium can exist in 120 different states.

Radionuclides can transfer from one state to another within each compartment as a result of processes such as deposition on the walls or spray water droplet pickup. They can also transfer from one compartment to another through inter-compartmental flows.

These transfers among the various radionuclide states within a given containment system are expressed as first order rate equations that can be expressed in matrix form as:

$$\frac{dC}{dt} = AC + S \qquad (3\text{-}1)$$

where C is a vector whose components are the radionuclide masses in various radionuclide states. S is also a vector whose components give the source rates into respective radionuclide states. As pointed out above for a 3-volume, 10-particle size case, C and S have dimensions of 12 for species that exist as vapor and dimensions of 120 for species that exist as particles.

The matrix A is constructed by considering the various intra-compartmental and inter-compartmental transfers among the radionuclide states. How one arrives at the individual rate coefficients for each transfer is discussed in Chapters 5 and 6.

Once constructed, however, the structure of the A matrix is as follows. It consists of (NV) X (NV) sub-blocks as shown in Figure 4.1. Here NV is the number of volumes considered. Each sub-block is dimensioned to (NS) X (NS) where NS is the number of radionuclide states in each volume. For a chemical species existing as vapor, NS = 4, and for a species in particle form, NS = NPS X 4, where NPS is the number of particle size classes considered. For a three volume (NV = 3), and 4 state (NS = 4) case, the A matrix looks as shown in Figure 4.2.

In Figure 4.2, the elements of the A matrix are grouped into appropriate sub-blocks. One can observe that the off-diagonal sub-blocks are all diagonal matrices. These sub-blocks are associated with the transfer of material from one volume to another due to atmospheric flow. The diagonal sub-blocks of the matrix A can have non-zero elements both on and off the diagonal. The off-diagonal elements of these sub-blocks are related to transfers among different states within a given volume, and the diagonal elements are the rate constants for the total rate of disappearance of the radionuclide mass from a particular state in a given volume.

If we assume that the matrix A displayed in Figure 4.2 is for a chemical species k, the rate equation for the mass of this species k in volume i and state m can be written as:

$$\frac{dC^k_{im}}{dt} = \sum_{n \neq m} {}^m\beta^k_{in} \, C^k_{in} + \sum_{j \neq i} {}^iF_{jm} \, C^k_{jm} + E^k_{im} \, C^k_{im} + S^k_{im} \qquad (4\text{-}1)$$

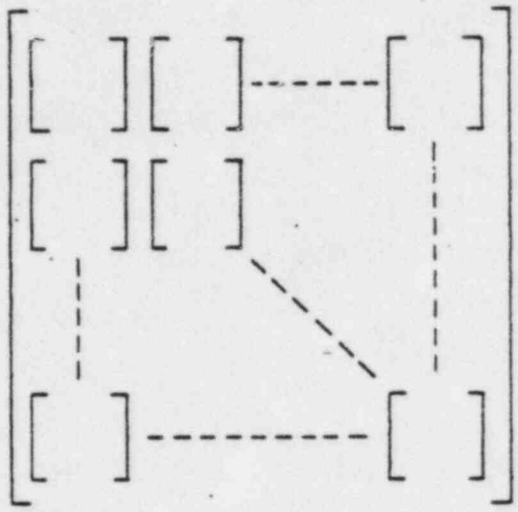

FIGURE 4.1. STRUCTURE OF THE COEFFICIENT MATRIX A IN EQUATION 3-1.

$$
\begin{bmatrix}
\begin{bmatrix} E_{11} & {}^1\beta_{12} & {}^1\beta_{13} & {}^1\beta_{14} \\ {}^2\beta_{11} & E_{12} & {}^2\beta_{13} & {}^2\beta_{14} \\ {}^3\beta_{11} & {}^3\beta_{12} & E_{13} & {}^3\beta_{14} \\ {}^4\beta_{11} & {}^4\beta_{12} & {}^4\beta_{13} & {}^4\beta_{14} \end{bmatrix} &
\begin{bmatrix} {}^1F_{21} & & & \\ & {}^1F_{22} & & \\ & & {}^1F_{23} & \\ & & & {}^1F_{24} \end{bmatrix} &
\begin{bmatrix} {}^1F_{31} & & & \\ & {}^1F_{32} & & \\ & & {}^1F_{33} & \\ & & & {}^1F_{34} \end{bmatrix} \\
\begin{bmatrix} {}^2F_{11} & & & \\ & {}^2F_{12} & & \\ & & {}^2F_{13} & \\ & & & {}^2F_{14} \end{bmatrix} &
\begin{bmatrix} E_{21} & {}^1\beta_{22} & {}^1\beta_{23} & {}^1\beta_{24} \\ {}^2\beta_{21} & E_{22} & {}^2\beta_{23} & {}^2\beta_{24} \\ {}^3\beta_{21} & {}^3\beta_{22} & E_{23} & {}^3\beta_{24} \\ {}^4\beta_{21} & {}^4\beta_{22} & {}^4\beta_{23} & E_{24} \end{bmatrix} &
\begin{bmatrix} {}^2F_{31} & & & \\ & {}^2F_{32} & & \\ & & {}^2F_{33} & \\ & & & {}^2F_{34} \end{bmatrix} \\
\begin{bmatrix} {}^3F_{11} & & & \\ & {}^3F_{12} & & \\ & & {}^3F_{13} & \\ & & & {}^3F_{14} \end{bmatrix} &
\begin{bmatrix} {}^3F_{21} & & & \\ & {}^3F_{22} & & \\ & & {}^3F_{23} & \\ & & & {}^3F_{24} \end{bmatrix} &
\begin{bmatrix} E_{31} & {}^1\beta_{32} & {}^1\beta_{33} & {}^1\beta_{34} \\ {}^2\beta_{31} & E_{32} & {}^2\beta_{33} & {}^2\beta_{34} \\ {}^3\beta_{31} & {}^3\beta_{32} & E_{33} & {}^3\beta_{34} \\ {}^4\beta_{31} & {}^4\beta_{32} & {}^4\beta_{33} & E_{34} \end{bmatrix}
\end{bmatrix}
$$

FIGURE 4.2. THE A MATRIX FOR A CHEMICAL SPECIES IN VAPOR FORM IN A 3-VOLUME CONTAINMENT SYSTEM

with

$$E^{k}_{im} = - [\sum_{n \neq m} {}^{n}\beta^{k}_{im} + \sum_{j \neq i} {}^{j}F_{im}] \quad (4-2)$$

C^{k}_{im} = mass of radionuclide species k in volume i and state m

${}^{n}\beta^{k}_{im}$ = transfer coefficient for transport of species k in volume i from state m to state n

${}^{j}F_{im}$ = transfer coefficient for transport of fission product in state m from volume i to volume j

S^{k}_{im} = source rate of species k in volume i and state m.

The summations in Equations (4-1) and (4-2) are either over the radionuclide states within a given volume or over the control volumes within the containment system under consideration.

The set of equations of the form of Equation (4-1) are solved over a finite timestep with a given initial condition and assuming that the elements of the matrix A and vector S remain constant over the given timestep.

In Equations (4-1) and (4-2), F's are calculated from inter-compartmental flow rate data supplied to the code as input. The calculation of β's for various deposition and transport mechanisms are outlined in Chapters 5 and 6.

The aerosols in the containment atmosphere, in addition to plating out on the walls and being removed by engineered safety systems. also go through the processes of agglomeration and settling due to gravity. Naturally all processes are active simultaneously. However, due to the modeling difficulties and long execution times associated with the agglomeration calculations of multi-size-group particles, the two processes are separated and the calculations are done consecutively. However, care is taken that within any given timestep the aerosol mass and particle density suspended in the containment atmosphere do not change by more than a predetermined amount so that one phase of calculations does not unduly affect the results of the other phase.

After equations of the type of Equation 4-1 are solved for aerosols, the total particle number density for each particle size class is calculated. The particle number densities for discrete particle size classes within each containment volume are then folded into a log-normal distribution with an average particle volume and standard deviation. Particle coagulation and gravitational settling calculations are done using this log-normal distribution of particle density. The details of these calculations and the models used are given in chapter 7.

After the coagulation calculations are completed, the modified particle number density distribution is converted back to discrete number densities for discrete particle size classes. It is assumed that coagulation does not affect the chemical composition of aerosols but only the number density and mass if gravitational settling occurs. The number density conversions between the discrete sizes and log-normal distribution conserve the mass of aerosols. The end point radii of discrete particle size classes usually are not the same before and after the coagulation calculations but vary with the accident time. The number of particle size classes stays the same, however. The code takes the range of 3 standard deviations to either side of the mean in the log-normal distribution and calculates the discrete particle densities from the particles that fall within that range.

Noble gases are treated in MATADOR similarly to CORRAL. They are assumed to simply transfer in phase with the fluid flow and not deposit on the surfaces or be affected by engineered safety systems.

5.0 VAPOR DEPOSITION AND REMOVAL MODELS

The only natural vapor deposition process modeled in CORRAL-2 is natural convection onto the containment system surfaces. It was assumed that the temperature difference between the bulk fluid and the surfaces provided a driving force and a heat transfer/mass transfer analogy was used to develop a model for this process. In addition, several engineered safety features are also modeled in the code: reactor building sprays, filters, and suppression pools.

It is now clear that other natural and engineered processes, such as forced convection and removal by containment cracks can be expected to contribute to the removal of vapors from the containment atmosphere. Additionally, several models now used in CORRAL can be replaced by newer and better ones. In this chapter, we present the correlations that are now used in CORRAL and discuss the ones that have been included in MATADOR.

5.1 Natural Deposition on Surfaces

The CORRAL computer code utilizes the concept of a deposition velocity to quantify the deposition rate of a radionuclide from the bulk of a well-mixed volume to the containment surface. The deposition velocity is calculated in CORRAL using mass transfer correlations. Natural convection due to temperature differences between the bulk fluid and the containment surface is assumed to provide the gradient for the transfer of iodine vapor to the walls upon which it deposits. Accordingly, the mass transfer coefficient, k, for vapor deposition in well-mixed compartments is calculated using the following correlation:

$$Sh = \frac{k\ell}{D_g} = \frac{\ell - 10}{\ell} Sh_2 + \frac{10}{\ell} Sh_1 \quad , \qquad (5\text{-}1)$$

where

$$Sh_1 = 0.59\ (Gr \cdot Sc)^{1/4},\ \text{if } Gr < 10^9 \qquad (5\text{-}2)$$

$$Sh_2 = 0.13\ (Gr \cdot Sc)^{1/3},\ \text{if } 10^9 < Gr < 10^{12} \qquad (5\text{-}3)$$

and -

Sh_1, Sh_2, and Sh = Sherwood numbers ,

$$Gr = \text{a Grashoff number} = \frac{\ell^3 \left(T_{wall} - T_{bulk}\right) g}{(\mu/\rho)^2 \; T_{bulk}} ,$$

Sc = a Schmidt number = $\mu/(D_g \rho)$,

ℓ = length of wall,

T = temperature,

μ = viscosity of fluid,

ρ = density of fluid,

g = acceleration due to gravity,

D_g = diffusivity of iodine in the gas phase,

and the subscripts "wall" and "bulk" refer to the conditions at the surfaces and in the bulk fluid, respectively.

The mass transfer coefficient for iodine deposition in the BWR annular region (where the fluid is not well-mixed) is calculated using correlations for forced convective mass transfer. These correlations are:

$$Sh = \frac{k(4R_h)}{D_g} = 0.026 \; Re_F^{0.8} \cdot Sc^{1/3} \quad (5\text{-}4)$$

if $2100 < Re < \infty$,

and

$$Sh = 1.86 \{Re_F \cdot Sc \cdot (4R_h/\ell_{Ann})\}^{1/3} \quad (5\text{-}5)$$

if $0 < Re < 2100$,

where

ℓ_{Ann} = length of the annulus,

Re_F = a Reynolds' number = $[\rho U(4R_h)/\mu]$,

U = bulk velocity of fluid in the annulus, and

R_h = hydraulic radius of annulus = cross sectional flow area/wetted perimeter = annular width/2.

In each instance, the calculated mass transfer coefficient can be used to compute a deposition coefficient ($\lambda_{vapor,\ nat.}$) using:

$$\lambda_{vapor,\ nat.} = (A/V)k \quad , \tag{5-6}$$

where

A = surface area of deposition, and

V = volume of compartment.

The Reactor Safety Study assumed that natural convection due to the gradient created by the temperature difference between the bulk fluid and the containment surfaces is the dominant mechanism for vapor deposition. This assumption appears to be unjustifiable in several instances. For example, thermal-hydraulic data for several accident scenarios show that there are time periods when the fluid flow rates are high and temperature gradients small. Under these circumstances, forced convection would also contribute to the vapor deposition rates. MATADOR therefore incorporates models both for natural and forced convection of iodine vapor in the well-mixed compartments. CORRAL also assumes that fluid flowing in the well-mixed volumes develops turbulence at a distance of 10 feet from the leading edge of the containment wall. This assumption, implicit in Equation (4-3), was justified on the basis of data obtained in the Containment Systems Experiments [10]. MATADOR uses correlations that do not require the use of such an assumption and, therefore, can be expected to better model situations where the conditions are different from those in the Containment System Experiments. Finally, CORRAL uses correlations for the calculation of the mass transfer coefficient for iodine vapor based on data obtained for mass transfer to dry surfaces. There are accidents where significant condensation of steam on the containment walls can be expected and where correlations for mass transfer to wetted walls would be more appropriate. MATADOR provides for their use when significant steam condensation is predicted for an accident.

The fraction of the containment surfaces that are wet is input by the code user and MATADOR appropriately weights the two depositon velocities, i.e., to the dry and wet surfaces, using the input value for the wetted fraction.

MATADOR utilizes the correlations discussed below to calculate the mass transfer coefficient for vapor deposition onto the containment surfaces [11,12,13]. These correlations are more recent and therefore are expected to better represent available experimental data. They are:

a) for vapor deposition due to natural convection:

$$Sh_L = 0.678 \left[\frac{Sc}{0.952 + Sc} \cdot Gr_L \cdot Sc\right]^{1/4} \text{ if } 0 < Gr_L Sc < 10^8 \quad , \tag{5-7}$$

$$Sh_L = 0.555(Gr_L \cdot Sc)^{1/4} \text{ if } 10^8 < Gr_L Sc < 10^9 \quad , \tag{5-8}$$

$$Sh_L = 0.021(Gr_L \cdot Sc)^{0.4} \text{ if } 10^9 < Gr_L Sc < 10^{10} \quad , \text{ and} \tag{5-9}$$

$$Sh_L = 0.0246\left[\frac{Gr_L}{1 + 0.494\ Sc^{2/3}}\right]^{0.4} Sc^{7/15} \quad \text{otherwise,} \tag{5-10}$$

b) for vapor deposition due to forced convection:

$$\frac{kL}{D_g} = 0.664(Re_L)^{1/2}(Sc)^{1/3} \text{ if } Re_L < 320{,}000 \quad , \text{ and} \tag{5-11}$$

$$\frac{kL}{D_g} = 0.037\ Sc^{1/3}\left[Re_L^{0.8} - 15{,}500\right] \text{ if } Re_L > 320{,}000 \quad . \tag{5-12}$$

c) for deposition in the BWR annulus, where the well-mixed assumption is not valid:

$$Sh_i = 0.046\ Re_F^{0.8}\ Sc^{0.4}(d_2/d_1)^{0.45} \quad \text{for the inner surface,} \tag{5-13}$$

$$Sh_o = 0.046\ Re_F^{0.8}\ Sc^{1/3}(\mu_{bulk}/\mu_{wall})^{0.14} \quad \text{for the outer surface,} \tag{5-14}$$

and

$$Sh = 1/2(Sh_i + Sh_o) \quad .$$

$$\left.\begin{array}{l}(5\text{-}13),\ (5\text{-}14),\ Sh\end{array}\right\} Re_F > 2100$$

$$Sh = 1.86 \{Re_F \cdot Sc \cdot (4R_h/\ell_{ann})\}^{1/3} (\mu_{bulk}/\mu_{wall})^{0.14} \qquad (5\text{-}15)$$

$$Re_F < 2100 \quad .$$

d) for transfer to wet containment surfaces:

$$\frac{kD_{eq}}{D_g} = 0.046(Re_{eq})^{0.83}(Sc)^{0.44} \qquad (5\text{-}16)$$

In all of the above equations, it is assumed that the rate determining step for deposition is gas phase mass transfer. For vapors such as iodine, this assumption is believed to be justified in most cases. However, there are some cases, especially following high energy releasing events such as hydrogen deflagration or detonation when resuspension of the deposited radionuclide vapors may occur. The data available at this time cannot support the development of models for these processes. The MATADOR code, however, has been written in such a manner that it is possible to include models to describe resuspension processes with little effort at a later date.

The mass transfer coefficient calculated for the transfer of iodine to the containment surfaces from the bulk fluid is converted to a deposition velocity through the use of Equation (5-6).

In Equations (5-7) through (5-16) above, normal engineering nomenclature is used. The symbols used are:

Sh_L = average sherwood number for length of surface

$= \dfrac{k(\text{characteristic length})}{D_g}$,

Gr_L = Grashoff number for length of surface

$= L^3 g\, \rho_{bulk} |(\rho_{bulk} - \rho_{wall})| / \mu^2$,

Re_L = Reynolds' number based on length of surface = $\dfrac{LU\rho}{\mu}$,

Re_F = Reynolds' number for BWR annulus; calculated using 4 x hydraulic radius as the characteristic length ,

Re_{eq} = Reynolds' number for a compartment calculated using the equivalent diameter as the characteristic length ,

L = length of the surface of a volume ,

k = a mass transfer coefficient, and

U = average velocity of fluid in volume.

5.2 Removal by Engineered Safety Systems

The removal of iodine by the containment sprays is modeled in CORRAL as a mass transfer process. The mass transfer coefficients for iodine in the gas phase and within the liquid droplet were calculated using standard correlations. They were then used in calculating a deposition coefficient ($\lambda_{vapor,\ spray}$) in terms of the volume of the sprayed compartment, the flow rate of the sprayed liquid, and the terminal velocity of the spray droplets. The model used is:

$$\lambda_{vapor,\ spray} = \frac{FH}{V}\left(1 - \exp\left(\frac{-6k_g t_e}{d(H + (k_g/k_\ell))}\right)\right) \quad , \qquad (5\text{-}17)$$

where

F = spray flow rate, cm^3/sec = gm/sec if ρ_{spray} = 1 gm/cc,

H = equilibrium Henry's Law constant for iodine (ratio of liquid phase concentration to gas phase concentration of iodine at equilibrium),

V = volume of sprayed compartment,

d = diameter of sprayed droplets,

t_e = fall time (height of fall of drop/terminal velocity of droplets, V_t)

D_ℓ = diffusivity of iodine in the droplet

k_g = gas phase mass transfer coefficient of iodine $= \frac{D_g}{d}(2.0 + 0.6\ Re^{1/2}\ Sc^{1/3})$, and

k_ℓ = liquid phase mass transfer coefficient of iodine = $6.58\ D_\ell/d$.

The value of V_t is found by matching the velocity independent dimensionless number:

$$f_D Re^2 = 4\rho(\rho_\ell - \rho)d^3 g/3\mu^2$$

with the appropriate range of Reynolds' number. For $10<Re<100$, $f_D Re^2 = 15.71\ Re^{1.417}$ and for $100<Re<700$, $f_D Re^2 = 6.477\ Re^{1.609}$. ρ_ℓ is the density of the liquid droplets and Re is defined by:

$$Re = d\rho V_t/\mu \quad .$$

This model for calculating the rate of iodine vapor removal by the containment sprays is believed to be adequate. It was developed on the basis of observations in the Containment System Experiments, and the data show that the model describes the actual behavior of iodine very well. It was therefore decided that no major modification to this model was necessary and it has been retained in MATADOR.

Removal by other engineered safety features such as filters, ice condensers, and suppression pools are modeled in CORRAL-2 utilizing the concept of a decontamination factor (DF). Attenuation of the concentration of iodine vapor due to passage through the filters or the suppression pool is not modeled as a rate process; rather the value of the DF is used to take out some of the iodine and deposit it in the filter or the suppression pool. The value of this factor is input to the code.

The decontamination factor approach has been retained in MATADOR for treating vapor removal by the filters, ice condensers, suppression pool, containment cracks, etc. These processes are called "adhoc" processes and they alter the airborne mass of vapors in a containment volume in the following way. If, at the beginning of timestep Δt, the airborne mass in volume s is C_{so} and in volume r is C_{ro}, and if the adhoc process takes its inlet from volume s and releases its output to volume r, then the airborne masses of the radionuclide in volumes s and r are changed over the time-step Δt according to

$$C_s = C_{so}\left(1 - \frac{F\,\Delta t}{V_s}\right) \qquad (5\text{-}18)$$

$$C_r = C_{ro} + C_{so}\,\frac{F\,\Delta t}{V_s\,D_{cf}} \qquad (5\text{-}19)$$

where C_s and C_r are the airborne masses of the radionuclide in volumes s and r at the end of timestep, F is the volume flow rate from volume s to volume r through the adhoc process under consideration, V_s is the volume of volume s, and D_{cf} is the decontamination factor. In the code, D_{cf}'s are input as a function of time for each adhoc process and for each chemical species. The source and receiver volumes s and r could be the same volume, in which case the function of the adhoc process is simply to take out some of the airborne radionuclide mass from that volume.

There are several reasons for modeling some vapor removal processes using decontamination factors rather than rate expressions. In the case of suppression pool scrubbing, there are not, at present, sufficient experimental data available to provide a sound basis for developing models to estimate vapor removal rates by the pool water. In the case of the filters and the ice condensers, the decontamination factor approach probably models the actual removal process more realistically than a rate expression. This is because the process of radionuclide removal by these systems probably cannot be modeled as a first-order process for inclusion in the transport and deposition equations. It is appropriate to point out here that all designs of the filters and pools can be modeled using this treatment. In all instances, the value of the decontamination factor is input to MATADOR as a function which depends on both time and radionuclide species.

Several other processes not included in CORRAL-2 could contribute to radionuclide removal and thereby reduce the levels of radioactivity released to the environment during an accident. These processes include filtration by ice condensers, vent filters, and containment cracks. The MATADOR code provides for modeling these processes by using decontamination factors. A more mechanistic approach was not practical at this time due to lack of experimental data.

5.3 Iodine Equilibrium

When airborne molecular iodine is depleted by either sprays or depositon on the water, the depletion rate becomes independent of these mechanisms when the concentration falls below about 1 percent of the initial value plus the sum of sources up to that time [1,10]. At concentrations below this level, an apparent equilibrium situation exists where the concentrations in liquid and gas phases are related by an equilibrium distribution constant, $H = C_\ell / C_g$. H is a function of time (probably due to slow liquid phase chemical reaction) and has been experimentally determined. In MATATOR it has been possible to incorporate H = H(t) when equilibrium conditions exist. This treatment is similar to that in CORRAL.

To get the equilibrium described quantitatively, an equivalent lambda for depletion of gas phase I_2 had to be developed. Since the value of H increases with increasing time, the gas phase is being depleted as time goes on. To get this equivalent lambda, we can write a mass balance for I_2. If C_{go} is the initial airborne concentration, then

$$C_{go} V_g = C_\ell V_\ell + C_g V_g \quad . \tag{5-20}$$

or

$$\frac{C_g}{C_{go}} = \frac{C_g V_g}{C_\ell V_\ell + C_g V_g} = \frac{1}{\frac{C_\ell V_\ell}{C_g V_g} + 1} = \frac{1}{H \frac{V_\ell}{V_g} + 1} \quad . \tag{5-21}$$

Then for H = H(t), we can write the removal rate of I_2 by

$$d\,\frac{C_g/C_{go}}{dt} = -\frac{1}{\left(H \frac{V_\ell}{V_g} + 1\right)^2} \left(\frac{V_\ell}{V_g}\right) \frac{dH}{dt} \tag{5-22}$$

where the equivalent lambda is

$$\frac{dC_g}{C_g} = -\left\{ \frac{1}{\left(H \frac{V_\ell}{V_g} + 1\right)} \frac{V_\ell}{V_g} \frac{dH}{dt} \right\} dt = -\lambda dt \tag{5-23}$$

$$\frac{dC_g}{C_g} = -\lambda dt \tag{5-24}$$

$$C_g(t) = C_{go} e^{-\lambda t} \tag{5-25}$$

where C_{go} is the concentration of airborne molecular iodine that would have existed if there were no iodine depletion.

Data shows that $H \ V_\ell/V_g >> 1$ for boric acid and caustic solutions in equilibrium with I_2, so that

$$\lambda = \frac{1}{H} \frac{dH}{dt} \quad . \tag{5-26}$$

Typical data for sprays are shown in Tables 5.1 and 5.2.

TABLE 5-1. EQUILIBRIUM DATA FOR I_2 WITH BORIC ACID SPRAYS [10]

Time, min	H	C_g/C_{go}
0	2676	0.01
100	1.5×10^4	1.8×10^{-3}
500	4.0×10^4	6.75×10^{-4}
1000	7.0×10^4	3.86×10^{-4}
2000	$1.5 \times 10^{+5}$	1.8×10^{-4}
4000	$5 \times 10^{+5}$	5.4×10^{-5}
≥7000	1×10^6	2.7×10^{-5}

TABLE 5-2. EQUILIBRIUM DATA FOR I_2 WITH CAUSTIC SPRAYS [10]

Time, min	H	C_g/C_{go}
0-100	Constant H, $\lambda = 0$	0.01
100-1000	Variable H, $\lambda = .095\ hr^{-1}$	
1000	7.0×10^4	3.86×10^{-4}
2000	1.5×10^5	1.8×10^{-4}
4000	5×10^5	5.4×10^{-5}
7000	1×10^6	2.7×10^{-5}

6.0 AEROSOL DEPOSITION AND REMOVAL MODELS

Deposition and removal mechanisms depleting aerosol concentrations in the containment are modeled in CORRAL-2 in a manner similar to that for vapors. Mass transfer coefficients are calculated using simple models which give deposition velocities for incorporation into the main structure of the CORRAL code. Removal due to natural processed and to engineered safety features is considered.

The models currently included in CORRAL-2 to simulate aerosol behavior need modification to enable the code to better simulate conditions likely to be present in a containment atmosphere during degraded core accidents. Accordingly, MATADOR utilizes a different treatment of particle size, employs different correlations for modeling processes currently in CORRAL, and includes processes for aerosol removal not present in CORRAL. These modifications are now discussed in detail.

6.1 Particle Size

Currently, the CORRAL code permits the existence only of time varying, single-size aerosols. The initial size of the particles is taken as 15 um, and it is assumed to decrease to 5 um over a certain time period which is chosen by the user. Thereafter, the particle size remains constant. This treatment of particle size is consistent with the results obtained in the Containment Systems Experiments [10] for the removal of the suspended aerosol mass from the system. It is not expected, however, that this treatment is an accurate reflection of aerosol behavior in situations where conditions in the containment are very much different from those in the Containment Systems Experiments. One can rectify these shortcomings with a complex treatment of the problem involving a large number of aerosol particle sizes; however, the model development, computer storage requirements, and code execution costs become considerable. Therefore, we limited the number of particle sizes that coexist at any given time to ten. Using more than 10 particle sizes would be highly desirable from a design point of view. However, for a systems study code such as MATADOR, 10 particle sizes should be adequate to show the effect of particle size on various aerosol transport and deposition processes in LWR containments. One can also employ less than ten particle sizes as an input option. The code calculates the particle sizes and number densities at later times assuming Brownian, turbulent, and gravitational coagulation to have occurred. The initial particle sizes and densities are input by the user.

In addition to the radionuclides and structural and control component materials which are vaporized and result in aerosol formation, very large quantities of water may be released to the containment with the particles. The injection of this very hot water vapor into the cooler environment of the containment is expected to lead to supersaturation with respect to water in the immediate vicinity of the release. The high concentration of aerosol particles in this region will provide a large number of condensation sites to relieve the supersaturation. The amount of water which will condense on the particles is determined by the mass release rate of water vapor, the initial size and number concentration of the aerosol, and the nature of the concentration fields of particles and water vapor. The simulation of this aspect of aerosol behavior in the post-accident containment in a mechanistic fashion is extremely difficult. After the aerosol particles leave the region where the supersaturation exists, the suspending atmosphere will very likely be at or very near saturation. If this is the case, and if the particles have grown to a size large enough so that the Kelvin effect does not significantly increase the vapor pressure of the water associated with the particles, thereby causing their evaporation, there will not be much further change in the size of the aerosol particles due to condensation or evaporation. Also, if the particles are released with the condensing water vapor, as during the melt phase, the mechanism of condensation at the point of release tends to make the aerosol size distribution narrower. Since steam condensation is not modeled in MATADOR, the user is required to specify an initial size and density of the radionuclide particles, with steam condensed on them.

Providing the code with the capability of handling up to 10 user specified particle sizes makes it feasible for one to simulate aerosol particles released through different mechanisms. If, for example, dry particles are released at some time during the accident but larger water jacketed particles at some other time one can simulate both releases by the use of different size classes and different material densities for different size particles.

The sizes specified by the user for the particles at the time they are emitted into the containment atmosphere will affect the rates of aerosol removal by the mechanisms considered in the code. Different removal rates will be calculated for particles in different size classes. Changes in particle size are accommodated through shifts in particle number concentrations between the number of size classes under consideration and through changes of the particle radii permitted. Brownian, turbulent and gravitational coagulation are assumed to be the three mechanisms causing particle agglomeration. Models used for coagulation processes are explained in detail in Chapter 7.

6.2 Natural Removal Processes

6.2.1 Gravitational Settling

Gravitational settling of the particles is the only natural removal process currently considered in CORRAL-2. The terminal velocity of the particles in the steam-air atmosphere is calculated assuming that the particles are spherical. MATADOR determines the aerosol loss rate due to gravitational settling according to the following relations:

$$\lambda_{gi} = \frac{4gd_{pi}^{2}(\rho_{pi}-\rho)}{72\mu} \frac{A_f}{V} \quad \text{for } K < 3.3 \tag{6-1}$$

$$\lambda_{gi} = \left[\frac{4gd_{pi}^{1.6}(\rho_{pi}-\rho)}{55.5\mu^{0.6}\,\rho^{0.4}}\right]^{\frac{1}{1.4}} \frac{A_f}{V} \quad \text{for } 3.3 < K < 43.6 \tag{6-2}$$

$$\lambda_{gi} = \left[\frac{4gd_{pi}(\rho_{pi}-\rho)}{1.32\,\rho}\right]^{0.5} \frac{A_f}{V} \quad \text{for } 43.6 < K < 2360 \tag{6-3}$$

where

A_f = floor area of containment (or more accurately, the sum of all horizontal areas)

V = volume of containment

g = acceleration due to gravity

μ = fluid viscosity

ρ_{pi} = density of particle of size d_{pi}

ρ = fluid density

and

$$K = \left[\frac{d_p^{3}\{g\rho(\rho_p - \rho)\}}{\mu^2}\right]^{1/3}$$

CORRAL-2 used equation (6-1) at all times to calculate the settling velocity of the radionuclide particles, which means that the aerosol is always assumed to be such that the Stokes' Law of settling applies. The MATADOR model is more general since it is able to describe particle settling for all three ranges of K values in equations (6-1) to (6-3).

As explained in Chapter 4, agglomeration is superimposed on the transport and deposition of particles. Since gravitational settling is affected most by particle size, and since particle size is altered due to agglomeration, it is more appropriate to include the gravitational settling as part of agglomeration calculations. For this reason, if the aerosol coagulation is assumed to take place in any compartment, the settling of particles due to gravity in that compartment is taken into account with the coagulation calculations. This is explained more fully in Chapter 7. Otherwise, if there is no coagulation, models explained here are used.

In addition to gravitational settling, other processes of particle deposition onto the containment surfaces could be important in certain accident scenarios. When the particle size is in the submicron range, Brownian diffusion becomes an important mechanism and when there are large temperature gradients between the bulk fluid and the surfaces, diffusiophoretic and thermophoretic disposition are important. MATADOR models these processes as well.

6.2.2 Diffusional Deposition

The removal of particles from a volume due to their diffusion to the internal surfaces of the containment is now considered. The flux of particles to a surface is given by Fick's law and one can derive

$$\frac{\partial n_i}{\partial t} = \frac{kTC_i}{6\pi\mu r_i} \frac{A_w}{V} \frac{\partial n_i}{\partial y} \qquad (6\text{-}4)$$

where k = Boltzmann's constant,

C_i = particle slip correction factor,

A_w = vertical or wall deposition areas,

and the subscript i is used to indicate the size class to which the particle belongs.

The particle concentration gradient near the wall of the containment, $\partial n_i/\partial y$, needs to be specified and is user input in the code. As in most mass transfer analyses, the particle concentration is assumed to be zero at the wall, and n_i far from the wall. The containment is considered to be well mixed up to within a small distance from the wall. So the particle concentration changes from 0 at the wall to n_i at distance Δ from the wall. Since the choice of Δ is left of the user, one obtains:

$$\lambda_{iD} = \frac{kTC_i A_w}{6\pi\mu r_i V\Delta} \quad . \tag{6-5}$$

6.2.3 Thermophoretic Deposition

Aerosol deposition on internal surfaces of a container due to temperature gradients normal to those surfaces is termed thermophoretic deposition. The theory of this process, due to Brock [14], yields the following expression to describe the rate of decrease of particle concentration:

$$\lambda_{it} = \left[\frac{3A_w \mu \Delta T}{2V\rho\ T}\right]\left[\frac{1}{1 + 2C_m Kn_i}\right]\left[\frac{C_t Kn_i + k_f/k_s}{1 + 2C_t Kn_i + 2k_f/k_s}\right] \tag{6-6}$$

where C_m is a constant associated with the Cunningham correction factor and for the low Knudsen number, Kn_i, particles can be taken as 1.66 by approximating the expression of Fuchs [15]. C_t is a constant associated with the thermal accommodation coefficient at the particle thermal conductivity, and a value of 0.05 is used [16] and ΔT is the normal component of the temperature gradient at the wall.

6.2.4 Diffusiophoretic Deposition

The diffusiophoretic deposition of aerosol particles on containment surfaces is a process which, it has been suggested, may be of potential importance in post-accident containment atmospheres [17] but is not currently included in CORRAL. Aerosol losses can be brought about by this process since the particles find themselves in a hot steam-air atmosphere bound by a relatively cold-walled container. This temperature difference leads to water condensation on the walls and sets up the conditions appropriate for diffusiophoresis of the particles to occur. Specifically, the partial pressure of the water vapor in the containment atmosphere far from the cold walls is expected to be equal to the saturation vapor pressure of water at the prevailing gas temperature. Very near the cold walls, where condensation has established a water film, however, the partial pressure of water will correspond to the saturation vapor pressure of water at the temperature of the walls. Since the total pressure in the containment is uniform, a concentration gradient of water vapor is established, the vapor concentration increasing with distance from the walls. This leads to a diffusive flux of water vapor towards the walls which will be maintained as long as the temperature differential remains and the containment atmosphere remains saturated with water vapor.

An aerosol particle present in such a diffusing binary gas mixture will experience a diffusiophoretic force, in this case directed towards the wall. For the theory of this process the reader is referred to Waldmann and Schmitt [18] and Goldsmith and May [19] and references therein. The theory predicts that diffusiophoresis will result in the particle having a deposition rate coefficient given by:

$$\lambda_{id} = \left[\frac{\sqrt{M_1}}{\gamma_1\sqrt{M_1} + \gamma_2\sqrt{M_2}}\ \frac{D}{p_2}\ \frac{p_1(T) - p_1\ (T_w)}{\Delta}\right] \frac{A_w}{V} \qquad (6\text{-}7)$$

where M_1, M_2 are the masses of the water vapor and air molecules,

γ_1, γ_2 are the mole fractions of water vapor and air,

D is the diffusion coefficient of water vapor in the air,

$p_1(T)$ is the partial pressure of water vapor at the temperature of the containment atmosphere,

p_2 is the partial pressure of air in the containment atmosphere

$p_1(T_w)$ is the partial pressure of water vapor in equilibrium with water at the temperature of the wall, and

Δ is the user specified boundary laver thickness.

This equation describes the observed behavior of particles smaller than the mean free path of the molecules of the suspending medium quite well but is not as accurate for larger particles. It is worth noting that the particle size and shape are not expected to influence the diffusiophoretic deposition of particles.

The correlations presented above are applicable only to the well mixed control volumes within the containment. For regions such as the BWR annulus where the fluid moves more like plug flow, the concept of a decontamination factor is invoked to simulate particulate deposition. This treatment is similar to that used to treat vapor removal by filters, for example.

6.3 Removal by Engineered Safety Systems

Removal of particles by sprays is currently modeled in CORRAL using the data obtained in the Containment Systems Experiments [10]. An analysis of these data allows the calculation of a deposition rate coefficient, λ , for particulate removal by sprays using the equation

$$\lambda_{\text{spray, particles}} = \frac{3FEh}{2Vd} \qquad (6\text{-}8)$$

where

F = spray flow rate

h = spray fall height

d = spray drop diameter

V = compartment volume, and

E = spray collection efficiency.

The functional dependence of E on (Ft/V) was arrived at from an examination of the results of the Containment Systems Experiments and is given as

$$E = \begin{cases} -15.825\ (Ft/V) + 0.055;\ 0<Ft/V<0.002 \\ 0.04125 - [0.08626 + 42.68\ (Ft/V)]^{1/2}/21.34;\ 0.002<Ft/V<0.0193 \\ 0.0015;\ Ft/V>0.0193 \end{cases} \qquad (6\text{-}9)$$

This treatment of particle attenuation by sprays is modified somewhat in the MATADOR code.

The loss rate coefficient for aerosol removal due to water spraying is as follows for more than one particle size:

$$\lambda_{is} = \frac{3Fh}{2d} \frac{\varepsilon_i}{V} . \tag{6-10}$$

The important consideration now is to describe the collection efficiency, ε_i, as a function of aerosol and drop sizes. Because of hydrodynamic interaction between the two particles, only a certain fraction of those in the "sweep out area" of a large particle will actually be contacted. If we define the "sweep out area" as the area of a circle with the radius of the the larger particle, then the collision efficiency, ε, is defined as the fraction of the small particles in the sweep out area which are collected. Furthermore, the smaller particle must stick to the larger one to complete the collision process. Here, the sticking or attachment probability is assumed to be unity, since this value is likely and very little theoretical or experimental evidence concerning this phenomenon exists.

In general, there are two major pertinent collision mechanisms which enable a particle to overcome the hydrodynamic repulsion and collide with the water drop. The first mechanism is inertial impaction, which accounts for the deviation of a particle from a steamline due to its inertia. The other mechanism is called the interception effect, which takes into account the increase of collision probability due to the finite extent of small particles. Thus, we write

$$\varepsilon_i = \varepsilon_{1i} + \varepsilon_{2i} \tag{6-11}$$

where ε_1 is the collision efficiency due to particle inertia and ε_2 is the collision efficiency due to interception.

For relatively low particle velocities an empirical formula for the efficiency of inertially caused particle collisions is reported by Fuchs [15] and is given by:

$$\varepsilon_1 = \left[1 + \frac{0.75 \ \ln (2 \text{ Stk})}{\text{Stk} - 1.214}\right]^{-2} \tag{6-12}$$

Here, Stk is the Stokes number defined by

$$Stk = \frac{2(V_g - V_{gi})r_i^2\rho_{pi}}{9\mu R} \tag{6-13}$$

where ρ_p is the particle density, V_g is the settling velocity of the water drop, V_{gi} that of the particle, r_i and R the radii of particle and water droplet. The efficiency ε_1 is taken as zero when Stk ≤ 1.214.

For viscous flow about a spherical collector, Lee and Gieseke [20] present an equation for the interceptional collision efficiency which is valid for small values of the ratio r_i/R:

$$\varepsilon_2 \approx \frac{3}{2} \frac{(r_i/R)^2}{(1 + r_i/R)^{1/3}} \tag{6-14}$$

It is clear from the expressions for ε_1 and ε_2 that separate efficiencies are calculated for each particle size in MATADOR.

Removal by the other engineered safety features like the filters and ice condensers are treated in the new code using the concept of decontamination factors. Decontamination by the containment cracks and vent filters are also modeled. This treatment is similar to that used for vapor species. The only difference is that different decontamination factors are used for different size particles.

7.0 AEROSOL COAGULATION AND GRAVITATIONAL SETTLING MODELS

The agglomeration of aerosols takes place in the containment atmosphere as a result of aerosols moving and colliding with one another in Brownian motion or under the influence of forces that affect the different size particles differently. While the coagulation preserves mass and therefore does not alter the amounts of radionuclide aerosol directly, it does reduce the number concentration and modify the aerosol size distribution and thereby alter the rates at which the particles are removed by processes which depend on either particle size or concentration.

The governing integro-differential equation describing the rate of change of particle concentration due to various agglomeration and deposition mechanisms can be written in the following form [21]:

$$\frac{\partial}{\partial t} n(x,t) = [1/2 \int_0^x \phi(\xi,x-\xi)\ n(\xi,t)\ n(x-\xi,t)\ d\xi$$

$$- n(x,t) \int_0^\infty \phi(x,\xi)\ n(\xi,t)\ d\xi]$$

$$- n(x,t)\ R(x) + S(x,t) \quad , \qquad (7\text{-}1)$$

where

t = time

$\phi(x,\xi)$ = the normalized collision kernel predicting the probability of collision between two particles of volume x and ξ due to Brownian motion, gravitational settling, and turbulent gas motion.

$x = \frac{4}{3}\pi r^3$ = volume of particle with radius r

$\xi = \frac{4}{3}\pi r'^3$ = volume of particle with radius r'

$n(x,t)$ = the size distribution function

$R(x)$ = the removal rate of particles due to gravitational settling to the floor, diffusion to the walls (wall plating), turbulent motion of gas, thermophoresis and leakage

$S(x,t)$ = the source rate of particles introduced to the enclosed space of the vessel.

The first integral in Equation (7-1) represents the formation rate of particles between the sizes x and x + dx as a result of collisions between particles of volumes ξ and $x - \xi$. Similarly, the second integral represents the disappearance rate of particles in the size range between x and x + dx due to collisions with all other particles.

The functional form of the collision kernel $\phi(x,\xi)$ depends upon the coagulation mechanisms present in a given system. In an enclosed containment vessel, possible mechanisms causing relative motion between particles, and thus coagulation, include Brownian motion of the particles, gravitational settling, and turbulent gas motion. In most analyses where more than one of these mechanisms are present, they are assumed to be separable and additive such that

$$\phi(x,\xi) = K_B(x,\xi) + K_G(x,\xi) + K_T(x,\xi) \quad . \tag{7-2}$$

where

K_B = collision kernel due to Brownian diffusion
K_G = collision kernel due to gravitational settling
K_T = collision kernel due to turbulent gas motion.

The aerosol deposition mechanisms to be included in R(x) depend on gravitational settling, Brownian diffusion to the walls and deposition due to thermophoresis. These mechanisms are also assumed to take place separately.

The only mechanism included in R(x) is settling due to gravity. S(x,t) is always set equal to zero. The source term and the other mechanisms in R(x) are taken into account in solving the rate equations described in Chapter 4.0.

To convert Equation (7-1) into a set of first order differential equations, the equation is multiplied by x^k and integrated over x. After some manipulation, the following general form for the moment equations results:

$$\frac{dX_k}{dt} = \frac{1}{2}\int_0^\infty d\xi\ n(\xi,t) \int_0^\infty d\zeta\ n(\zeta,t)\ \phi(\xi,\zeta)][(\xi+\zeta)^k - \xi^k - \zeta^k]$$

$$- R_k(t) + S_k(t) \quad , \tag{7-3}$$

where

$$X_k = \int_0^\infty n(x,t)\, x^k\, dx \quad \text{is termed the } k^{th} \text{ moment of the size distribution} \tag{7-4}$$

$$R_k(t) = \int_0^\infty R(\xi)\xi^k\, n(\xi,t)\, d\xi \tag{7-5}$$

and

$$S_k(t) = \int_0^\infty S(\xi,t)\xi^k\, d\xi \quad . \tag{7-6}$$

The solutions of Equation (7-3) can be analytically obtained by assuming that the airborne particle concentration is represented by a log-normal distribution function at all times. Hence, in terms of particle volumes, the number distribution may be written

$$n(x,t) = \frac{N(t)}{\sqrt{2\pi}\, u(t)} \exp\left\{ - \frac{\ln^2 \dfrac{x}{\bar{x}(t)}}{2u(t)} \right\} \frac{1}{x} \tag{7-7}$$

where

$N(t)$ = the total number concentration of suspended particles

$\bar{x}(t)$ = geometric mean particle volume

$u(t)$ = logarithmic variance.

Then X_o, X_1, and X_2 are related to the three parameters of the log-normal aerosol size distribution by the following relations:

$$X_k(t) = N(t)\ \bar{x}(t)^k [\exp \frac{k^2}{2} u(t)] \quad , \tag{7-8}$$

so that

$$X_o(t) = N(t) \tag{7-9}$$

$$X_1(t) = N(t)\ \bar{x}(t)\ e^{u(t)/2} \tag{7-10}$$

and

$$X_2(t) = N(t)\ \bar{x}(t)^2\ e^{2u(t)} \quad . \tag{7-11}$$

Alternatively,

$$N(t) = X_o \tag{7-12}$$

$$\bar{x}(t) = X_1^2/[X_o^3 X_2]^{1/2} \tag{7-13}$$

and

$$\sigma(t) = \ln(X_o X_2/X_1^2) \ . \tag{7-14}$$

Equation (7-3) is converted into a set of three simultaneous first order differential equations for k = 0, 1, and 2. Using equation (7-7) and after some manipulation, the following three equations are obtained [21,22, 23,5].

$$\frac{dX_o}{dt} = S_o - R_o - B_1[X_o^2 + X_{1/3}X_{-1/3} + A(X_o X_{-1/3} + X_{1/3}X_{-2/3})]$$

$$- \varepsilon T_2 J_o - \varepsilon T_1(X_o X_1 + 3X_{1/2}X_{2/3}) - GAGGO \tag{7-15}$$

$$\frac{dX_1}{dt} = S_1 - R_1$$

$$\frac{dX_2}{dt} = S_2 - R_2 + 2B_1[X_1^2 + X_{4/3}X_{2/3} + A(X_1 X_{2/3} + X_{4/3}X_{1/3})]$$

$$+ 2\varepsilon T_2 J_1 + 2\varepsilon T_1(X_1 X_2 + 3X_{5/3}X_{4/3}) + GAGG2 \tag{7-17}$$

Here,

S_i = moments of source term

R_i = moments of the removal terms

B_1 = (2/3)(kT/μ) = Brownian coagulation coefficient

k = Boltzmann constant

μ = dynamic viscosity of steam

$T_1 = \frac{4}{3}\sqrt{\frac{8\pi^3\varepsilon_T}{15\nu}}$ = first turbulent coagulation coefficient

ε_T = turbulent energy dissipation rate

ν = kinematic viscosity of steam

$$T_2 = 0.0717 \frac{\rho_p}{\mu} \frac{\varepsilon_T^3}{15\nu}^{1/4} = \text{second turbulent coefficient}$$

ρ_p = particle material density

ε = collision efficiency

A = first order slip correction factor

$$J_\ell = X_o^2 \exp[(2\ell + \ell)\mu + (\ell^2 + \ell + \tfrac{1}{2})u]\cdot[e^{1/3(\mu+\ell u)}F(u) + AG(u)]$$

where

$$F(u) = e^{u/18}[e^{u/3} \operatorname{erf}(\tfrac{2}{3}\sqrt{u}) + 2 \operatorname{erf}(\tfrac{1}{3}\sqrt{u})], \text{ and}$$

$$G(u) = \operatorname{erf}(\tfrac{1}{2}\sqrt{u}) + e^{-2u/9} \operatorname{erf}(\tfrac{1}{6}\sqrt{u}) \quad .$$

In equations (7-15) and (7-17), the terms with square brackets are Brownian agglomeration terms, terms containing T_1 and T_2 are turbulent agglomeration terms, and GAGGO and GAGG2 are the gravitational agglomeration terms. The remaining variables are defined as

$$X_{1/3} = X_o\, e^{(\frac{1}{3} \ell n\, \bar{x} + \frac{u}{18})}$$

$$X_{-1/3} = X_o\, e^{(-\frac{1}{3} \ell n\, \bar{x} + \frac{u}{18})}$$

$$X_{2/3} = X_o\, e^{(\frac{2}{3} \ell n\, \bar{x} + \frac{2u}{9})}$$

$$X_{-2/3} = X_o\, e^{(-\frac{2}{3} \ell n\, \bar{x} + \frac{2u}{9})}$$

$$X_{4/3} = X_o\, e^{(\frac{4}{3} \ell n\, \bar{x} + \frac{4u}{9})}$$

$$X_{5/3} = X_o\, e^{(\frac{5}{3} \ell n\, \bar{x} + \frac{25u}{8})}$$

$$\text{GAGGO} = 0.75(6.84169 \times 10^{-14}) \frac{\rho_p}{\mu} X_o X_1[e^{\frac{\ell n\, \bar{x}^2}{6}} e^{-\frac{u}{18}} (1 - e^{\frac{4u}{9}})$$

$$(1 - \operatorname{erf}(\frac{2\sqrt{u}}{3})) + A\, e^{-\frac{2u}{9}} (1 - \operatorname{erf}(\frac{\sqrt{u}}{6})) - (1 - \operatorname{erf}(\frac{\sqrt{u}}{2}))]$$

$$GAGG2 = 2(6.84169 \times 10^{-14}) \frac{\rho_p}{\mu} X_1 X_2 \left[e^{\frac{\ln \bar{x}^{-2}}{6}} e^{\frac{5u}{18}} (1 - e^{\frac{4u}{9}}) \right.$$

$$(1 - \mathrm{erf}\,(\frac{2\sqrt{u}}{3})) + A\, e^{-\frac{2u}{9}} (1 - \mathrm{erf}\,(\frac{\sqrt{u}}{6}))$$

$$\left. - (1 - \mathrm{erf}\,(\frac{\sqrt{u}}{2}))\right] \quad .$$

The source terms in equations (7-15) to (7-17), S_o, S_1 and S_2 are always zero.

The removal terms due to gravitational settling are

$$R_o = F^* X_o\, e^{\left(\frac{2 \ln \bar{x}}{3} + \frac{2u}{9}\right)}$$

$$R_1 = F^* X_o\, e^{\left(\frac{5 \ln \bar{x}}{3} + \frac{25u}{18}\right)}$$

$$R_2 = F^* X_o\, e^{\left(\frac{8 \ln \bar{x}}{3} + \frac{32u}{9}\right)}$$

and

$$F = \frac{2}{9} \frac{\rho_p\, g}{\mu} \frac{A}{V}$$

with

g = gravitational acceleration

A = sedimentation area

V = compartment volume

The three differential equations (7-15) to (7-17) are solved simultaneously to obtain X_o, X_1, X_2 using the initial conditons at the beginning of the timestep. Once X_o, X_1 and X_2 are known, N, $\bar{X}$ and u are calculated from equations (7-12) to (7-14).

8.0 INTERFACES WITH OTHER CODES

MATADOR requires a variety of thermal-hydraulic parameters to perform the radionuclide transport and deposition calculations. These parameters are all functions of time and are calculated by the MARCH code. However, MARCH takes hundreds, or even thousands, of timesteps to determine these quantities. Because of computer storage space limitations, a user must choose at most twenty values of these parameters for input to MATADOR so as to provide an adequate linear approximation to the function.

An algorithm which was originally written for the CORRAL-2 code provides the necessary rules for picking the appropriate values from the output of the MARCH code. If we donate the thermal-hydraulic parameter by P and let $\overline{p}$ represent the vector of parameter values at each MARCH timestep, i.e.,

$$\overline{p} = (P_1, P_2, \ldots, P_m) \equiv f\ (t) \qquad (8\text{-}1)$$

then we wish to devise an algorithm for defining a vector $\overline{c}$

$$\overline{c} = (C_1, C_2, \ldots, C_N) \equiv g\ (t) \qquad (8\text{-}2)$$

where

$$2 \leq N \leq 20$$

and

$$C_i \in \overline{p} \quad \forall\ i \quad .$$

The functions $f(t)$ and $g(t)$ are discrete, however, and we make them continuous by connecting each successive point with a straight line. The problem is to choose the vector $\overline{c}$ such that $f(t)$ and $g(t)$ are approximately equal. In order to do this we define a linear operator, L_t,

$$L_t\,(\cdot) = {}_o\int^t (\cdot)\,dt \quad . \tag{8-3}$$

Next we begin at the initial time step and calculate a least squares fit of a linear function to this and the successive point. Denoting this function $Y(t)$ we have

$$Y_1\,(t) = a_1 t_i + D_1 \quad , \; i = 1,2 \quad . \tag{8-4}$$

Finally we calculate a function $R(t)$ as

$$R(t_2) = \frac{L_{t_1}\; f(t) - L_{t_2} Y_1(t)}{L_{t_2}\; f(t)} \; , \; t_1 \leq t \leq t_2 \quad . \tag{8-5}$$

If $R(t)$ is greater than R_o, which is supplied by the user, the program choses t_2 as its first point. If $R(t)$ is less than R_o, (as it must be for the first time step) then a third point is added and we have

$$R(t_3) = \frac{L_{t_3}\; f(t) - L_{t_3}\; Y_2(t)}{L_{t_3}\; f(t)} \quad . \tag{8-6}$$

This procedure is continued until the program reaches the final value in the $\overline{p}$ vector. If more than twenty points are chosen before the time t_i reaches t_m the value of R_o is increased by 10 percent and the algorithm is restarted. At the end of the calculations two arrays are returned to the main program:

$$XR = (T_1, T_2, \ldots, T_N), \; 2 \leq N \leq 20 \tag{8-7}$$

$$YR = (Y(T_1), Y\,(T_2), \ldots, Y\,(T_N)) \quad . \tag{8-8}$$

The user has the option of requesting integral values rather than point values, in which case the YR array is given by:

$$YR = (L_{T_1} \ (Y_1(t)), L_{T_2} \ (Y_2(t)), \ldots, L_N \ (Y_N(t))) \quad . \qquad (8\text{-}9)$$

An example of this procedure is shown in Figure 8.1. In this figure, the containment temperature during an accident sequence is shown. The solid boxes indicate the points chosen from this curve by the algorithm when the convergence criterion, R_o, was one percent. When using the MATADOR code, the user has the option of either selecting to input thermal-hydraulic data or to allow the code to read a tape on which output from the MARCH code has been written, use the algorithm just described to select an appropriate number of them and use them for input.

The source rates of the various radionuclides that enter the containment through the breach or release point in the reactor primary system have for most accidents been assumed to be equal to the release rate from the fuel with no allowance made for primary system deposition. Recent calculations performed using the TRAP code have indicated, however, that the assumption of negligible primary system deposition is not always justified, particularly for the less volatile radionuclides [24]. It therefore becomes important that, in future calculations, the source term reflect radionuclide depletion during transport through the reactor primary system. The MATADOR code has been written such that it can directly accept source terms calculated by such codes as TRAP.

The output of the MATADOR code consists of environmental radionuclide release fractions for each of the radionuclide groups. These releases can then be used in a radiological consequence code such as CRAC to calculate the health effects of reactor accidents. CRAC, in its present version, performs atmospheric diffusion calculations using burst releases, whereas MATADOR predicts radionuclide releases to the environment over several hours. Different approaches to modify these output data into a form suitable for input to CRAC will have to be evaluated before an interface with the health effects code can be constructed. A better approach would be to suitably modify CRAC to treat continuous releases of radioactivity to the environment since burst releases would not be expected to occur in all possible accidents.

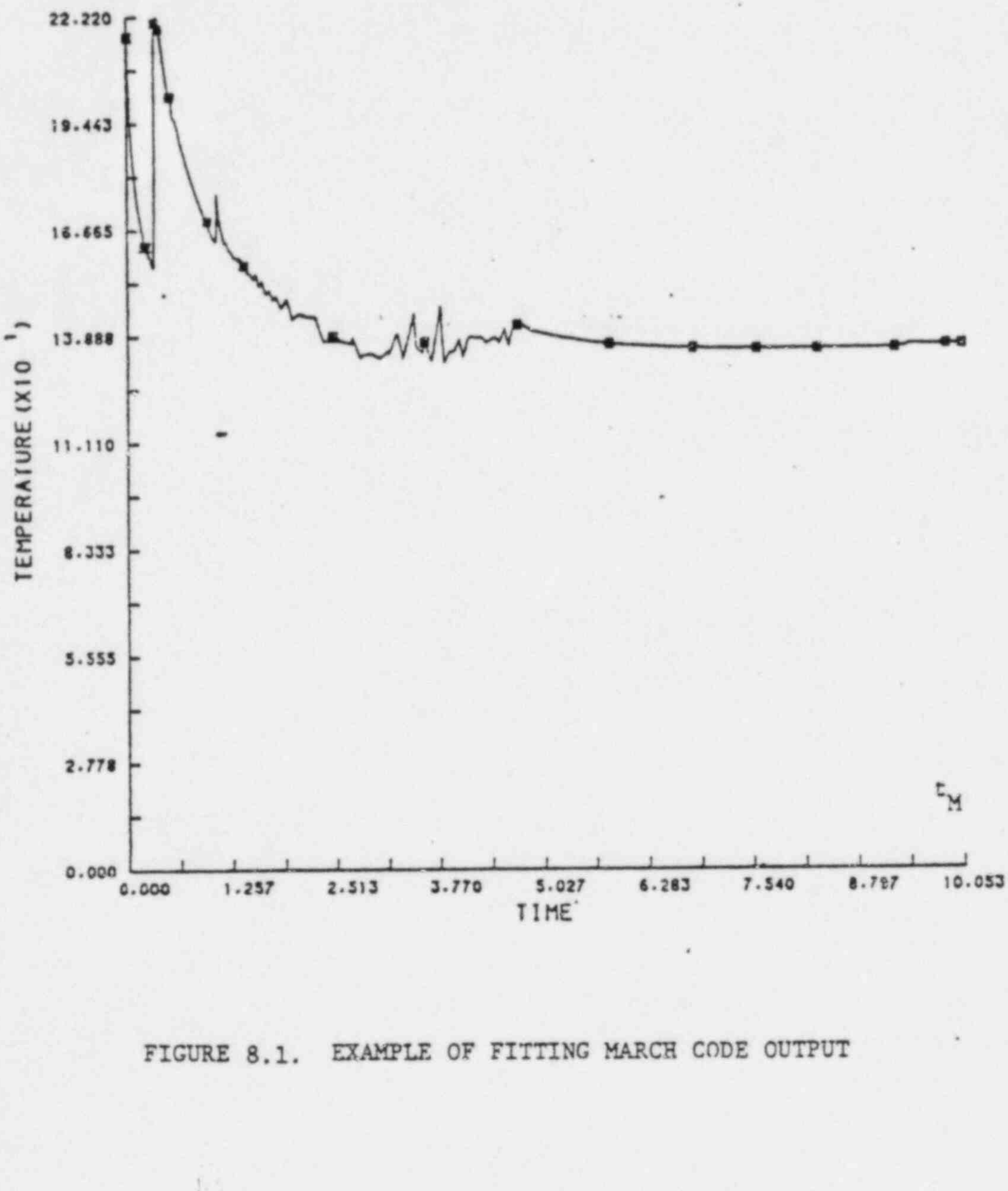

FIGURE 8.1. EXAMPLE OF FITTING MARCH CODE OUTPUT

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APPENDIX A

SOLUTION TECHNIQUE USED IN SOLVING TRANSPORT AND DEPOSITION EQUATIONS

The set of differential equations describing the transport and deposition of a radionuclide species in the containment may, conveniently, be expressed in the following compact form:

$$\frac{dM}{dt} = AM + S \quad . \tag{A-1}$$

In the above equation,

M is a vector of radionuclide masses in each state in each control volume,

S is vector of radionuclide source rates to each state in each control volume,

A is a matrix of intrastate and intravolume transport coefficients, and

T is time.

The solution to the set of equations (A-1) under the assumption of constant A and S over a timestep of integration, Δt, is

$$M = M_o + A^{-1}\Delta t^{-1} \, (e^{A\Delta t} - I)(AM_o + S)\Delta t \tag{A-2}$$

where

$$M_o = M \text{ at } t = 0 \quad .$$

Equation (A-2) may be rewritten in the following form:

$$M = M_o + \left[I + \frac{A\Delta t}{2} + \frac{A^2(\Delta t)^2}{3!} + \text{---}\right]\left[AM_o + S\right]\Delta t \tag{A-3}$$

Equation (A-3) may also be written in the following form:

$$M = M_o + \left[X_o \Delta t + \frac{AX_o \Delta t^2}{2} + \frac{A^2 X_o (\Delta t)^3}{3!} + \text{---}\right] \tag{A-4}$$

where

$$X_o = AM_o + S \ .$$

The expression (A-3) has been coded in the computer code as the subroutine ALCEMY. The subroutine sums the series to an appropriate number of terms in order to calculate the value of the vector M at the end of a time-step using a known M_o.

The suboutine scales the elements of the A matrix in order to ensure that the series summation converges regardless of the value of the time-step Δt. The elements of the A matrix are scaled by powers of 2 if

$$\Delta t || A || > 1$$

where

$$||A|| = + \sqrt{\sum_{ij} a^2_{ij}} \tag{A-5}$$

and a_{ij} are the elements of A.

The solution is obtained using the expression in Equation (A-4) if the A matrix is not scaled. Powers of A are not evaluated. Rather the jth term in the series within the square brackets is computed from the (J - i)th term by multiplying it by $A\Delta t/j$. If the elements of the A matrix are scaled, the solution in obtained by using the expression in Equation (A-3). Assuming that Z is the scaled A matrix such that

$$z_{ij} = \frac{a_{ij}}{2^n} \qquad i,j \tag{A-6}$$

where the z_{ij}'s are the elements of Z, the subroutine evaluates the sum

$$Z^{-1} \Delta t^{-1} \left(e^{Z\Delta t} - I\right) = A^{-1} t^{-1} 2^n \left(e^{\frac{A\Delta t}{2^n}} - I\right) \ .$$

The sum

$$2^{n-1} A^{-1}\Delta t^{-1} \left(e^{\frac{A\Delta t}{2^{n-1}}} - I \right)$$

is obtained from the value of the sum

$$2^{n} A^{-1}\Delta t^{-1} \left(e^{\frac{A\Delta t}{2^{n}}} - I \right) = B$$

as the value of the expression

$$\frac{1}{2^{n+1}} B^2 A\Delta t + B \quad .$$

A repeated application of this formula 'n' times allows the calculation of $A^{-1}\Delta t^{-1} (e^{A\Delta t} - I)$ from the computed value of $Z^{-1}\Delta t^{-1} (e^{Z\Delta t} - I)$. The value of M is then evaluated simply by substitution into Equation (A-3).

APPENDIX B

MATADOR ASSUMPTIONS

MATADOR is intended to describe the transport and depositon behavior of radionuclides within LWR containment buildings under accident conditions. Its intended role is to predict the important characteristics of the airborne release from the reactor building for reactor risk studies given the release from the primary system as input. In order to achieve widespread acceptance of MATADOR, potential users must believe that the code predictions are sufficiently credible so that MATADOR can be used with confidence in reactor risk studies. The credibility of the code calculations can be established by:

1. Suitable integral validation of the code calculations. This could include comparison of MATADOR results with data from suitable experiments and/or comparison with the results of other more accepted code calculations.
2. Examination and evaluation of the MATADOR models and assumptions.

In using the second of these approaches, it should be remembered that the approach adapted from the outset, in developing MATADOR has been to include adequate descriptions of all of the important processes which affect the transport and deposition of airborne radionuclides while at the same time avoiding the detailed analysis and more complex models that would result from a careful consideration of the microscopic details of the processes involved. This approach was consistent with the intended code application. With this design basis it can be expected that the code is based, to some extent, on the intuition and judgement of the authors. We therefore emphasize that the credibility of the MATADOR results should, for the most part, be established through the integral validation approach mentioned above. However, we also believe that the following discussion of some of the key assumptions which are implicit in the code can with proper interpretation give the user some insight into the code output credibility.

Implicit in the use of MATADOR are the following assumptions:

1. All of the important phenomena are described.
2. All of the phenomena descriptions (models) are adequate.

The following list identifies some of the key phenomenological and simplifying assumptions implicit in the code use.

List of Assumptions

- The flow paths in the containment building can be treated as a series of well mixed control volumes
- The radionuclides in the containment can be treated as noninteracting species, e.g., chemical reactions are not treated

  NOTE: Species coupling is implicit in the way the aerosol particles are treated .
- Transformations that result from radioactive decay are not treated
- The transport and deposition behavior of vapors and aerosols in the reactor building can be adequately treated by assuming a limited number of allowed "states" for each species
- All vapor deposition processes are assumed to be mass transport rate limited
- Resuspension is not treated except insofar as it is implicit in the equilibrium behavior of iodine
- Condensation and evaporation from the aerosols in the containment atmosphere is not treated
- The geometric and other similarity considerations which would completely justify the application of the individual process models have not been studied in detail
- Aerosol particles are spherical
- Coagulation does not alter the chemical composition of the aerosols within a size class over a timestep
- Noble gases transport through containment in phase with fluid flow with no deposition
- Organic iodide is not treated in a special way. It could either be included with noble gases or molecular iodine or both.