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ACCIDENT-INDUCED FLOW AND MATERIAL TRANSPORT IN NUCLEAR FACILITIES--A LITERATURE REVIEW

by

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ABSTRACT

The reported investigation is part of a program that was established for deriving radiological source terms at a nuclear facility's atmospheric boundaries under postulated accident conditions. The overall program consists of three parts: (1) accident delineation and survey, (2) internal source term characterization and release, and (3) induced flow and material transport. This report is an outline of pertinent induced-flow and material transport literature. Our objectives are to develop analytical techniques and data that will permit prediction of accident-induced transport of airborne material to a plant's atmospheric boundaries.

Prediction of material transport requires investigation of the areas of flow dynamics and reentrainment/deposition. A review of material transport, fluid dynamics, and reentrainment/deposition literature is discussed. In particular, those references dealing with model development are discussed with special emphasis on application to a facility's interconnected ventilation system.

I. INTRODUCTION

Nuclear facilities must be designed to protect the general public from the consequences of accidents that could result in a release of radioactive material to the environment. Regulatory agencies are reponsible for reviewing proposed facility designs to that end. The degree of conservatism and the related risk also must be evaluated for these accident conditions. Designers and analysts must have methods and data that permit a systematic approach to estimating accident effects.

Assessment of the environmental consequences of an accident requires an estimate of release rate, which is basic to calculating the radioactive dose to the public. Much uncertainty lies in the estimate of release rate. Therefore, we are undertaking a program to provide more realistic estimates of accident-induced release rate and to better characterize source terms. The program to obtain and process data is divided into three major research areas: (1) accident delineation and survey of literature, (2) source-term and release characterization, and (3) material transport.

Battelle Pacific Northwest Laboratories (PNL) and Oak Ridge National Laboratory (ORNL) share responsibility for research areas (1) and (2), and the Los Alamos National Laboratory is responsible for research area (3). Tasks in research areas (1) and (2) involve identifying the accidents to be studied and the primary source-term data to be used in the transport models. Los Alamos will study transport of the released material through the nuclear facility. The objective is to develop mathematical models and computer codes that will predict material transport through a complex of rooms, gloveboxes, ductwork, filtration systems, and other components commonly found in ventilation systems.

In this report we review some material transport models that may be applicable to modeling material transport within nuclear facilities. Work in the supporting areas of accident-induced flow dynamics and reentrainment/deposition also is reviewed. In flow dynamics, existing one- and multidimensional models are discussed. We believe that these models will provide the basis for computer codes tailored to predict accident-induced phenomena.

II. ACCIDENT-INDUCED MATERIAL TRANSPORT WITHIN STRUCTURES

This section is an outline of a review of the literature and approaches for developing material transport models to be used in analyzing the effects of accidents within nuclear facilities. We have identified significant parameters and effects that must be considered for one-, two-, and three-dimensional material transport models.

A review of literature pertaining to material transport is presented below. This survey is sufficient to describe material transport for nuclear facilities. Discussed in some detail are articles that are especially relevant to our approach in model development. The discussion is organized under the divisions of general theory, concentration equation concepts, and single-particle tracking concepts.

A. General Theory

Several texts that describe the theory of aerosol transport were reviewed. Although we did not attempt to discuss all of the many references concerning material transport, we will discuss several of the better texts that outline the fundamentals of particle transport and important parameters to be considered.

One of the more useful articles selected for review is a reference by R. Dennis,[1] Chap. 3, "Dynamic Behavior of Aerosols," by C. E. Billings and R. A. Gussman, which provides a review of the phenomena producing particle motion. These phenomena have been divided and categorized by the authors as interfacial phenomena (evaporation, condensation, nucleation, and adhesion) and aerosol dynamics (settling, impaction, diffusion, coagulation, electrostatics, and filtration). The authors state that analysis of aerosol behavior requires simultaneous consideration of the following phenomena:

- interaction of particles with gas constituents,
- interaction of particles with other suspended particles,
- motion of individual particles or clouds in a defined flow field under the influence of one or more forces, and
- motion of particles with respect to immersed obstacles or flow boundaries.

The authors also list important characteristics that must be known about the particles in addition to the characteristics of the flow field that contains the suspended particles. In later sections, the authors point out the difficulties associated with mathematical modeling systems where flow, coagulation, settling, and diffusion effects are interacting. They state that a completely satisfactory model has not been developed yet. However, empirical formulas and equations describing material transport are given.

Billings and Gussman describe formulations that can be used with the time-dependent concentration equation given below.[1]

$$\frac{dc}{dt} = S_+ - S_- \quad , \qquad (1)$$

where

c = material concentration,
t = time,
S_+ = source of material, and
S_- = sink of material.

The formulations outlined by the authors allow approximations for settling, coagulation, or other aerosol dynamics phenomena to be used for the terms S_+ and S_-.

Other references reviewed offer a more rigorous approach to the theory of material transport. These approaches are described in texts by S. L. Soo,[2] H. E. Hesketh,[3] and R. G. Boothroyd.[4] Basically, they attempt to consider the forces acting on an individual aerosol particle and write equations of motion that allow calculation of particle velocity and trajectory. The basic equation used in these approaches is written as

$$m_p \frac{dv_p}{dt} = \quad F_i \;, \tag{2}$$

where

m_p = particle mass,
v_p = velocity of the particle,
t = time, and
F_i = forces acting on the particle.

In addition to boundary and multiparticle effects, the effect of the flow field is discussed in the referenced texts. Also, these analyses assume that the particle concentration is dilute enough so that the particle has little effect on the flow field. Clearly, many approximations are necessary in these approaches, particularly when interparticle interactions are considered.

B. Concentration Equation Concepts

The need to predict the fate of accidentally released aerosols within reactor containments has led to the development of several material transport models. The HAA-3 code has been used extensively in the past.[5] This code was developed to simulate liquid-metal fast-breeder reactor (LMFBR) accidents but has been applied to other containment volumes.[6] The HAA-3 code simulates the changes in size distribution and concentration of a well-mixed, log-normally distributed aerosol with time. The code uses a time-dependent concentration equation similar to Eq. (1) to describe aerosol motion within a large cylindrical container. The influence of gravity or particle deposition and collisions between particles (agglomeration) are considered. The model can account for wall interactions (such as plating) in addition to providing for leakage removal mechanisms. A uniform mixture is assumed, with wall plating, agglomeration, and gravity being the predominant phenomena. However, when agglomeration proceeds to a point where the size distribution is no longer log-normal, the calculative method is changed to a stirred settling model where only settling and leakage are considered. The empirical constants needed for the code were developed using experimental data from Atomics International.

H. Jordon and C. Sack have developed a code called PARDISEKO that is similar to HAA-3.[7] This code is used extensively in the Federal Republic of Germany's fast breeder reactor safety programs.

F. Gelbard has developed a computer code called AEROSOL that simulates size distribution dynamics for a spatially homogeneous aerosol.[8] The code assumes a single volume containing the aerosol mixture, and it appears to be similar to HAA-3 in applicability. That is, the code places special emphasis on coagulation and agglomeration mechanisms.

A. K. Postma, P. C. Owczarski, and D. L. Lessor have developed a computer code called CORRAL to simulate material transport behavior in reactor containments following a postulated accident.[9] The code provides removal mechanisms for fission products in the form of elemental iodine, methyl iodide, and solid particles. The authors have structured the code to predict internal movement of the aerosol material to a reactor's atmospheric boundary. As in HAA-3, a time-dependent concentration equation is used to describe the aerosol behavior within the reactor containment. A well-mixed volume is assumed with empirical terms added to the concentration equation that account for particle removal by filters, sprays, deposition onto surfaces, and gravitational settling. In contrast to other aerosol models that were reviewed, CORRAL includes capabilities for simulating transport through several internal subcompartments within the general containment system. The multicompartment feature was developed specifically to model transport in a boiling water reactor (BWR) containment system.

A two-dimensional, time-dependent computer program that models chemically reactive mixtures has been reported by Rivard, Farmer, and Butler.[10] A concentration or species equation is used for aerosol transport in this code. It has been applied to flows within chemical lasers, but there seems to be no reason why it could not be applied to the containment problems outlined above. However, it does not include capabilities for predicting agglomeration or wall plateout, and it is not suitable for multiple-volume analysis.

R. J. Fluke has reported the use of a computer code call FISSCON to simulate the movement of fission products inside the containment of a Canadian reactor system under accident conditions.[11] He reports that transport of fission products can be calculated to determine filtration, wall plating, and water absorption. Personal communication with the author indicates that the code is a modification and extension of the CORRAL computer code.

C. Single-Particle Tracking Concepts

Another body of literature involves calculative methods that simulate material transport phenomena by solving the equations of motion for individual particles. That is, given the flow field, the velocity of a single particle can be calculated while accounting for forces such as gravity, drag, buoyancy, and inertia. The equations solved are similar to Eq. (2). The turbulent diffusion of an individual particle also has been included, but very little in the way of interparticle forces or wall surface forces has been modeled. However, the essential point is that the species or concentration equation is solved by tracking many thousands of particles to simulate movement of material. The particles can be tracked throughout a system by using a large number of particles of varying sizes and densities.

Particle tracking schemes to simulate material transport have been advanced primarily by the fluid dynamics group at Los Alamos. R. S. Hotchkiss and C. W. Hirt explained the principles of the technique with reference to the species or concentration equation method that has been discussed above.[12] The technique discussed by the authors was applied to atmospheric dispersion in a highly distorted flow field where the flow field was calculated using the SOLA-3D code.

C. W. Hirt and L. R. Stein have reported application of the above method to aerosol transport within rooms.[13] In this case, the normal ventilation airflow for a room in the Los Alamos plutonium handling facility was calculated using SOLA-3D. Particles then were injected into the room, and their movement was observed to locate dead zones and areas of high aerosol concentration within rooms.

Other applications of the technique have been reported by J. R. Zurewicz and D. E. Stock at Washington State University.[14] Their application was for modeling aerosol transport in an electrostatic precipitator. A term that calculates the force on a particle from an electric field was added to the equation of motion for the particles. Their numerical calculations compared quite well with experimental data.

Calculation of gas/droplet flows that allow the particles to be liquid droplets also has been reported.[15] In this two-dimensional application, the droplet size history, temperature, and trajectory were calculated. The authors used the technique to simulate spray drying systems. Similar calculations have been reported by C. T. Crowe of Lawrence Livermore National Laboratory (LLNL).[16]

Applications of the HAA-3 code using the time-dependent concentration equation and a SOLA code using particle-tracking methods were reported by D. H. Mitchell.[17] The codes were used to predict aerosol behavior in gloveboxes. Mitchell notes that although HAA-3 appears to be limited, it was useful to indicate the relative importance of agglomeration, which was not taken into account by the SOLA code. No direct comparison of material transport calculations for the two codes was reported.

D. Assessment of Literature

In this section we will discuss our assessment of the articles reviewed. Also, plausible approaches will be discussed with particular reference to how they can guide our development of one- and multidimensional material transport models for nuclear facilities.

Although the literature review presented here is relatively limited, we believe that two basic approaches to predicting material transport have been outlined in the selected references. The methods vary from those using the conventional concentration equation for a system to those that involve calculating the movement of individual aerosol particles.

We did not find any codes or models that described the transport of combustion products in our literature review. However, in our review of fire-induced flow dynamics, several researchers noted that this type of work needed to be done or was in progress. Combustion products are made up of solids, liquids, and gases with a range of physical properties. The characteristics of some combustion products may be too complex to approximate very well with the most simple models. Researchers have tried to model both solid and liquid movement, and their work may provide some insight into the problem of modeling combustion product movement. Some of this work is discussed below.

The established aerosol transport codes have been specially tailored to model LMFBR or light-water reactor (LWR) containments. All but one of these codes are applicable only to single volume conditions and do not have provisions for large convective effects that could be expected in accident situations. The only exception is the CORRAL code, which allows for multiple volumes and convective flux between these volumes. However, the CORRAL code and associated empirical relationships also are tailored to simulate BWR conditions rather than the more arbitrary conditions that may be found in many nuclear facilities, particularly fuel cycle facilities. None of these codes include the effect of multiple blowers or fans that move air through interconnected compartments. Therefore, we believe that the traditional and established aerosol codes are not suited totally for our application in their current form. However, there are many desirable or essential elements in these codes that should be retained and used.

Using the time-dependent species or concentration equation contained in the established aerosol codes offers a logical and straightforward approach to developing a material transport code. Little difficulty would be encountered in coupling the required set of concentration equations to existing lumped-parameter or quasi-one-dimensional ventilation network codes. In certain areas, single volume aspects of the aerosol codes would be essential for proper development of quasi-two-dimensional aspects of the material transport code. Also, the application of these codes to modeling multidimensional effects in single volumes may offer the only practical approach that also provides correlations with other types of codes.

The particle-tracking approach being developed and used by some researchers is especially promising for modeling multidimensional movement of material.

The major drawback of this approach is the lack of interparticle effects. This method would be unsatisfactory for modeling material transport very near the accident source. However, in regions farther away from the material source where particle concentration is sufficiently dilute, this approach may be very useful. In the past, researchers have neglected this concept because it required vast computer storage and run time to account for the movement of individual particles. However, recent advances in computer systems now allow consideration of this approach.

III. ACCIDENT-INDUCED FLOW DYNAMICS WITHIN STRUCTURES

This section of the report is a review of analytical models that are applicable to flow induced by postulated fire, explosion, or other accidents within nuclear facilities. Lumped-parameter and multidimensional models are considered, with emphasis on existing computer codes that can provide a basis for developing models of accident-induced flow dynamics.

A. Existing Computer Codes

A Los Alamos report by F. H. Harlow and A. A. Amsden provides a discussion of basic physical fluid dynamics.[18] In this report, general solutions to fluid phenomena are considered with an introduction to numerical techniques using high-speed computers.

The earliest and most well-known fluid dynamic codes using numerical techniques are the MAC and SMAC codes developed at Los Alamos.[19,20] These codes solve the Navier-Stokes equations and the continuity equation using finite differences for two-dimensional, transient, incompressible flow. A series of computer codes called SOLA has evolved from the early MAC and SMAC codes. These codes are simplified versions for the less experienced user. The SOLA-ICE code[21] has the capabilities outlined above but also is capable of handling compressible flow.

In England, D. P. Spalding developed multidimensional codes called GENMIX and CHAMPION that may be applicable.[22,23] They will handle two-dimensional parabolic and elliptical compressible flows. GENMIX also has particle transport modeling capability.

The computer codes discussed above are primarily multidimensional, but SOLA-ICE can be used to simulate one-dimensional phenomena. Characteristically, ventilation systems in nuclear facilities are essentially one-dimensional with many branching and looping ducts. Therefore, simulation of accident-induced flow phenomena within ventilation systems requires a computer code that can simulate one-dimensional effects. Furthermore, the most cost-effective approach in analyzing accident-induced flows is to first perform an analysis with fast, one-dimensional computer codes and then follow up with more detailed analyses if required.

The TVENT computer code is designed specifically for nuclear facility ventilation systems.[24] The code was developed to predict the effect of tornado-induced depressurization within such systems. TVENT features user-oriented input/output, portability, and applicability to a large number of ventilation systems. In addition to the one-dimensional simulation, assumptions include incompressible and isothermal flow, system components treated as lumped parameters, and compressibility allowed at rooms or gloveboxes. Inertia and shock effects are neglected. TVENT's use in safety analysis has been demonstrated in addition to its coupling with the SOLA-ICE code.[25]

B. Explosion-Induced Flow Dynamics

TVENT has been extended to predict propagation of explosively driven transients within a ventilation system.[26] As the explosion code evolved from the TVENT code, the basic input/output format and the steady-state portions of the code were retained. However, the transient analysis portion of the code was modified extensively. The transient analysis is subdivided into two major categories, the near field and the far field, and these categories apply to regions of the ventilation system that are near to or far away from the explosive event.

Depending on the characteristics of the explosive event, a deflagration, detonation, or transition to detonation will take place in the near field. The far-field analysis is treated as a gas-dynamics problem with the explosion modeled parametrically. This analysis is particularly suitable when the flow dynamics are relatively insensitive to the explosive event or when there is little detailed information about the explosion conditions. The far-field version of the code has been used on several simple problems. The results compare well with experimental results.

Some experimental data can be found in Ref. 27, which describes the discharge of high-pressure gas (air) from a vessel to the atmosphere. It also describes the pressurization of a vessel by a high-pressure air supply reservoir. These are interesting cases for initial tests of an explosion computer code, especially in the areas of mass and energy conservation, orifice flow relations, and choked flow conditions. The effect of dissipation during choked flow is shown in Ref. 28.

C. Fire-Induced Flow Dynamics

This section describes selected works (both experimental and analytical) that have a bearing on an approach for a fire-induced flow dynamics code. The main emphasis is placed on analytical models developed and used by others to predict fire effects. However, because fire modeling is so difficult, we find that many of the models rely on or reduce to correlations of experimental data. Therefore, we will discuss various sets of available experimental data as well.

The results of the literature survey are divided into the general categories of experimental and analytical investigations. These references summarize previous work that has been performed in areas related to the subject of interest. This review of the literature is not exhaustive but rather is an overview of the state of the art as it relates to facility fires.

1. Experimental Investigations.

a. Enclosure Fires. There are many references in the literature to measurements of parameters in enclosure fires. These experiments are typically performed for both full-scale and scale-model rooms or enclosures. The geometry of the test typically involves a room containing a fire source near one end and a doorway at the other end. Variations in the tests consider doorway size, magnitude of heat source, types of combustible materials present, and scale. McCaffrey and Rockett[29] show measurements of ceiling and floor temperatures and pressures for both full-size and scale-model rooms. Steady-state measurements are given using an adjustable number of gas burners as the heat source.

Gross and Robertson[30] present experimental measurements of burning rates, temperatures, and gas compositions in model enclosures of three sizes. Again interest was confined to the fully developed period of burning. They found that the burning rate was dependent on the size and shape of the ventilation opening. Thus, they showed that the gas-dynamics effects are coupled intimately to the heat release rate of the combustible material. Further, the major portion of the generated heat is transferred by radiation from the flames and glowing fuel.

Parker and Lee[31] have studied the transient nature of the fire build-up process in a room. Heat transfer from conduction and radiation as well as temperature, air velocity, fuel supply rate, and oxygen concentration were measured in the transient mode. The tests showed that a large fraction of the heat generated in the fire was lost through conduction and radiation even 5 min after initiation of the tests. The heat absorbed by the air and carried out the doorway was only about 56% of the heat generated in the fire. These tests also demonstrated a two-layer effect (a layer of hot gas near the ceiling and a layer of cold gas near the floor).

b. Duct Fires. McCaffrey and Quintiere[32] report that the flow patterns for fire-induced flows in corridors may be as complicated as those for enclosures. Their tests were performed with a 1/7-scale and a full-scale corridor. Detailed measurements indicate a complex, recirculating, three-dimensional flow field with a four-layer flow pattern. Furthermore, the flow field and temperature were strongly influenced by the size of the corridor doorway.

Two sets of experiments on fires in ducts indicate that modeling this physical situation poses equally severe problems. Roberts and Clough[33] experimentally studied the propagation of fires along a duct lined with wood. Their experiments indicated a strong coupling between the fire growth rate and the airflow rate; that is, the growth of a fire affects the ventilation, and conversely the growth of the fire is strongly dependent on the ventilation rate. Their experiments also show that in the early stages, the heat release rate is determined by the fuel supply, whereas the heat release rate is controlled by the supply of oxygen later on. Further, the heat release rate can differ by a factor of 10 or more between these two conditions.

Chaiken et al.[34] experimentally investigated the nature of coal mine fires in a 23-cm^2 duct under the influence of a forced-ventilation airflow. The experiments showed that the fire passed through both stages described by Roberts and Clough. Furthermore, the experiments indicated stratification and reverse flow in the upper level upstream of the fire zone. Also, the reverse flow in the upper portion of the duct is greater than the forward flow in the lower portion of the duct for several time periods.

c. Combustion Experiments. Many experiments have been performed in which the rate of burning of cellulosic fuel in a controlled environment was studied.

Parker[35] performed basic studies in which he showed that the oxygen depletion measured in an exhaust duct downstream from a fire correlated with the total rate of heat production of the specimens. This basic correlation has been used by others to obtain the heat release rate for burning materials for experiments in which this quantity could not be measured directly.

The burning mechanism for fully developed fires in a ventilation-controlled compartment has been studied by Harmathy.[36] Data are shown for the results of over 250 full-scale and scale-model tests performed by others. A fully developed combustion model that correlates with the multitude of experimental findings for cellulosic fuels with reasonable accuracy is derived. The model probably is not applicable to other fuel types.

The difference in burning rates between wood cribs and some synthetic polymers under forced-ventilation conditions also was studied by Harmathy.[37] The experiments showed that the burning rate of the polymers was not affected significantly by the ventilation rate. In contrast, the burning rate of the wood cribs showed a definite dependence on the ventilation rate.

The determination of the size distribution and mass concentrations of the products of combustion is important in the prediction of fire effects. The mass concentration and size distribution for soot particles is given by Prado et al.[38] as a function of a number of variables for both kerosene and benzene. The experimental device was a turbulent continuous flow combustor. Additional information on the size distribution of combustion aerosols is given by Pourprix et al.[39] and Alvares et al.[40] Alvares shows the size and mass distribution of smoke aerosols at the exit of a test cell for a variety of combustible materials. As discussed in this reference, it is difficult to obtain these type of data, and the accuracy is not good because of the many processes that cause the aerosol to change its character during the sampling and measurement procedures.

d. Component Response. The effects of smoke aerosols on high-efficiency particulate air (HEPA) filters have been reported by Gaskill et al. [41] and by Beason and Alvares.[42] A series of experiments were performed in the LLNL Full-Scale Fire Test Facility. The facility has a full-sized test apparatus with a complete ventilation system, including a HEPA filter. The fires were located in a room upstream from the filter. Some important observations about fire effects in ventilation systems were noted. First, an almost immediate overpressurization of the fire compartment was observed. This implies that the ventilation system is compromised because air leakage from the room or flow reversal through the intake can occur. Second, because of the large quantities of smoke particulates, filter plugging and a subsequent decrease in the ventilation rate were observed.

The above experiments were performed to determine the lifetime of HEPA filters exposed to fire-generated aerosols. Additional information was reported by Alvares et al.[40] on various methods used to reduce the aerosol exposure by installing engineering countermeasures in the duct between the filters and the fire source. These countermeasures included water scrubbing sprays, rolling prefiltration systems, and sprinkler systems.

The duct spray techniques did not increase the filter lifetimes appreciably; rather, they tended to enhance the condensation of volatile aerosols, which made filter plugging more likely. The rolling prefiltration system showed the most promise because it enhanced filtration and it extended HEPA filter lifetimes by a factor of 2 or more at the same time.

2. Analytical Investigations.

a. Enclosure Fires. Several methods are used to predict the effects of fire in enclosed spaces analytically. The first of these is the simplest, and much is assumed about the geometry of the enclosure and the fully developed flow patterns in the enclosure. In this method (two-layer model), the gas in the enclosure is assumed to be stably stratified with a layer of hot gas above and a layer of cool ambient air below. We usually assume that air enters the room (cold layer) from an opening in one wall and approaches the fire, where it is entrained in the gas plume. Hot gas enters the upper layer, where it flows out the upper part of the wall opening. A review of the models, assumptions, and state of the art in this type of fire modeling is given by Rockett.[43] In its simplest form, such a model is amenable to hand calculations.

As more effects are included in such a model (especially time-dependent effects), we eventually have to solve the resulting equations with a computer. The most encompassing and sophisticated model along these lines (that is, two-layer models) that we are aware of is the Harvard Computer Fire Code.[44] Even so, it has drawbacks with regard to the current application. The model is limited to the prediction of the development of a fire ignited on a horizontal surface in a rectangular enclosure with open doors or windows. The fire must be away from the walls for the model to work well. Because of the complexity of combustion phenomena, the burning rate and fire growth are not predicted from first principles, but the code uses empirical correlations obtained from open burn tests carried out over a limited time.

Another approach to the problem is to derive and solve the fundamental equations that govern the gas dynamics in an arbitrary three-dimensional system explicitly. Such equations are presented by Rehm and Baum.[45] The equations are tailored explicitly to the prediction of gas flows caused by fires. Caretta et al.[46] and Patankar and Spalding[47] present several techniques for the solution of such equations. These equations and techniques are not tailored necessarily to fire-induced flows. As pointed out by Hjertager and Magnussen, although computational procedures for flow have been available for some time, there have been relatively few applications to ventilation systems. Hjertager and Magnussen[48] do apply the Patankar and Spalding algorithm to flows in ventilated rooms with good agreement for some problems (not fire-induced flow).

Another recently developed analytical model that shows promise for fire-induced flows is presented by Doria.[49] A compilation of results obtained using this model is given by Doria and Ku.[50] A number of two-dimensional problems were calculated, and excellent agreement with existing analytical and experimental results was obtained.

This method eventually became the basis for the UNDSAFE-1 computer code,[51] which predicts the flow, temperature, and pressure fields in a two-dimensional rectangular enclosure that result from a volumetric heat source. An improved version of the code with additional physical models has been released.[52] This code has been found to be suited to applications to the fire problem in enclosures. The fire source itself is not modeled, but the code is useful for predicting temperatures away from it. Applications of the code to experiments performed at the National Bureau of Standards and Notre Dame University show a consistency between the experiments and code predictions.[53]

Tanaka presents a model that attempts to deal with more than a single enclosure.[54] This model is a computer simulation of the movement throughout a building of hot gas and smoke caused by a fire source in an arbitrary room. This model shows how it may be possible to incorporate some of the specific models treated here into a more general code that can handle networks and ventilation systems of increasing complexity.

b. Duct Fires. Much work has been reported on the analytical modeling of fuel-rich fires spreading within ventilated fuel-lined ducts. These works generally are concerned with fires in mine shafts, tunnels, and air spaces between stored materials. An early example of this is shown in the work of De Ris[55] in an analytical treatment of fuel-rich duct fires. The theory is in general agreement with experimental data for duct fires that do not exhibit reverse or stratified flow.

A one-dimensional model is not adequate to describe duct fires in which reverse stratified flow takes place. Under these conditions, smoke may form a layer near the ceiling and flow in the opposite direction of the ventilation flow. Hwang et al.[56] developed a two-dimensional mathematical model of the phenomenon to gain some understanding of it. The detailed behavior of gas plumes and stratified layers can be studied with this model. Hwang and Chaiken[57] applied this theory to mine-related ventilation systems that use an exhaust fan to supply forced ventilation. The coupling between the fire and the ventilation airflow was analyzed to relate the air velocity in normal operation to the air velocity during a fire for a single entry duct. By combining Hwang's and Chaiken's theory, we can calculate critical flow velocities that will prevent reverse stratified flow in the event of a duct fire. The resulting theory agrees with experimental results available from small-scale tunnel fires.

References 55--57 (discussed above) deal with the fully developed (steady-state) condition. Edwards et al.[58] analyzed the time-dependent problem of fire spread along the walls of a ventilation duct using a two-dimensional model. The model applies during the initial stages of a fire build-up during which the flame spread is governed by energy transport rather than the later stationary state controlled by the air supply. During this initial stage, reverse stratified flow is not encountered.

<u>c. Combustion Theory.</u> The theory of combustion has been studied, and models have been suggested for the free burning of particles or gaseous elements in controlled conditions. For example, Lowe et al.[59] model a large pulverized coal furnace with data for single char particles and an assumed gas flow pattern to predict local combustion heat release rates of the furnace. Magnussen and Hjertager[60] developed a mathematical model that predicts the rate of combustion and soot formation of reacting species in turbulent flames.

Roberts[61] shows that deriving an analytic model for the burning of a larger solid, such as a piece of wood, is much more complicated. He states that the problem is not so much computational but is rather in the formulation of a mathematical model from the complex chemical and physical processes occurring and in the availability of data for use in a mathematical model. Block[62] reports on the more complicated problem of developing models for the free-burning behavior of piles (cribs) of wood. The crude model developed is guided by quantitative and qualitative experimental observations. Here he notes that the crib model could be greatly improved if a model that could predict the burning rate of a single piece of wood could be developed.

d. Component Behavior. Liu[63] has reported on a theoretical and experimental investigation to evaluate the effects of a corridor sprinkler system on the cooling and suppression of a fire in an adjacent compartment connected by an open doorway. A simplified, one-dimensional mathematical model is presented to predict the net reduction of the corridor ceiling hot gas temperature by evaporative cooling. The effect of the spray droplet size on the cooling and suppression of fire is discussed.

Fuel cycle facility ventilation systems include components designed to mitigate the effects of postulated accident conditions (for example, HEPA filters, water-spray heat exchangers, and mist and debris eliminators). If the operation of this equipment affects the transport of material, then this equipment must be simulated under accident conditions along with the more obvious components such as ducts and blowers. So far, we have not found existing models to predict the behavior of this type of equipment under accident conditions. The degree to which such models are required depends to a great extent on the detailed accident definition for a particular facility.

There is a scarcity of information about analytical models that predict the interaction of combustion phenomena with the flow field. A good review of the state of the art of modeling of fire-flow fields has been reported by Emmons.[64] He states that the understanding of the basic elements of the combustion process presents insurmountable difficulties in analytical modeling where turbulent flow is encountered. This is because the performance of the system is controlled as much or more by the way gases move about before and after combustion as by the combustion process itself, and solutions for turbulent flow fields may not be obtained. Emmons adds that the key to our predictive understanding of turbulent combustion is the correlation of experimental data, and although some model studies have been made, in no case are these adequate.

IV. REENTRAINMENT/DEPOSITION

A. General Theory

This section presents the results to date of our literature survey in the areas of reentrainment and deposition and literature cited in the areas of aerosol measurements (including techniques, devices, and data analysis) and particle characteristics in fuel cycle facilities. The survey is performed to assure that previous work is used to the fullest extent possible. We have found monographs, journal articles, and technical reports in the areas of fluid mechanics, multiphase flow, aerosol science, nuclear safety, ceramics and power metallurgy, health physics, atmospheric science, soil science, and space science (geophysical aspects). A number of key articles that are being studied will be identified, but the survey is not exhaustive.

In fuel cycle safety assessment, we are interested ultimately in defining the radioactive aerosol flux at the atmospheric boundaries of a plant under accident conditions. This means that we must be able to estimate material transport through the ventilation system or other pathways. However, before any material is transported, it must somehow be made airborne. One mechanism for aerosolizing particles from a surface is aerodynamic stress; that is, if the air velocity impinging on a bed or pile of particles is sufficiently high because of an explosion, fire, or tornado, some of the particles may be entrained or reentrained. These are the particles that are made available for possible transport and deposition.

B. Reentrainment

Over a period of more than 30 yr, Bagnold has produced an important series of papers[65-68] and a classic monograph[69] on this subject. His work includes analysis of the requirements for motion of dust and sand. He has performed many experiments with dust and sand particles under both cohesive and cohesionless conditions. Bagnold has shown us how to collapse experimental particle threshold speed data with variations in particle size and density onto a single curve. (We emphasize the importance of this procedure.) This similitude approach is extremely valuable in understanding the physics of small, heavy particle reentrainment and development of a mathematical formulation for the process. If the experimental data can be represented with a single curve, this curve can be used to describe material movement for a wide range of material sizes and weights. This suggests that we bracket the materials of interest, such as PuO_2 or UO_2. Bagnold has been concerned primarily with dust-, sand-, or soil-type materials.

Raudkivi[70] has summarized ideas on the transport of solids by fluids, including threshold of particle transport in a single volume. Halow[71] has done a number of experiments to measure rolling, sliding, and suspension of particles in turbulent airflow in pipes. He has developed expressions for initiation fluid velocities for a number of material sizes and densities. However, his data for heavy particles are limited to very large size (2700 μm or greater).

Lyles and Krauss[72] have performed experiments to investigate the effects of turbulence intensity in a wind tunnel boundary-layer on soil particle movement, threshold friction speed, and mean flow speed. For a given particle size, the threshold mean windspeed decreased with increasing turbulence intensity. This paper demonstrates the importance of flow conditions on reentrainment, whereas Wasan et al.[73] discuss the effects of particle charge. Additional experiments to determine particle movement and reentrainment criteria for soil-type particles in air were carried out by Punjrath and Heldman[74] and earlier by Zingg.[75] White[76] measured threshold conditions in water.

A very important series of experiments and similitude analyses has been underway for the past several years at Iowa State University (ISU) and at the National Aeronautics and Space Administration (NASA) Ames Research Center.[77-81] The team conducting these experiments is associated with J. D. Iversen at ISU. This team has studied a wider range of particle sizes and densities than Bagnold and the other experimenters cited above, and it has collapsed the data successfully. However, the data are sparse for small, heavy particles, and the team has not considered the effect of varying bed thickness (light loadings). Iversen and his colleagues have been correlating particle erosion rate (reentrainment) and horizontal flux (material transport). They also have made predictions of the air speeds required for particle motion and reentrainment from their data.

Another ongoing experimental and analytical program is being conducted at the National Center for Atmospheric Research at Boulder, Colorado, by Gillette and his co-workers.[82-87] Although Gillette's measurements have been restricted to soil-type particles under atmospheric boundary-layer conditions, his theoretical analyses have included development of semi-empirical correlations of vertical aerosol flux (reentrainment) as well as horizontal aerosol flux (material transport). An older but important sequence of experiments was performed by Chepil[88-91] at the Wind Erosion Laboratory at Manhattan, Kansas. Chepil observed a quantitative correlation between material in suspension with surface horizontal flux. For dry soils, he found that the horizontal flux of particles varied directly as the cube of the threshold friction speed[92] as Bagnold found earlier for desert sand.[69] Gillette[86] later modified this relationship to include the difference between the local friction speed and the threshold friction speed. These semi-empirical erosion rate (transport) functions are summarized by Iversen et al.[78]

An important symposium devoted to the atmosphere-surface exchange of particles by dry deposition and resuspension was held at Richland, Washington, in September 1974.[93] One contribution to this symposium was a paper by Travis[94] detailing a computer model he developed to describe the reentrainment, transport, and deposition of soil-contaminant mixtures. Travis' model is based on conserving mass within a matrix of control volumes with reentrainment close to the surface governed by a combination of the semiempirical formulations of Bagnold and Chepil for horizontal flux and Gillette for vertical flux. Other noteworthy contributions to the symposium in the area of reentrainment are Refs. 94-97. Horst[98-100] has developed a model for estimating atmospheric aerosol concentrations accounting for resuspension, diffusion, and deposition. Mills and Olson[101] have modeled suspension and atmospheric transport.

We cite two references that treat the subject of calculating individual particle trajectories.[102,103] These two papers, as well as the three important works that follow,[104-106] deal with concepts necessary for the calculation of individual particle trajectories in shear flow. Thus, in contrast to the semiempirical approach to reentrainment, one can calculate individual particle trajectories through the boundary layer (by integrating the equations of motion) if the initiation phenomena are known from experiment or are assumed. The Morsi and Alexander paper[102] gives particle drag coefficients as a function of the Reynolds number up to 50 000. The Saffman paper[103] formulates the lift force generated in shear flow as being proportional to the square root of the vertical velocity gradient.

Corn has produced a number of articles dealing with particle-surface phenomena.[107-111] In Ref. 107 he makes an important distinction between cohesive bonds between particles and adhesive bonds between individual particles and a surface. He points out many factors that influence the strength of the bonds. References 108-111 report the results of Corn's experiments to determine the nature and magnitude of adhesive force.

The Symposium on Surface Contamination held at Gatlinburg, Tennessee, in June 1964 resulted in a number of pertinent papers[112-118] with many measurements of resuspension factors for normal nuclear facility conditions.

C. Deposition

Many forces can contribute to mass transport across a surface boundary layer, including eddy diffusion, velocity gradients, turbulence gradients, gravity, impaction, irregular surfaces, Brownian motion, diffusiophoresis, thermophoresis, interception, electrostatic effects, and shear-flow-induced lift forces. These mechanisms are discussed in detail in Refs. 3, 119, and 120. Davies[119] and Billings and Gussman[121] present deposition equations for specific situations, such as diffusion through a turbulent boundary layer, inertial deposition from turbulent flow, and deposition of aerosol from turbulent pipe flow.

Liu and Agarwal[122] have performed aerosol deposition studies for liquid particles ranging in size from 1.4 to 21 μm in vertical turbulent pipe-flow. They found the predominant mechanism to be an inertial effect resulting from the particle mass being acted on by the fluid turbulence for this flow. This had been suggested earlier by Friedlander and Johnstone,[123] who ran experiments in a similar test setup using fine metal powders (iron and aluminum). The preceeding two papers expound the "diffusion free-flight" model in which the particle diffusivity in the boundary layer is assumed equal to the eddy momentum-diffusivity of the flow up to very near the surface. Near the surface, the particles are assumed to "free-flight" to the wall. Reference 122 describes 12 previous experiments on turbulent deposition in tubes and channels and compares the results with theory.

An important series of papers by Sehmel[124-128] presents equations for and experimental determinations of aerosol particle eddy diffusivities. These equations and experiments will be useful in calculating particle removal rates from turbulent air to vertical and horizontal surfaces. Clough[129] has conducted experiments that have supported Sehmel's theory.[124]

Slinn, Sehmel and Hodgson, and Horst discussed problems and predictive modeling of deposition in the atmosphere in their 1974 Atmosphere-Surface Exchange of Particulate and Gaseous Pollutants Symposium papers.[130-132] Gillette and Porch[133] recently reported their experimental results on the effects on dust deposition of velocity fluctuations and particle concentration in the atmosphere.

Cleaver and Yates[134] have studied the influence of particle removal on deposition rate. They identify wall shear stress (friction velocity) as the controlling parameter for deposition when reentrainment is occurring simultaneously. The works by Fuchs[135] and Soo[2] are classic treatises dealing with many aspects of the mechanics (and dynamics) of multiphase systems, including aerosol deposition. After studying these books, one cannot help but appreciate the breadth of scope of two-phase systems. In general, these two volumes provide rigorous background material, which is a necessary foundation for practical applications. Chapter 8 in Brodkey's book[136] also should be mentioned because it provides a good review of laminar viscous flow (which, by virtue of small particle size or slow flow speed and therefore low Reynolds number, is often the case for aerosols). Stokes' drag formula for spheres and the resulting terminal velocity expression for a nonaccelerating particle are derived here. The modifications to Stokes' law, such as those of Oseen and Cunningham, are discussed here and elsewhere.

The book Surface Contamination contains several articles[137-139] dealing with the concept of deposition velocity (analyses and measurements are included). Van der Hoven[140] has presented deposition velocity results from field experiments using radioisotopes.

Koontz[6] has developed a computer code (HAA-3) that calculates suspended mass concentration, mass of fallout material, mass of wall plateout material, and median size by volume of the particle distribution as functions of time for sodium or uranium oxide aerosols in a vessel of a given size. HAA-3 solves an integro-differential equation that models aerosol coagulation or agglomeration with removal and source terms. The removal processes are leakage (input as a table), fallout, and plating. A source rate can be input as a table. When the aerosol concentration decreases to the point where agglomeration is no longer important, the program uses a stirred-settling model (Stokes' corrected).

HAA-3 neglects resuspension. It uses a log-normal aerosol number concentration during agglomeration, and the particle density is assumed to be 1/4 of the theoretical density. A wall plating factor must be determined experimentally. The HAA-3 code does not account for changing flow velocity, material transport (other than settling and plate-out in a vessel), or initial mass (that is, it will not calculate reentrainment under flow conditions). Parametric studies using the code allowed comparison with experimental data.

Castleman et al.[141] have produced a code similar to HAA-3 to predict the vertical (downward) transport of radioactive aerosols (PuO_2 and UO_2). Again, both theoretical and experimental results are presented.

Deposition phenomena in turbulent boundary flows are very complex, as Sehmel's work will attest.[124-128] Of course, eddy diffusivities are dependent on a particular flow configuration and must be assumed or measured experimentally. Although complex, aerosol concentration reduction phenomena have been modeled successfully in the past, as in HAA-3.[5] One noticeable area where experimental data are lacking is in deposition of small, heavy particles from accident-induced flows in ducts.

D. Aerosol Measurements

A number of references concerning aerosol measurement devices and techniques are reviewed in this section. The Davies,[142] Mercer,[143] and Hesketh[3] books are helpful for properties, size classification, and sampling of aerosols. Reference 144 and the notes on the course on aerosol measurement[145] are particularly useful for understanding the limitations of aerosol measuring devices and their selection. References 146-148 deal specifically with optical devices. Sehmel[149-152] has written several articles on the errors and pitfalls that await the experimenter in acquiring samples of aerosols isokinetically through nozzles and probes. He discusses his work on sampling of aerosols on wires (by impaction) in Ref. 152. Two chapers in the book Handbook on Aerosols are pertinent, Sampling and Particle Size Measurement[153] and Aerosol Generation.[154] We have a number of books that are helpful in understanding the statistics of aerosol size analysis.[155-159] Reference 160-162 are reports that deal with aspects of size distribution determination, and Refs. 163-165 deal with various aspects of aerosol measurement.

E. Particle Characteristics in Fuel Cycle Facilities

References 166-176 compose a partial list of articles that concern reentrainment, transport, and deposition for selected materials. These papers and reports, as well as a long list of others obtained from a computer search, are being studied to gain information on powder and dust in fuel cycle facilities. The computer search was based on the following descriptors and authors.

Descriptors	Authors
Fuel reprocessing plants	G. A. Schmel
Reprocessing	T. W. Horst
Radioactive aerosols	C. N. Davies
Aerosols	T. T. Mercer
Radioactive effluents	M. Corn
Plumes	
Particle size	
Particle resuspension	

We are interested primarily in the potentially hazardous powders PuO_2 and UO_2. However, we also are interested in characterizing combustion products. In Sec. III, we emphasized the need for and lack of available data characterizing combustion products from fires, except in the area of fire detection, which emphasizes relatively young and therefore small particles ($d_p < 1 \mu m$).

V. SUMMARY

A program to determine the effect of postulated accident source terms on a nuclear facility's confinement system has been established by the NRC. The program consists of three investigative areas: (1) accident delineation, (2) internal source term characterization at point of origin, and (3) transport through the ventilation system or other pathway to a facility's atmospheric boundary. Three contractors have responsibility for undertaking this program; Los Alamos is responsible for the area of transport. In this report, we described our initial review of the literature, including experimental data that will permit characterization of accident-induced source terms after passing through a facility's confinement system.

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The reported investigation is part of a program that was established for deriving radiological source terms at a nuclear facility's atmospheric boundaries under postulated accident conditions. The overall program consists of three parts: (1) accident delineation and survey, (2) internal source term characterization and release, and (3) induced flow and material transport. This report is an outline of pertinent induced-flow and material transport literature. Our objectives are to develop analytical techniques and data that will permit prediction of accident-induced transport of airborne material to a plant's atmospheric boundaries.

Prediction of material transport requires investigation of the areas of flow dynamics and reentrainment/deposition. A review of material transport, fluid dynamics, and reentrainment/deposition literature is discussed. In particular, those references dealing with model development are discussed with special emphasis on application to a facility's interconnected ventilation system.

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