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Literature Survey of Aerosol and Iodine-Vapor Deposition Models Relevant to TVA Radiation Monitor Sampling Line Conditions

A. L. Wright

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Chemical Technology Division

LITERATURE SURVEY OF AEROSOL AND IODINE-VAPOR DEPOSITION
MODELS RELEVANT TO TVA RADIATION MONITOR SAMPLING LINE CONDITIONS

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HOLDUP IN AIR MONITORING SAMPLING LINES

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LITERATURE SURVEY OF AEROSOL AND IODINE-VAPOR DEPOSITION
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A. L. Wright

ABSTRACT

This report describes work performed as part of a project entitled "Investigation of the Degree of Iodine Holdup in Air Monitoring Sampling Lines." The work was sponsored by the Tennessee Valley Authority as project TVA-58784A. This report, the first in a series, summarizes the available modeling data base for predicting iodine aerosol and vapor deposition in air-monitoring sampling lines. Sample aerosol and vapor deposition calculations are presented for conditions that might simulate those present in a sampling line during severe accident conditions.

1. INTRODUCTION

The Nuclear Regulatory Commission (NRC) is concerned that gas effluent sampling lines in nuclear power plants are not well characterized as to the vapors and aerosols that can be deposited in them during sampling. In response to this concern, the Tennessee Valley Authority (TVA) is involved in a program to determine how to characterize the capabilities of the sampling lines at TVA nuclear power plants. This program, in general, involves studies related to the following issues: (1) determination of the ability to obtain "representative" samples from the present sampling line configurations, (2) development of the capability to calculate iodine species vapor and aerosol deposition for representative sampling line conditions, and (3) performance of experiments to verify that the models developed to calculate iodine vapor and aerosol transport are adequate. The "representative" sampling line conditions that are important include conditions that could occur under normal plant operation and conditions that could occur during severe (core-melt) accidents.

This report summarizes the available models for the major iodine aerosol and vapor deposition mechanisms, based on evaluation of the available literature. The second section of this report summarizes

models and data for iodine aerosol and vapor deposition. The third section presents some sample calculations for conditions that might simulate those present in one of the sampling lines in the Watts Bar nuclear plant. Finally, the results and conclusions from the study are presented.

2. REVIEW OF IODINE AEROSOL AND VAPOR DEPOSITION MODELS

2.1 AEROSOL DEPOSITION MODELS

Aerosol deposition in sampling lines could occur by some combination of the following mechanisms:

1. gravity settling in horizontal lines,
2. laminar diffusion,
3. turbulent diffusion and inertial effects,
4. thermophoresis,
5. inertial deposition in bends, or
6. diffusio-phoresis.

A summary of the available correlations for calculating aerosol deposition by these mechanisms follows.

2.1.1 Gravity Settling in Horizontal Lines

Aerosol settling in horizontal sample lines occurs as a result of particles settling due to their "Stokes settling velocity," defined as

$$V_{st} = \frac{\rho_p d^2 g C}{18\mu}, \quad (1)$$

where

- g = acceleration of gravity,
 - ρ_p = particle density,
 - d = particle diameter,
 - μ = carrier-gas dynamic viscosity,
 - C = the Cunningham "slip-correlation factor," defined as
- $$C = 1 + Kn(1.257 + 0.4e^{-1.1/Kn}), \quad (2)$$
- Kn = particle Knudsen number = $2\lambda/d$,
 - λ = gas mean-free-path between molecular collisions.

Some aerosol transport computer codes calculate settling in horizontal lines by assuming that the Stokes velocity is the settling deposition

velocity and that the effective pipe settling area is DL , where D is the pipe diameter and L is the pipe length. A more rigorous relationship for the deposition efficiency for aerosol flow through a pipe under laminar-flow conditions was presented in Fuchs' book:¹

$$E_{1s} = \frac{2}{\pi} [2S(1 - S^{2/3})^{1/2} - S^{1/3}(1 - S^{2/3})^{1/2} + \sin^{-1}(S^{1/3})], \quad (3)$$

where

- E_{1s} = aerosol deposition efficiency for settling in laminar flow,
- S = $3V_{st}L/(4UD)$,
- U = average gas-flow velocity through the pipe,
- L = horizontal length of pipe section,
- V_{st} = Stokes settling velocity (Eq. 1),
- D = pipe diameter.

2.1.2 Laminar Diffusion

The most widely used formulation for calculating laminar diffusion in pipe flow comes from the work of Gormley and Kennedy:²

$$E_{1m} = 0.8191e^{-7.31h} + 0.0975e^{-44.6h} + 0.0325e^{-114h} \quad \text{for } h > 0.0156, \quad (4)$$

$$E_{1m} = 1 - 4.07h^{2/3} + 2.4h + 0.446h^{4/3} \quad \text{for } h < 0.0156, \quad (5)$$

where

- E_{1m} = transport efficiency for laminar diffusion in pipe flow,
- h = $2LD_p/(UD^2)$,
- D_p = diffusion coefficient for particle of diameter d , defined as
- $D_p = kTC/\pi\mu d$, (6)
- k = Boltzmann constant,
- T = gas temperature (K),
- C = Cunningham slip-correction factor [Eq. (2)],
- U = average gas-flow velocity through the pipe.

2.1.3 Turbulent Diffusion and Inertial Effects

Turbulent flow effects can cause deposition of aerosol particles in pipes through either diffusive (for "small" particles) or inertial (for "large" particles) mechanisms. The parameter that governs the approximate boundary between whether diffusive or inertial effects are important is the particle "dimensionless relaxation time," which is defined as

$$\tau^+ = \frac{\rho_p \rho_g d^2 U^* C}{18\mu^2}, \quad (7)$$

where

$$\begin{aligned} \tau^+ &= \text{dimensionless relaxation time.} \\ U^* &= U \sqrt{f/2}, \\ U^* &= \text{carrier-gas friction velocity,} \\ f &= \text{flow friction factor.} \end{aligned} \quad (8)$$

For values of $\tau^+ > 0.1$, inertial effects typically dominate over pure diffusion.

A relationship developed by Davis³ for turbulent deposition by diffusion is as follows:

$$V_{tu,d} = \frac{U^* (D_p/\nu)^{2/3}}{14.5 \left[\frac{1}{6} \ln \left(\frac{(1+\phi)^2}{1-\phi+\phi^2} \right) + \frac{1}{\sqrt{3}} \tan^{-1} \left(\frac{2\phi-1}{\sqrt{3}} \right) + \frac{\pi}{6\sqrt{3}} \right]}, \quad (9)$$

where

$$\begin{aligned} V_{tu,d} &= \text{turbulent diffusion deposition velocity,} \\ \phi &= 1/[2.9(D_p/\nu)^{1/3}], \\ \nu &= \text{carrier-gas kinematic viscosity, and} \\ Re &= \text{flow Reynolds number.} \end{aligned}$$

For turbulent diffusion due to inertial effects, the most reliable experimental data have been those of Liu and Agarwal.⁴ The deposition correlation developed from their data is

$$V_{tu,i} = 6(10^{-4})\tau_+^2 U^* \quad \text{for } \tau^+ < 12.9, \quad (10)$$

$$V_{tu,i} = 0.1U^* \quad \text{for } \tau^+ > 12.9, \quad (11)$$

where

$$V_{tu,i} = \text{turbulent inertial deposition velocity.}$$

Equations 9-11 can be combined to provide a unified correlation for turbulent deposition. As was noted in a report by Gieseke et al. and in a paper by Matsui et al., measurements of turbulent deposition in the transition region between pure diffusive and pure inertial deposition tend to be greater than predicted by available models.^{5,6}

2.1.4 Thermophoresis

Thermophoretic deposition driving forces result from temperature gradients at wall surfaces (heat losses to walls). The formula used to calculate thermophoretic deposition in almost all aerosol deposition computer codes is that based on Brock's theoretical expression:⁷

$$V_{th} = -2C_s \psi C \frac{\nabla T}{T}, \quad (12)$$

$$\psi = \frac{1}{1 + 2C_m Kn} \cdot \frac{(k_g/k_p + C_t Kn)}{(1 + 2k_g/k_p + 2C_t Kn)}, \quad (13)$$

where

- V_{th} = thermophoretic deposition velocity,
- C_s = thermal slip coefficient,
- C_m = momentum accommodation coefficient,
- C_t = thermal accommodation coefficient,
- k_g/k_p = gas-to-particle thermal conductivity ratio,
- ∇T = gas-wall temperature gradient.

The values recommended for C_s , C_m , and C_t are those based on the paper published by Talbot et al.:⁸ $C_s = 1.17$, $C_m = 1.14$, and $C_t = 2.18$. Using these values rather than the original ones from the Brock paper leads to an increase in calculated deposition velocities of roughly 40%.

2.1.5 Inertial Deposition in Bends

Deposition of aerosols in bends can be calculated using a simple formula developed by Crane and Evans:⁹

$$E_{db} = St \frac{\theta}{2}, \quad (14)$$

where

E_{db} = deposition efficiency for aerosol retention
in bends,

θ = bend angle, in radians,

St = particle Stokes number, defined as

$$St = \frac{\rho_p d^2 U}{9\mu D}. \quad (15)$$

Equation 14 holds when the ratio of the bend radius of curvature to the pipe radius is less than about 50. It does not hold for conditions in which secondary (recirculating) flows occur in the bends.

2.1.6 Diffusiophoresis

Diffusiophoretic aerosol deposition occurs as the result of condensation of a vapor (typically steam) onto a colder surface. The equation that is used in aerosol transport codes to calculate diffusiophoretic deposition is¹⁰

$$V_{df} = V_s \frac{\gamma_s \sqrt{M_s}}{\gamma_s \sqrt{M_s} + \gamma_a \sqrt{M_a}}, \quad (16)$$

where

V_{df} = diffusiophoretic deposition velocity,

V_s = diffusion velocity of condensable steam
to a surface,

M_s, M_a = molecular weights of steam and noncondensable gas, respectively,

γ_s, γ_a = airborne mole fractions of steam and noncondensable gas, respectively.

To be able to calculate diffusio-phoretic deposition, it is necessary to calculate V_g from the rates of steam condensation onto surfaces.

2.1.7 Other Considerations

As the preceding equations show, aerosol deposition mechanisms are dependent on aerosol particle sizes. An important consideration, then, in being able to characterize any sampling line is the ability to know the aerosol sizes input to the line. An associated consideration is whether aerosols that enter a sampling line will agglomerate, or grow larger, as they are transported through the line. If so, and if this agglomeration is significant, then any model used to calculate aerosol retention in sampling lines may also need to have the capability to calculate aerosol agglomeration.

For sampling under normal plant operating conditions, agglomeration during sampling is not likely to be important because amounts of airborne aerosol would be expected to be small. However, under severe accident conditions, aerosol concentrations in containment could reach values as high as 10 g/m^3 ; for such airborne concentrations, agglomeration effects could be important in sample lines. This issue needs further investigation.

Another unaddressed issue is the potential for resuspending aerosols that are deposited inside the sampling lines. As will be discussed in Sect. 3, at least one of the Watts Bar sampling lines may have gas flow velocities in the range of 4 m/s , and flow conditions will be turbulent. Although the likelihood is not great, there is the potential that resuspension could occur in the sample lines, particularly for deposited particle sizes that are much greater than $1 \text{ }\mu\text{m}$ diam. However, this potential will be much less for sample line conditions where steam condensation occurs within a line.

2.2 IODINE VAPOR DEPOSITION MODELS

Deposition of iodine vapor species in sampling lines depends on (1) the vapor species of iodine that are sampled; (2) the thermal-hydraulic conditions in the sampling line, including whether water is present; and (3) the type of steel used for the sample line and the condition of the sample line surface. An additional complication is that simultaneous adsorption of iodine species on the surface and desorption of previously deposited iodine from the surface may be occurring, which is analogous to deposition and resuspension of aerosols within the sampling line.

A major consideration in being able to characterize nuclear plant sampling lines is the species of iodine airborne in the plant under operating and accident conditions. Some previous investigations have indicated that the vapor species airborne in containment under plant operating conditions would consist of elemental iodine (I_2), hypiodous acid (HOI), and organic iodides (typically CH_3I).^{11,12} Discussions with an ORNL staff member (E. C. Beahm) involved with investigating iodine behavior in severe power plant accidents, however, indicate that the airborne vapor species in containment would consist largely of elemental iodine, hydrogen iodide (HI), and methyl iodide.¹³

The difference in behavior of I_2 -HOI- CH_3I and I_2 -HI- CH_3I mixtures would be significant. For the I_2 -HOI- CH_3I mixture, I_2 would be the most reactive species, and the deposition of the other species on steel surfaces would be minor. However, for the I_2 -HI- CH_3I mixture, HI is the most reactive species, so deposition of both HI and I_2 would need to be investigated. In this report we will present sorption and desorption data for I_2 and HI and will assume that these are the major species to be investigated in sampling-line calculations. The next phase of our sampling-line characterization effort (to be summarized in a future report) will concentrate on a more detailed discussion of the chemical species that may be transported within the sampling line.

2.2.1 I_2 and HI Vapor Deposition

Unrein et al. and Burchfield and Voilleque presented results from measurements of molecular iodine deposition velocities derived from tests

in which iodine vapor was passed through sampling lines meant to simulate those in nuclear plants.^{11,12} Kabat measured molecular iodine deposition velocities from deposits formed on steel coupons.¹⁴

Table 1 presents the molecular iodine results summarized in the three preceding papers. Overall, the measured deposition velocities varied between 0.0088 and 0.2 cm/s. The data show (as might be expected) no trends in dependence of deposition velocity values on the sampling line diameter. The highest measured values, those from Kabat, were measured for sampling system humidities of 97%; high humidity did not appear to increase the deposition velocity.¹⁴

Table 1. Summary of molecular iodine deposition velocity measurement results

Reference	Range of test conditions	Range of deposition velocity values (cm/s)
11	Tube diameters used ranged from 0.64 to 2.22 cm diam. Sampling temperatures were 25–30°C. Relative humidities were 25–70%.	0.0088–0.054
12	Tube diameters used were 1.57, 3.48 cm diam. Sampling temperature, humidity conditions not given.	0.038–0.076
14	Stainless steel coupons used. Temperature range of 20–24°C. Relative humidities were 5–97%.	0.018–0.2

An additional source of data on the sorption of I_2 and HI on stainless steel surfaces is included as a data base within the TRENDS (Transport and Retention of Nuclides in Dominant Sequences) computer code being developed at ORNL.¹⁵ Development of the code was begun in 1981 to investigate fission product transport for analyses performed in the NRC-funded ORNL Severe Accident Sequence Analysis (SASA) program, which is to analyze accident sequences associated with the TVA Browns Ferry Unit 1 plant. The code is currently being used for iodine behavior modeling associated with both pressurized water and boiling water reactor severe accidents.

In terms of I_2 sorption on steel surfaces, the data obtained by Genco et al. were used by Wichner to develop the following deposition velocity correlation,^{16,17} which is valid for I_2 deposition on 304 stainless steel in a steam environment for temperatures ranging from 423 to 823 K:

$$\log_{10}(V_{I_2}) = 2140/T - 7.8 \quad (\text{cm/s}), \quad (17)$$

where

$$\begin{aligned} V_{I_2} &= \text{molecular iodine vapor deposition velocity,} \\ T &= \text{steam temperature (K).} \end{aligned}$$

If we attempt to apply this correlation to predict the I_2 deposition velocity at a temperature of 298 K, we obtain a value of 0.24 cm/s. This value seems somewhat high, but is comparable to the higher values in Table 1.

Genco et al. also performed experiments to measure HI sorption on stainless steel in steam.¹⁶ Wichner¹⁷ developed a correlation for this data for temperatures between 423 and 1023 K:

$$\log_{10}(V_{HI}) = 1300/T - 4.3 \quad (\text{cm/s}), \quad (18)$$

where

$$\begin{aligned} V_{HI} &= \text{hydrogen iodide vapor deposition velocity,} \\ T &= \text{steam temperature (K).} \end{aligned}$$

Applying this correlation to HI deposition at 298 K, we obtain a value of 1.15 cm/s; this illustrates that HI is more reactive than I_2 .

2.2.2 I₂ and HI Desorption from Surfaces

Desorption data for I₂ were obtained from the works of Unrein et al. and Burchfield and Voilleque (desorption was called "resuspension" in these papers).^{11,12} After deposition velocity measurements were made, desorption was measured by passing an inert gas through the test pipes, measuring the outlet iodine concentration, and determining the desorption rates from these results. A summary of the measured desorption rate results is presented in Table 2. Note that the measured rates are very small, ranging from roughly 10⁻⁷ to 10⁻⁵ s⁻¹.

Table 2. Summary of measured molecular iodine desorption rate results

Reference	Range of measured desorption rates (s ⁻¹)
11	5 • 10 ⁻⁶ to 1 • 10 ⁻⁵
12	7.1 • 10 ⁻⁸ to 9.1 • 10 ⁻⁷

To my knowledge, no data base is available from which data for HI desorption from surfaces can be obtained.

2.2.3 Other Considerations

For a number of situations, small pools of water may exist in portions of nuclear plant sampling lines. If such conditions exist, then iodine "partitioning" in the water pools may be a significant mechanism for trapping I₂ before it passes through the line. Discussions with E. C. Beahm at ORNL indicate that the lowest values of molecular iodine "partition coefficient" - defined as the ratio of iodine in the water to iodine airborne in the gas phase - that might exist in sampling lines would be about 90.¹³ This suggests that almost all of the vapor species I₂ would be scavenged by water pools. This topic will be investigated in the next project report.

3. SIMPLE MODEL CALCULATIONS FOR IODINE AEROSOL AND VAPOR DEPOSITION

As a basis for sample calculations of aerosol and vapor deposition in sampling lines, data was obtained from Birney Fish of TVA for two of the containment air sample lines in the Watts Bar plant.¹⁸ A summary of important sample-line data on which sampling line transport calculations can be based is presented in Table 3. Note that there are a significant number of bends in each of these sampling lines. For the conditions listed in Table 3, the calculated flow Reynolds number is about 10,000, so turbulent flow will exist in the lines.

We will examine aerosol deposition in the sample lines first, under the assumption that no aerosol resuspension of deposits will occur and that steady-state deposition and transport conditions exist in the line. In terms of the simple analysis that follows, we will also consider that aerosol deposition in bends can be modeled separately from aerosol deposition by turbulence, settling, and thermophoresis. In terms of modeling deposition by turbulence, settling, and thermophoresis, the steady-state mass balance equation that governs aerosol behavior for each aerosol size is

$$0 = -q \frac{dC}{dx} - \pi D(V_{tu} + V_{th})C - DV_{st}C, \quad (19)$$

where

- C = airborne aerosol concentration,
- x = axial distance from pipe inlet,
- q = volume flow rate through pipe,
- V_{tu}, V_{th} = deposition velocities for turbulent deposition and thermophoresis, respectively,
- V_{st} = deposition velocity for settling (Stokes), and
- D = sampling line diameter.

Table 3. Summary of Watts Bar containment sampling line conditions; lines 1-RE-90-112-1, 1-RE-90-112-2

SAMPLE LINE 1-RE-90-112-1

Horizontal line length	4305 cm
Vertical line length	2446 cm
Line diameter	3.48 cm
Sampling flow velocity	496 cm/s
Gas sampling temperature, accident conditions	49°C
Number of "equivalent" pipe bends ^a	36

SAMPLE LINE 1-RE-90-112-2

Horizontal line length	4458 cm
Vertical line length	1836 cm
Line diameter	3.48 cm
Sampling flow velocity	496 cm/s
Gas sampling temperature, accident conditions	49°C
Number of "equivalent" pipe bends ^b	40

^aThis sample line has 24 actual bends and 4 globe valves. Birney Fish of TVA has estimated that each globe valve is equivalent to 3 bends in terms of aerosol deposition; therefore, we assume that there are 36 "equivalent" bends in this sample line.

^bThis sample line has 28 actual bends and 4 globe valves. Birney Fish of TVA has estimated that each globe valve is equivalent to 3 bends in terms of aerosol deposition; therefore, we assume that there are 40 "equivalent" bends in this sample line.

Equation (19) was derived by assuming the deposition area for turbulence and thermophoresis is equal to $\pi D x$, and the area for settling is equal to $D x$. The solution to Eq. (19) for C_{out} , the aerosol concentration at the pipe outlet, is

$$C_{out} = C_i \exp - \left[\frac{\pi D L}{q} (V_{tu} + V_{th}) + \frac{D L_s}{q} V_{st} \right], \quad (20)$$

where

C_{out} = aerosol concentration at outlet ($x = L$),

C_i = inlet aerosol concentration ($x = 0$),

L_s = horizontal sampling-line length, for settling.

The transport efficiency for turbulent deposition, settling, and thermophoresis, E_{t1} , is C_{out}/C_i , as defined by Eq. (20).

In terms of pipe bends, the deposition efficiency for each pipe bend, E_{db} , is defined in Eq. (14). The aerosol transport efficiency for one bend, E_{tb} , is equal to $(1 - E_{db})$. It follows that the transport efficiency for N pipe bends, $E_{t,Nb}$, is

$$E_{t,Nb} = (1 - E_{db})^N. \quad (21)$$

Finally, the total aerosol transport efficiency through the sampling line, $E_{t,tot}$, which is the ratio of the aerosol concentration measured at the line outlet to the concentration at the line inlet, is

$$E_{t,tot} = E_{t1} E_{t,Nb}. \quad (22)$$

Calculations were performed for each of the two sampling lines, with particle size as a variable. An additional input needed was the temperature gradient for thermophoresis; this was assumed to be $54^\circ\text{C}/\text{cm}$, based on a calculated turbulent boundary-layer thickness of 0.09 cm and an assumed gas-wall temperature difference of 5°C . Tables 4 and 5 present summaries of calculated aerosol transport efficiencies for each deposition mechanism and the overall transport efficiency as a function of assumed aerosol particle size. Figures 1 and 2 restate Tables 4 and 5 in a graphical format.

Table 4. Summary of calculated aerosol transport efficiencies for Watts Bar sampling line 1-RE-90-112-1

Particle diameter (μm)	Calculated aerosol transport efficiency				Overall
	Turbulence	Settling	Thermophoresis	Bends	
0.01	0.512	1.0	0.687	1.0	0.352
0.02	0.773	1.0	0.692	1.0	0.535
0.05	0.925	1.0	0.705	1.0	0.652
0.1	0.967	1.0	0.720	1.0	0.696
0.2	0.984	0.999	0.741	0.999	0.728
0.5	0.993	0.997	0.779	0.995	0.770
1.0	0.996	0.990	0.821	0.980	0.801
2.0	0.997	0.963	0.866	0.921	0.795
5.0	0.965	0.800	0.910	0.595	0.523
10.0	0.588	0.416	0.930	0.120	0.066

Table 5. Summary of calculated aerosol transport efficiencies for Watts Bar sampling line 1-RE-90-112-2

Particle diameter (μm)	Calculated aerosol transport efficiency				Overall
	Turbulence	Settling	Thermophoresis	Bends	
0.01	0.536	1.0	0.704	1.0	0.378
0.02	0.786	1.0	0.709	1.0	0.558
0.05	0.930	1.0	0.722	1.0	0.671
0.1	0.969	1.0	0.737	1.0	0.713
0.2	0.985	0.999	0.756	0.999	0.744
0.5	0.994	0.997	0.792	0.994	0.783
1.0	0.996	0.990	0.832	0.977	0.810
2.0	0.997	0.962	0.874	0.912	0.795
5.0	0.967	0.794	0.916	0.562	0.498
10.0	0.610	0.403	0.934	0.095	0.054

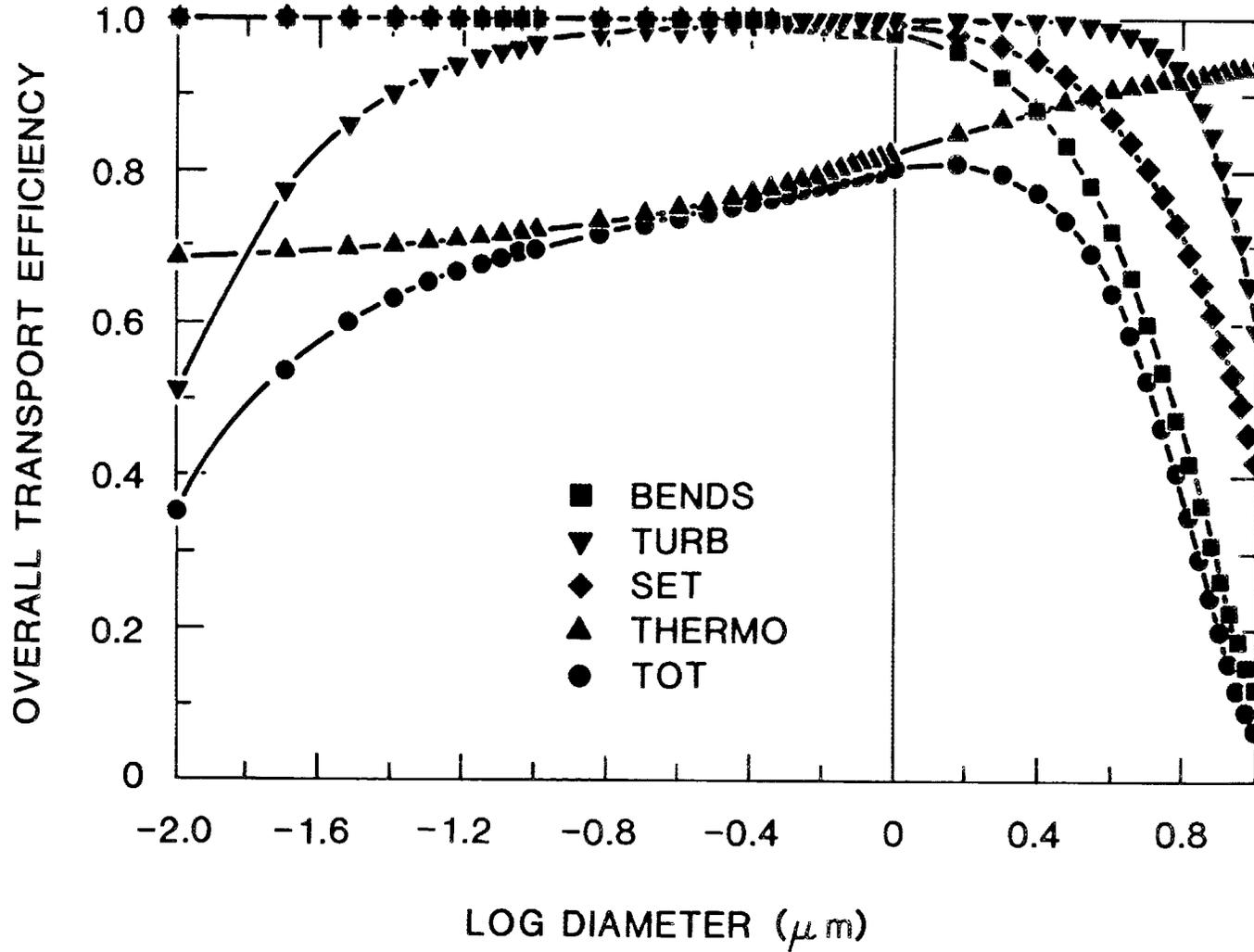


Fig. 1. Overall transport efficiency for TVA Watts Bar Line No. 1.

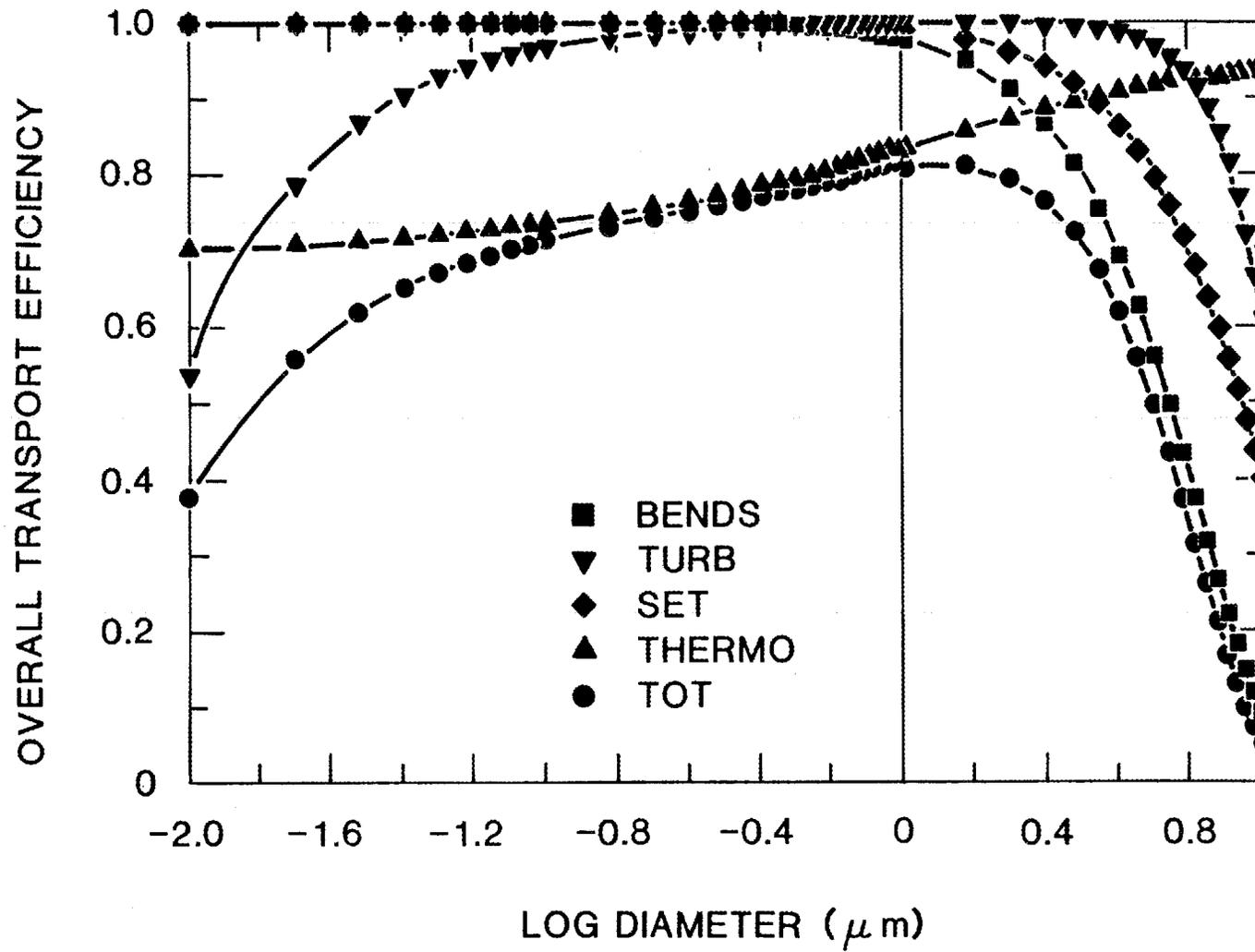


Fig. 2. Overall transport efficiency for TVA Watts Bar Line No. 2.

Tables 4 and 5 and Figs. 1 and 2 illustrate the following important points:

1. In these calculations, the dominant aerosol deposition mechanism for particle sizes between 0.01 and about 2.5 μm diam. (and these sampling line configurations) is thermophoresis. For particle sizes larger than 2.5 μm , aerosol deposition is dominated by deposition in pipe bends. Remember, however, that these calculations were performed for severe accident conditions, when temperature gradients between the flow gas and the sampling line walls would be expected to exist. For sampling under normal operating conditions, temperature gradients would be negligible, as would thermophoresis. However, under accident conditions gas-wall temperature gradients could be even larger than assumed in these calculations, and thermophoresis could be even more important.
2. The calculated results illustrate that, for particle sizes between about 0.02 and 4 μm , line losses are calculated to always be less than 50%. For sizes below and above this range, calculated losses were greater than 50%.
3. Finally, there was little difference in the calculated overall transport efficiencies for the two sampling lines.

Sample calculations of iodine deposition and transport in the Watts Bar sampling lines are complicated by the fact that deposition and desorption would be occurring simultaneously in the lines. The governing mass-balance equations for calculating simultaneous vapor deposition and desorption in sampling lines can be written as follows:^{19,20}

$$\left(\pi \frac{D^2}{4}\right) \frac{\partial C}{\partial t} = -q \frac{\partial C}{\partial x} + \pi DEW - \pi DV_d C, \quad (23)$$

$$\frac{\partial W}{\partial t} = V_d C - EW, \quad (24)$$

where

- C = airborne vapor concentration in line;
 W = vapor mass deposited per unit surface area;
 x = axial distance from pipe inlet;
 D = sampling line diameter;
 V_d = vapor deposition velocity, cm/s;
 E = desorption coefficient, 1/s;
 q = volumetric gas flow rate through line.

These coupled partial differential equations do not have a closed solution; however, an approximate solution can be obtained by making a "control volume" assumption - that is, that the airborne vapor concentration in the pipe is uniform. With this assumption, the equations reduce to

$$V_p \frac{dC}{dt} = EA_s W - (q + V_d A_s) C + M_i, \quad (25)$$

$$\frac{dW}{dt} = V_d C - EW, \quad (26)$$

where

- V_p = pipe volume,
 A_s = pipe surface area,
 M_i = vapor source rate to the pipe.

Analytical solutions of these equations can be obtained and are presented in ref. 20. The equations can be solved for $E_{\text{vap}} = C_{\text{pipe}}/C_i$ (the vapor transport efficiency through the pipe) as a function of time.

Solutions for Eqs. (25) and (26) were obtained for four cases, using representative "low" and "high" values of molecular iodine vapor deposition velocities and desorption coefficients from Tables 1 and 2:

$$\text{CASE 1: } V_d = 0.009 \text{ cm/s, } E = 7 \cdot 10^{-8} \text{ s}^{-1};$$

$$\text{CASE 2: } V_d = 0.2 \text{ cm/s, } E = 7 \cdot 10^{-8} \text{ s}^{-1};$$

$$\text{CASE 1: } V_d = 0.009 \text{ cm/s, } E = 1 \cdot 10^{-5} \text{ s}^{-1};$$

$$\text{CASE 1: } V_d = 0.2 \text{ cm/s, } E = 1 \cdot 10^{-5} \text{ s}^{-1}.$$

Calculations were performed only for sampling line 1-RE-90-112-1 since similar results should be expected for the two lines. These calculations are summarized graphically in Fig. 3 and imply the following:

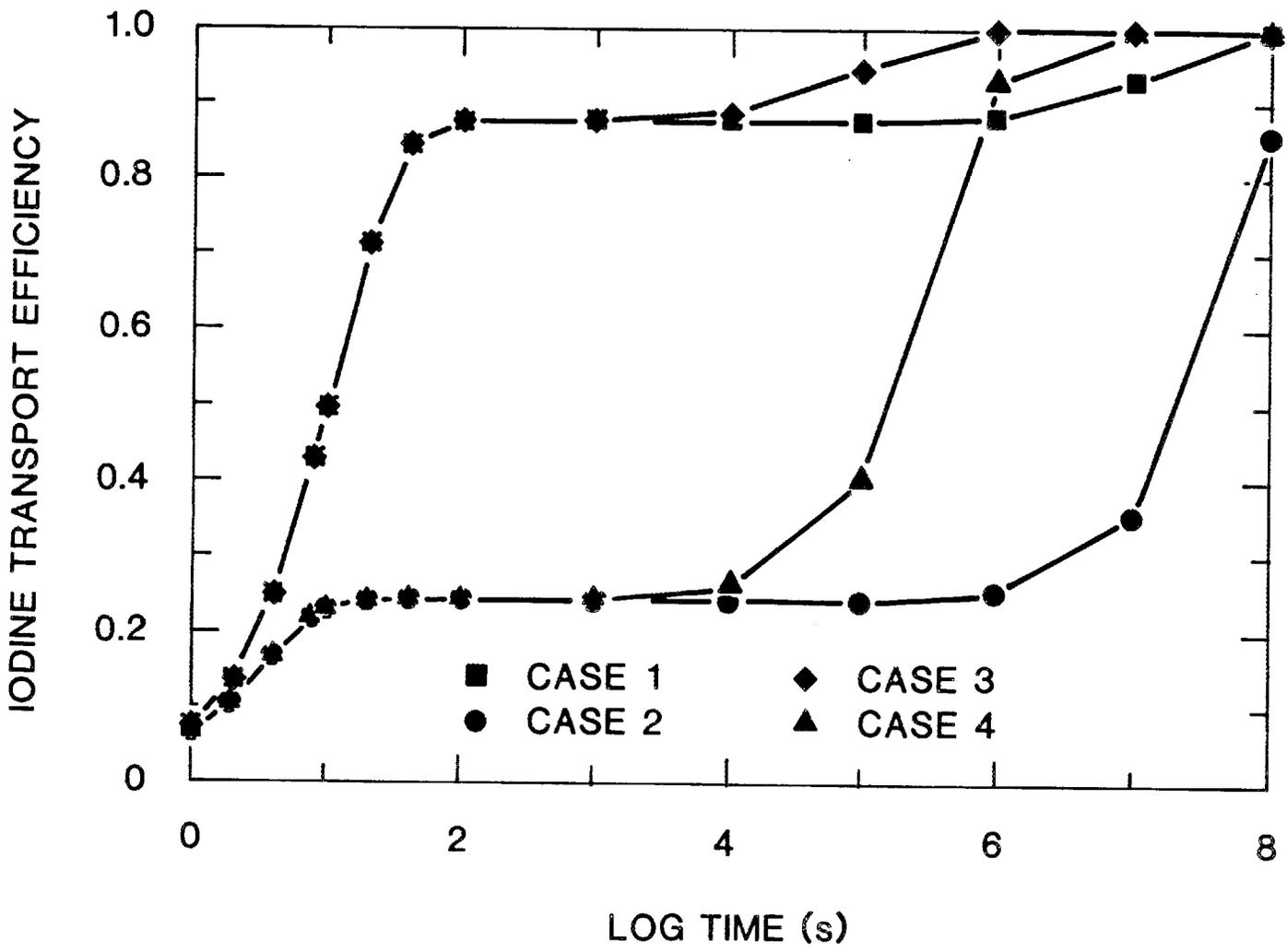


Fig. 3. Iodine deposition calculations for TVA Watts Bar Line No. 1.

1. As should be expected, an increase in the deposition velocity results in a decrease in the calculated transport efficiency of iodine through the sampling line. If molecular iodine deposition velocities are in the range of 0.2 cm/s, it might be expected that only roughly 20% of the inlet iodine would be transported through the line for sampling times less than 10,000 s.

HI deposition velocities at a given temperature are greater than those for I_2 . For example, for a gas temperature of 49°C, Eq. (18) gives an HI deposition velocity of 0.55 cm/s. We might infer from this that the calculated transport efficiency for HI in the sampling line would be less than 10%.

2. Figure 3 shows that modeling desorption affects the iodine transport efficiency for very long sampling times. For Cases 3 and 4, which had the larger values of desorption coefficient, iodine desorption from the surface starts to significantly contribute to vapor transport for sampling times greater than 10,000 s (roughly 3 h). For Cases 1 and 2, which had lower values of desorption coefficient, desorption does not influence iodine transport for times $<10^6$ s (less than 300 h).

4. SUMMARY AND CONCLUSIONS

The major results from this study are the following:

1. Models for calculating aerosol deposition under sampling line conditions are more mature than models for calculating sorption of iodine species. In particular, there is a major need for better-characterized experimental data and modeling of both I_2 and HI deposition and desorption on stainless steel surfaces. Although some data is available for sorption of these vapors, it is uncertain enough that results from vapor deposition calculations are questionable.

2. The aerosol transport results show that thermophoresis dominates the calculated deposition for small particle sizes, while deposition in bends dominates calculated deposition for large sizes. However, these are only sample calculations for one set of conditions; other sample line conditions in other plants might produce different results. The models presented here provide a framework for calculating aerosol deposition for other sampling-line conditions.

Aerosol deposition by diffusiphoresis was not considered; this could be a major source of aerosol deposition under accident conditions in which steam condensation occurs in sampling lines. In addition, thermophoretic deposition, which was significant for the accident conditions used for the calculations in Sect. 3, would not be expected to be important during normal plant operation sampling.

3. An important effect that was not investigated in this report (but will be discussed in detail in the next project report) is the potential influence of water in sampling lines on the transport of iodine species through the lines. Since molecular iodine partition coefficients are not likely to be less than 90, any condensed water in the lines could effectively inhibit the transport of I_2 to the sampling point. This effect may turn out to be more important than iodine sorption onto steel surfaces.

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