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DISPER—AN AEROSOL PARTICLE TRANSPORT CODE

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DISPER—AN AEROSOL PARTICLE TRANSPORT CODE

Douglas C. Hunt

Abstract. The code DISPER determines the aerosol particle-source strength outside an enclosure caused by a release of aerosol particles within the enclosure. The release is assumed to pressurize the enclosure and the airborne particles are carried by the escaping gas into leak paths in the enclosure walls. Here, the particles may be deposited on the leak-path walls or remain entrained and escape from the enclosure.

The report briefly describes the method of problem solution and summarizes the important equations involved. The code input and output are given in detail with comments on parameter interpretation which should assist in more general application of the code as, for example, to problems of reactor melt down with associated fuel or fission-product releases.

INTRODUCTION

The problem solved by the computer code DISPER^{1,2} is the determination of the source strength outside of a leaky enclosure caused by a release of aerosol particles within the enclosure. The release is assumed to pressurize the enclosure and the airborne aerosol particles are carried into leak paths in the enclosure wall by the escaping gas.

CODE DESCRIPTION

DISPER is written in FORTRAN 63 and is designed to run on a CDC Model-3800 machine. A block diagram of the code appears in Figure 1 and the details of the DISPER input and output appear in Tables I and II, respectively. The code operates in two modes: (1) pressure dependent (right hand

branch in Figure 1), and (2) pressure independent (left hand branch in Figure 1). In the pressure dependent mode (I FLAG = 1), an enclosure leakage flow rate (QT) at an enclosure overpressure (DELP) and two pressure response parameters (A and B) must be supplied as input. The pressure response parameters appear in Equation 1 (most equations are written in FORTRAN format using DISPER code names for the variables):

$$R(J) = A * SIG + B \quad (1)$$

In the equation, SIG is equal to a constant times DELP (in DISPER the constant relates to flexure cracks in a rebar strengthened concrete wall) and R(J) is the radius of a leak path. The code uses this input to compute the number of leak paths of radius R(J) required to give QT at the overpressure DELP.

In the pressure independent mode (I FLAG = 2), a number of leak path sets (I) are specified. Each set is defined by a number [XN(J)] of leakage paths of radius R(J). For both modes, once the leakage path model is established, the enclosure overpressure is computed using:

$$\Delta P = \frac{PCON * PATM}{TATM} * TCON * XMT \quad (2)$$

In Equation 2:

$$PCON = \frac{(TCON) - TCON MIN}{TCON MAX - TCON MIN} \quad (3)$$

The remainder of the terms are defined in Table I.

The rate at which particles enter leak paths [RH(J)] is then computed from:

$$RH(J) = \frac{XKG * XMT * ADM * FA}{[1.0 + ATOT * F/AH(J)]} \quad (4)$$

¹ Douglas C. Hunt. *The Possibility of Hazardous Environmental Plutonium Releases*. RFP-1543. Rocky Flats Division, The Dow Chemical Company, Golden, Colorado. April 14, 1971.

² D. C. Hunt. "Restricted Release of Plutonium-Part 2, Theory." *Nuclear Safety*, 12:203. May-June 1971.

FIGURE 1. Block Diagram for Calculations of Free-Release Source Strength.

In Equation 4, ATOT is the total interior enclosure area, AH (J) is the total leak-path entrance area, and the remainder of the terms are defined in Table I.

The leak path gas-flow velocity is then determined from the computed overpressure (Equation 2) and from either

$$VBAR(J) = \frac{R(J) ** 2 * (PO - PATM)}{8 * VISC * XL}, \quad (5)$$

for laminar flow or

$$VBAR(J) = \frac{RGAS * GAMMA * TO}{AMGAS * (GAMMA - 1.0) ** FFF * [1.0 - (PATM/PO) ** (GAMMA - 1.0)/GAMMA]}, \quad (6)$$

for turbulent flow, where TO and PO are the enclosure temperature and pressure, respectively and the remainder of the terms are input quantities described in Table I. Note that FFF (the Fanning Friction Factor) depends on the Reynolds Number and so an iterative process is required to use Equation 6.

Next, the leakage path nondeposition probability is obtained for each particle size and an average nondeposition probability is computed according to:

$$FTBAR(J) = \int_{DPMIN}^{DPMAX} F_{i,j}(\delta) g(\delta) \delta^Y d\delta \quad (7)$$

In Equation 7, $F_{i,j}(\delta)$ is the nondeposition probability for particles of diameter δ in leak paths of radius r_i and having j bends per leak path, $g(\delta) d\delta$ is a log-normal particle distribution, and δ^Y is a weighting function whose exponent is determined by the type of particle transport from the source to the leak-path entrances. The equations used to obtain $F_{i,j}(\delta)$ are too lengthy to detail here, but are given in RFP-1543.³ Five modes of deposition are considered:

1. Gravitational Settling
2. Brownian Diffusion
3. Inertial Impaction
4. Thermal Conduction
5. Turbulence

The first three only are assumed to be effective if the leak-path gas flow is laminar, while only the last two are assumed to act if the flow is turbulent.

The particle source strength outside the enclosure is obtained as the product of RH (J) (Equation 4) and FTBAR (J) (Equation 7).

³Loc. cit.

TABLE I. DISPER Input.

Card No.	Format	Quantity	Units	Description	Nominal Value and Comments
1	5E14.6	XKG	$\frac{\text{atoms}}{\text{cm}^2\text{-sec}}$	Release rate of aerosol atoms.	10^{13} for oxidizing plutonium.
		ADM	cm^2/kg	Area-to-mass ratio of aerosol-producing material.	10^4 for oxidizing plutonium. The product $XKG * ADM * XMT$ (see Card 12) is the release rate of aerosol particles within the enclosure. Once an XMT (see TCON description on Card 4) value is determined, this product may be adjusted to give the desired aerosol release rate.
		F	none	Fraction of airborne particles which strike interior enclosure and adhere.	Unity. Note $(1 - F)$ may be interpreted as an <i>additional entrainment probability</i> so that e.g., setting F to 0.75 means that 25 percent of the particles whose initial trajectories would not take them into a leak-path entrance will actually enter a leak path.
		FA	none	Fraction of released aerosol particles which are airborne.	Obtained in the calculations reported in Footnotes 1 and 2 (Page 1) by assuming all particles of diameter <10 microns are airborne.
		DMBAR	cm	Mass median aerosol-particle diameter.	2×10^{-4} for a plutonium dioxide aerosol. Log-normal particle distribution assumed.

(continued on next page) →

TABLE I. DISPER Input (continued).

Card No.	Format	Quantity	Units	Description	Nominal Value and Comments
2	5E14.6	DPMIN	cm	Minimum aerosol-particle diameter.	10^{-7} for the plutonium dioxide aerosol.
		DPMAX	cm	Maximum aerosol-particle diameter.	10^{-3} for the plutonium dioxide aerosol.
		XLEF	cm	Effective leak-path length for deposition by settling.	For gravitational settling, a path length averaged with respect to the vertical direction must be obtained. For a spherically symmetric distribution of paths of length L, the effective path length is $(\pi/4) * L$.
		XL	cm	Length of a leak path.	
		SIGG	none	Aerosol distribution geometric standard deviation.	2.0 for plutonium dioxide aerosol.
3	5E14.6	THETA	radians	Angle made by a bend in a leak path.	
		RBARC	none	Ratio of leak-path bend radius of curvature to leak-path radius.	About 3.0
		RHOP	g/cm ³	Mass density of aerosol particles.	Maximum value is the aerosol-particle crystal density. Any particle agglomeration will reduce this value.
		Y	none	Exponent of particle diameter used to specify the type of aerosol particle transport which takes particles to the leak-path entrances.	Settling Y = 4 Convection Y = 2 Diffusion Y = 0.5
		BEE	none	Number of bends per leak path.	Usually specify an even number to <i>straighten out</i> bends.
4	5E14.6	E	cm	Roughness of leak paths.	Varies from 0.304 for concrete to 0.00015 for drawn steel tubing.
		ERR	none	Convergence criteria for numerical integration over aerosol-particle diameter distribution.	0.01
		ERR 1	cm/sec	Convergence criteria on smooth leak-path flow velocity (VBARR) calculation.	1.0
		ERR 2	none	Convergence criteria on rough leak-path friction factor calculation for VBARR 1 calculation.	10^{-4}
		TCON	°K/mole	Constant used in computing enclosure temperature from the heat and aerosol producing material. Used in $TO - TATM = TCON * XNPU$, where XNPU is the total number of moles of material involved in the release, TO is the enclosure temperature, and TATM is the temperature outside the enclosure. TCON depends on the release rate and is a calorimetric constant which specifies the fraction of the enclosure material which is heated by the release. Note $XNPU = XMT / 0.239$ where XMT is the number of kilograms of plutonium.	The product $TCON * XNPU$ is the total heat generated in the release divided by the heat capacity of whatever fraction of the enclosure's contents has time to come to thermal equilibrium before significant enclosure leakage occurs. To generally specify the enclosure heat source, determine the total heat generated in the release and the relevant enclosure heat capacity. The equivalent XNPU is then the total heat generated divided by the heat per mole (252 kilocalories/mole for plutonium oxidation) and the equivalent TCON value is the heat per mole divided by the enclosure heat capacity.
5	5E14.6	RHOG	g/cm ³	Density of gas in leak paths.	1.182×10^{-3} at standard temperature or pressure (STP) for air.
		AMGAS	none	Molecular weight of gas in leak paths.	28.97 for STP air.
		GAMMA	none	Specific heat ratio of gas in leak paths.	1.41 for STP air.

TABLE I. DISPER Input (continued).

Card No.	Format	Quantity	Units	Description	Nominal Value and Comments
		TCONMIN	°K/mole	Minimum value of TCON.	
		TCONMAX	°K/mole	Maximum value of TCON.	
6	5E14.6	VISC	poise	Viscosity of gas in leak paths.	1.84×10^{-4} for STP air.
		TATM	°K	Temperature outside enclosure.	
		RGAS	$\frac{\text{ergs}}{\text{mole} \cdot ^\circ\text{K}}$	Molar gas constant of gas in leak paths.	8.32×10^7 for air.
		PATM	$\frac{\text{dynes}}{\text{cm}^2}$	Pressure of gas outside enclosure.	1.013×10^6 for STP air.
7	I2	I FLAG	none	Tells whether pressure dependent or pressure independent problem is to be performed.	Pressure Dependent I FLAG = 1 Pressure Independent I FLAG = 2.
8	2E14.6	A	$\frac{\text{cm}^3}{\text{dyne} \cdot \text{cm}}$	Pressure response parameters in $R(J) = A * \text{SIG} + B$. SIG = constant * enclosure overpressure.	For concrete: $A \sim 6 \times 10^{-12}$ $B \sim 1.4 \times 10^{-3}$
		B	cm		
9	2E14.6	QT	$\frac{\text{cm}^3}{\text{sec}}$ $\frac{\text{dynes}}{\text{cm}^2}$	Gas-flow rate (QT) at an overpressure (DELP) used to compute the number of leak paths in pressure dependent problems.	Cards 8 and 9 are omitted if I FLAG = 2.
10	I3	I	none	Number of sets of leak-path specifications (see Card 11) in pressure independent problems.	Cards 10 and 11 are omitted, if I FLAG = 1.
11	2E14.6	XN (J)	none	The number of leak paths with radius R (J) in a pressure independent calculation.	There will be I number 11 cards, one for each set of XN (J) and R (J) leak-path types desired in a pressure independent calculation.
		R (J)	cm	The radius of Type-J leak paths in a pressure independent calculation.	
12	F12.2	XMT	kg	Amount of aerosol producing material which is oxidized to produce the computed enclosure temperature and overpressure.	As many card 12's as desired may be input. For pressure dependent problems, an answer is generated for the input set and the computed XN and R value for each XMT. For pressure independent problems, an answer is generated for the input set and for each XN (J), R (J) set at each XMT value. The last Card 12 must be 999.
13	5E14.6	-	-	A blank card should follow the last XMT = 999 card. This calls exit for the program.	

Legend

cm = centimeters
g/cm³ = grams per cubic centimeter
kg = kilograms

TABLE II. DISPER Output.

Output Line No.	*Output Quantity	Input Quantity	**Description	Comment
1	KG	XKG	Aerosol release rate.	
2	Al/Ml	ADM	Area-to-mass ratio of source material.	
3	F	F	Particle sticking probability.	
4	FA	FA	Aerosol airborne fraction.	
5	DMBAR	DMBAR	Aerosol mass-mean diameter.	
6	DPMIN	DPMIN	Minimum aerosol-particle size.	
7	DPMAX	DPMAX	Maximum aerosol-particle size.	
8	LEF	XLEF	Effective leak-path length.	
9	L	XL	Leak-path length.	
10	SIGG	SIGG	Aerosol particle geometric standard deviation.	
11	THETA	THETA	Bend angle of leak path.	
12	RBARC	RBARC	Leak-path radius to radius of curvature ratio.	
13	RHOP	RHOP	Aerosol-particle density.	
14	Y	Y	Type of aerosol transport to wall exponent.	
15	Number of bends	BEE	Number of bends per leak path.	
16	E	E	Leak-path roughness.	
17	ERR	ERR	Numerical integration convergence criteria.	
18	ERR 1	ERR 1	Smooth leak-path flow velocity convergence criteria.	
19	ERR 2	ERR 2	Rough leak-path friction factor convergence criteria.	
20	TCON	TCON	Constant determining enclosure temperature.	
21	RHOG	RHOG	Leak-path gas density.	
22	MGAS	MGAS	Molecular weight of leak-path gas.	
23	GAMMA	GAMMA	Specific heat ratio of leak-path gas.	
24	TCONMIN	TCONMIN	Minimum possible TCON value.	
25	TCONMAX	TCONMAX	Maximum possible TCON value.	
26	VISC	VISC	Viscosity of leak-path gas.	
27	TATM	TATM	Temperature outside enclosure.	
28	RGAS	RGAS	Molar gas constant for enclosure gas.	
29	PATM	PATM	Gas pressure outside enclosure.	
30	pressure dependent	I FLAG = 1	Indicates the results of a pressure dependent calculation will follow.	
	pressure independent	I FLAG = 2	Indicates the results of a pressure independent calculation will follow.	Lines 31 through 34 are omitted in pressure independent (I FLAG = 2) calculations.
31	A	A	A and B are the leak-path radius pressure response parameters.	
32	B	B		
33	Q	QT	Input gas-leakage rate at an enclosure overpressure DELP.	
34	DELTA P	DELP		
35	MT	XMT	Amount of aerosol producing material.	
36	N, R	XN (J) R (J)	Number of leak paths and radius of each leak path.	For pressure dependent problems (I FLAG = 1), N, R are computed, while for pressure independent problems the N, R sets are input.

TABLE II. DISPER Output (Continued).

Output Line No.	*Output Quantity	Input Quantity	**Description	Comment
37f.f.	—	—	The code prints the number of integration intervals after each numerical integration attempt until convergence is achieved.	Two sets of integration intervals are printed out (single spaced), one for the numerator and one for the denominator (respectively) in the leak-path nondeposition probability [FTBAR (J)] formula: $\text{FTBAR (J)} = \frac{\int d\delta \varphi(\delta) \delta^Y F_T(\delta)}{\int d\delta \varphi(\delta) \delta^Y}$ where δ is particle diameter, $\varphi(\delta)$ is the particle distribution, and $F_T(\delta)$ is the total nondeposition probability for particles of diameter δ . Units are cm/sec. J goes from 1 to I (the number of input sets). For pressure dependent problems, J is always 1 since a new N, R set is computed for each XMT value. Units are cm ³ /sec. Units are cm ² . Dimensionless flow number. Determines frictional energy losses in fluid flow. Equals 16/Re for laminar flow. Dimensionless. If REO $\geq$ 2500, turbulent-flow velocity recipes are used.
38	VBAR	—	The flow velocity of the gas in the leak paths.	Units are cm/sec.
39	J = number	—	The leak path type number [radius = R (J)] in a set of pressure independent calculations.	J goes from 1 to I (the number of input sets). For pressure dependent problems, J is always 1 since a new N, R set is computed for each XMT value.
40	Q	—	Total flow rate of gas out of the enclosure.	Units are cm ³ /sec.
41	AH	—	Total entrance area of all leak paths.	Units are cm ² .
42	RE	—	Reynolds Number computed for leak-path flow.	Dimensionless flow number.
43	friction factor	—	Proportionality constant between frictional resistive shear to fluid flow and specific fluid kinetic energy.	Determines frictional energy losses in fluid flow. Equals 16/Re for laminar flow. Dimensionless.
44	REO	—	Test value of Reynolds Number computed in rough tube-flow calculations to determine whether laminar or turbulent flow velocity formulas apply.	If REO $\geq$ 2500, turbulent-flow velocity recipes are used.
45	integral 1	—	Denominator integral in formula used to compute average leakage path flow nondeposition probability. See output line 37 description.	
46	integral 2	—	Numerator integral in formula used to compute average leakage path flow nondeposition probability. See output line 37 description.	
47	HFTBAR (J)	—	Average leak path nondeposition probability for leak paths of radius R (J).	
48	S (J)	—	Total free-release source strength associated with the given source and leak path model for Type-J leak paths.	Units are atoms per second. This is the principle item of output.
49	S	—	Total free-release source strength summed over all leak-path types.	This output only appears in pressure independent problems. S is defined as:

$$\sum_J N(J) S(J)$$

*Units same as corresponding input quantities.

**See Table I for detailed description.