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A Computer Code for Calculating the Aerosol Behavior in Closed Vessels

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Table of Contents

Abstract

This report describes the PARDISEKO IV computer code. Its purpose is to calculate the behavior of a polydisperse aerosol system in a closed vessel as a function of the time. The main objective is to describe the extensions added, to compare them with the former version PARDISEKO IIIb, and to explain the input and output.

PARDISEKO IV - Ein Computerprogramm zur Berechnung des Aerosolverhaltens in geschlossenen Behältern

Zusammenfassung

Dieser Bericht beinhaltet eine Beschreibung des Computerprogramms PARDISEKO IV, dessen Aufgabe die Berechnung des zeitlichen Verhaltens eines polydispersen Aerosolsystems in einem geschlossenen Behälter ist. Der Schwerpunkt liegt dabei auf der Beschreibung der Erweiterungen im Vergleich zum Vorgängerprogramm PARDISEKO IIIb sowie auf der detaillierten Beschreibung der Ein- und Ausgabe.

1. Introduction

The PARDISEKO IV computer code describes the behavior of a polydisperse aerosol system in a closed volume. Although it is capable in principle of calculating the behavior of any aerosol system - with the restrictive prerequisites to be enumerated later in this work taken into account - the input and output of the code as well as a number of subprograms have been designed with special regard to the boundary conditions to be expected in a serious hypothetical accident taking place in the containment of a sodium cooled reactor.

The code has been developed from the former PARDISEKO IIIb code [1] whose numerical representation and structure have been taken over to a large extent. The main reason for improving the program had been that a group of experiments could not be verified with the previous code on the basis of input data lying within the range defined by the experiments. This implied that other physical effects not taken into account so far must have an influence on the aerosol behavior. Since in all experiments mentioned here the test vessel accommodated internal heat sources and every such heat source causes natural convection, mostly turning into turbulent flow, it suggested itself to consider the removal effects associated with this convection [2]. Following a number of experiments the statements derived by Sehmel in [3] seemed to be best suited for the computation, and the results obtained with them appeared to be the most reliable ones. These formulae are now available in the PARDISEKO IV code. Besides (as compared to PARDISEKO IIIb) quite a number of changes were made on the input and output which are intended above all to facilitate the comparability of computations with experiments.

2. Model Equation

PARDISEKO IV is essentially based on the same system of differential equations as PARDISEKO IIIb. The latter will be represented here once more just for the sake of completeness and only those details will be explained which deviate from the code described in [1]. Since linear discretization of the particle size range with respect to the logarithm of the mass equivalent radius has been found to be well suited for application in accident computations it has been kept. The model equation used in PARDISEKO IV can thus be put in the formulae

$$\frac{\partial n(r_i, t)}{\partial t} = S(r_i, t) - (\alpha_V(r_i) + \alpha_c(r_i) + \alpha_S(r_i) + \alpha_T(r_i) + \alpha_L(r_i)) \cdot n(r_i,t) + \frac{1}{2} \sum_{K=1}^{N} \sum_{j=1}^{N} K(r_K, r_j) \cdot \beta_{Kj}^{i} \cdot n(r_K, t) \cdot n(r_j, t) - n(r_i, t) \cdot \sum_{j=1}^{N} K(r_i, r_j) \cdot n(r_j, t) \cdot (1-\frac{1}{2}\delta_{ij})$$

$$i = 1, \ldots\ldots, N \qquad (1)$$

with

$$\beta_{Kj}^{i} = \begin{cases} \dfrac{V_{i\pm1} - (V_K + V_j)}{V_{i\pm1} - V_i} & + \text{ for } (V_K + V_j) \in (V_i, V_{i+1}) \\ & - \text{ for } (V_K + V_j) \in (V_{i-1}, V_i) \\ 0 & \text{in all other cases} \end{cases} \qquad (2)$$

and

$$\alpha_V(r) = \alpha_D(r) + \alpha_{VT}(r) = \left(\frac{k \cdot T \cdot B(r)}{\delta_D} + v_{VT}(r)\right) \cdot \frac{A_D}{V} \qquad (3)$$

$$\alpha_C(r) = \alpha_D(r) + \alpha_{CT}(r)$$

$$= \left(\frac{k \cdot T \cdot B(r)}{\delta_D} + v_{CT}(r)\right) \cdot \frac{A_C}{V} \qquad (4)$$

$$\alpha_S(r) = \frac{4\pi}{3} r^3 \cdot \rho \cdot g \cdot B(r) \cdot C_T(r) \cdot \frac{A_S}{V} \qquad (5)$$

$$\alpha_T(r) = \frac{9\pi\,\eta^2 r}{\rho_g} \cdot \frac{1}{1 + 3C_m \cdot Kn} \cdot \frac{\frac{k_g}{k_s} + C_t \cdot Kn}{1 + 2 \cdot \frac{k_g}{k_s} + 2C_t \cdot Kn}$$

$$\frac{B(r)}{\delta_T \cdot V \cdot T} \cdot \sum_{k=1}^{NT} \Delta T_k \cdot A_{T_k} \qquad (6)$$

The coefficients α_V, α_C, α_S and α_T are the coefficients of removal on the vertical walls, on the ceiling, on the bottom surface due to sedimentation, and on various wall zones as a result of thermophoresis. The coefficient α_L constitutes any leakage coefficient which, in principle, may depend also on the particle size. The equations governing the removal coefficients differ from those indicated in [1] as regards the following items:

(a) The new code makes a distinction between particle removal on vertical surfaces (index V) and on horizontal surfaces facing down (index C). In PARDISEKO IIIb removal by diffusion had been assumed to occur at the same rate on both surfaces.

(b) Regarding the vertical walls a second term is added to the previously considered removal by diffusion ($\alpha_D(r)$); it describes the transport to the wall due to turbulence. According to [4] this transport is expressed by:

$$v_{VT}(r) = u^*/\mathrm{Int}\ (r) \qquad (7)$$

It should be noted here that the definition of the sign of the diffusive resistance integral Int(r) is opposed to that given in [4].

(c) By analogy, another term, although different from (7), is added when dealing with the ceiling surfaces

$$v_{CT}(r) = \frac{v_{sed}(r)}{\exp(v_{sed}(r) \cdot \text{Int}(r)/u^*) - 1} \qquad (8)$$

(d) Since sedimentation towards the bottom is enhanced by turbulent flow, the normal rate of sedimentation

$$v_{sed}(r) = \frac{4\pi}{3} r^3 \cdot \rho \cdot g \cdot B(r) \qquad (9)$$

must be replaced by

$$v_{ST}(r) = v_{sed}(r) \cdot C_T(r) \qquad (10)$$

with

$$C_T(r) = (1-\exp(-v_{sed}(r) \cdot \text{Int}(r)/u^*))^{-1} \qquad (11)$$

(e) As different temperature gradients may prevail across different parts of the overall surface, the possibility was provided of taking into account via surfaces of different sizes the respective temperature gradients as a function of time. Therefore, $(T-T_W) \cdot A_T$ from [1] must be substituted by the sum

$$\sum_{k=1}^{NT} \Delta T_k \cdot A_{T_k}.$$

To describe the probability of coagulation K(r, r') an expression largely resembling that in [1] is used:

$$K(r,r') = 4\pi kTf\,(B(r) + B(r'))\,(r + r') + \varepsilon(r,r')\,\frac{4\pi}{3}\,f\,g$$

$$\left|r^3 B\,(r) - r'^3 B\,(r')\right| \cdot \pi \cdot (r + r')^2 \qquad (12)$$

Using the formula for the mobility of the particles according to [5] and combining it with [6] we obtain

$$B(r) = \frac{1}{\kappa 6\pi\eta r}\,(1 + AKn + QKn\,C^{-b/Kn}) \qquad (13)$$

Unlike in [1], the expression indicated in [7] will always be used to describe the probability of collision.

$$\varepsilon(r,\,r') = \frac{1}{2}\,\frac{(r'/r)^2}{(1 + r'/r)^2}\,,\quad r' < r \qquad (14)$$

This formula takes into account the hydrodynamic deflection of the approaching particles by the carrier gas flow around the settling particles. This implies an effective reduction of the cross section ($\pi(r+r')^2$) which would be obtained under conditions of exclusively geometrical interception and straight line fall. The prerequisites of Eq. (14) are, on the one hand, Stokesian flow around the particles, which, however, can be assumed to prevail for the Reynolds numbers applicable to the particles to be investigated with the help of PARDISEKO, and $r' \ll r$, on the other hand. As shown by the calculations by Davis [8] quoted in [7], Eq. (14) can nevertheless be extrapolated rather well up to the range $r' \approx r$. The assumption of Stokesian flow is valid up to particle radii of approx. 30 µm (corresponding to a Reynolds number of 0.4); for larger particles conversion into potential flow must be expected which implies a higher probability of capture.

This is true in particular for the capture of particles similar in size. However, since such large-sized particles have a relatively short residence time in the containment and, in addition, Eq. (14) underestimates the probability of capture for these particles so that the residence time would be even further shortened if the expression for this flow regime were used, application of Eq. (14) to all particle sizes should be considered as being on the safe side and consequently justified.

Values of $\varepsilon(r, r')$ which are constant over the whole range of particle sizes and had previously been used as parameters in certain cases are no longer permissible because they are not meaningful physically and give results which likewise make no sense. However, the computations performed with $\varepsilon(r, r') = 0$ should be considered in any case as being on the safe side which is true for all design calculations made earlier (e.g., [9]).

A separate computer code is necessary to calculate the resistance integrals Int(r) in Eqs. (7), (8), (11) because they can be calculated only numerically. Since, similar to [1], a fixed division of particle size classes is used in PARDISEKO IV too, these integrals can be calculated separate from the PARDISEKO computation proper for each particle size and stored on a file. This file can be reused in each new computation based on the same division of particle sizes (see also the description of the input).

3. Numerical Method of Solution

(a) Selection of the Independent Variables

Since the particle sizes encountered mostly extend over several orders of magnitude and log-normal distributions are used in the majority of cases to describe source size

distributions, the logarithm of the mass equivalent radius is still being used as an independent variable. Although this is by no means necessary on fundamental grounds, it seems reasonable to adhere to this choice because it represents best the whole range of particle sizes.

(b) Selection of the Size Range

As already mentioned a rigid division into size categories is defined at the beginning of each computation which is determined by the three input parameters RMIN and RMAX (minimum and maximum particle radii), and K2 (number of particle categories). The parameters RMIN and RMAX must be selected in such a way that the whole particles spectrum to be treated in the computation lies within the range defined by them. The parameter K2 should have a value greater than or equal to approx. 80, as shown by parameter computations relying on the similarly structured computer code ABC-3 [10] since otherwise the particle size distribution can no longer be approximated accurately enough which leads to a systematic deviation from the reference values. Reference values are understood to mean values which are obtained for a very great number (in the approximate limit cases ∞) and hence a correspondingly good approximation to the continuous spectrum.

Besides, the rules defined in [1] for selecting the size range continue to apply.

(c) Integration with respect to Time

As already described in [1], the N-dimensional differential equation system (Eq. (1)) is integrated by means of a self-controlled Euler-Canchy method. The stability of the method is ensured by the fact that the relative deviation of the results after one full and two half time steps must not exceed a given predefined value. In case this value is

exceeded the next time step is reduced accordingly; in case of deficiency the time step is enhanced. As experience has shown that the sequences to be computed with PARDISEKO are not very transient ones (which means that above all the time constants for the changes of particle source functions are great compared with the time steps) integration is possible by such an explicit method. An additional (logical "and") criterion applied for calculating the time steps while the particle source function is different from zero, is the time which is characteristic of changes of this function. Numerical instabilities which might still occur due to a selection of a too large accuracy parameter can be easily recognized from violations of the mass balance printed for each output cycle and from variations of the results not conditioned by physical events. In such a case the computation must be repeated with the smaller value for the accuracy parameter (EPS).

4. Code Input

The input for PARDISEKO is read from four units, namely:

(a) Unit 5

Data input by cards (LRECL = 80, RECFM = FB)
The whole input of this unit, except for the field TEXT, is by means of a list controlled input, i.e., the individual values must be separated from each other by a blank or a comma. It is intended that these cards are given numbers at the end and to use only the first 72 columns for data transfer. To guarantee that these numbers are bypassed the variable NDUMMY is read in addition at the end of each card which has no other meaning whatsoever. If non-numbered record (cards) are used for input, this variable must be deleted from the input list.

In the following listing the input variables will be described in the sequence they must be read in. The data types are abbreviated as follows:

R4: Real 4
I4: Integer 4
L4: Logical 4
Cn: Character n (n = any integral number)

Card No.	Variable	Type	Explanation
1 + 2	TEXT	C72	Any text for identifying the computation
3	K2	I4	Number of grid points for particle size distribution
	NWRITE(1)	I4	Number of time steps after which a small printout is produced
	NWRITE(2)	I4	Number of time steps after which a large printout is produced containing particle size distribution
	NTHERM	I4	Number (up to 5) of surfaces at different temperature levels for thermophoretic removal (see Eq. (6))
	LNOLK	L4	Taking into account leakage (=.TRUE.)
	LNOTE	L4	Taking into account thermophoresis (=.TRUE.)
	NCARD	I4	Number of time steps after which output on Plot-dataset (unit 1) takes place
	CPUZT	R4	Computer time [min.] after which computation is to be discontinued; should, if meaningful, be identical to the value on the job card
	RESTRT	L4	Computation constitutes a restart job (=.TRUE.)
	ZWCOMP	L4	Computation relates to a downstream compartment with leakage from an upstream compartment as particle source (=.TRUE.)
	GRAVK	L4	Taking into account gravitational coagulation according to Eq. (14) (=.TRUE)
	FUKS	L4	Taking into account the Fucks interpolation formula for the probability of coagulation (=.TRUE.)
4	VOL	R4	Containment volume [cm^3]
	FSED	R4	Bottom surface for removal through sedimentation [cm^2]
	FDIFF	R4	Vertical surface [cm^2]
			Remark: If removal through turbulence is not taken into account, the total surface can be entered here. In this case FCEIL must be set zero.
	FCEIL	R4	Horizontal surface facing down [cm^2]
	FTHERM(K) K = 1, NTHERM	R4	Surfaces for thermophoretic removal according to Eq. (6) [cm^2]
5	TT	R4	Containment temperature [K]
	P	R4	Containment pressure [bar]
	GASIN	C10	Nature of gas in the containment; possible gases are air, nitrogen and argon. Information serves to calculate the gas viscosity.

Card No.	Variable	Type	Explanation
6	DELD	R4	Diffusion boundary layer δ_D (Eq. (4)) [cm]
	DELT	R4	Thermophoretic boundary layer δ_T (Eq. (6)) [cm]
	CONS	R4	Ratio of thermal conductivities of particles and gas
	FORM	R4	Dynamic shape factor (Eq. (12))
	FORMC	R4	Coagulation shape factor f (Eq. (11))
7	UMLU	R4	Performance of recirculating air filter [m^3/s]
	UMLUZT	R4	Startup time of recirculating air filter [h]
	UMLEFF	R4	Removal efficiency of recirculating air filter [%]
8	RMIN	R4	Minimum particle radius [µm]
	RMAX	R4	Maximum particle radius [µm]
	TIME	R4	Total problem time [h]
	SZEIT	R4	Startup time [s]
	EPS	R4	Accuracy parameter (see Chapter 3c)
	DT	R4	Initial time step [s]
	ZLIM	R4	Lower level for number distribution [P/cm^3]
	GLIM	R4	Lower level for mass distribution [mg/m^3]
9	NVGL	I4	Number of points in time (up to 10) when output of particle distribution is to be produced in addition to printout as defined with NWRITE (2); besides optional output on a file for plotting of size distribution
10 to 10 + NVGL	TVGL(K), K =1,NVGL	R4	Points in time for output of size distribution [min]
11 + NVGL	K2T	I4	Number of grid points of the functions TE
$= N_1$	DELTT	R4	Time increment of the functions TE, the latter to be read in as a table equidistant in terms of time
$N_1 + 1$ to $N_1+1+K2T$ $= N_2$	TE(K,I), K=1, NTHERM, I=1,K2T	R4	Temperature differences above the individual surface areas normalized to gas temperature (values at a given point in time on one card)
$N_2 + 1$	NTURB	I4	Number of points in time when new (related to other new values of u*) removal factors must be read in
	FAKTVT	R4	Factor by which the turbulent removal coefficients on the vertical walls must be corrected (experimental: about 300)
$N_2 + 2$	TTUBB(K), K=1,NTURB	R4	Points in time when new turbulent removal coefficients must be read in [s]
$N_2 + 3$	NPHASE	I4	Number of release phases of the aerosol source

Card No.	Variable	Type	Explanation
	NUKLID	I4	Number of the nuclides for which balances should be established. Now NPHASE (NUKLID+2) cards defining the aerosol source will be indicated. The sequence of the cards is identical for each release phase so that it will suffice to describe one release phase (no. K). For the sake of simplicity separate card counting will be started at this point.
1	SRATE(1,K)	R4	Source rate for release mode 1 in phase K [g] or [g/s] (see KONTIN (1,K))
	FAKTOR	R4	Factor by which SRATE (1,K) is to be multiplied; can be used as a conversion factor in case that the source rate is not given in a CGS unit
	KONTIN(1,K)	L4	SRATE (1,K) is a rate (=.TRUE.) SRATE (1,K) is an instantaneous source (=.FALSE.)
	MESSI(1,K)	L4	For mode 1 a measured mass distribution still to be read in will be used as source particle size distribution (=.TRUE.) The two following parameters will then constitute a dummy input
	RG(1,K)	R4	Mean geometric radius of the number distribution of the source particles [µm]
	SIGL(1,K)	R4	Logarithm of the geometric standard deviation of the source particle distribution. From the two parameters RG(1,K) and SIGL(1,K) the size distribution is calculated assuming a log-normal distribution
	RHOQ(1,K)	R4	Material density of the source particles [g/cm^3]
2	SRATE(2,K)	R4	Meaning as above, but applicable to the second release mode in phase K
	FAKTOR	R4	
	KONTIN(2,K)	L4	
	MESSI(2,K)	L4	
	RG(2,K)	R4	
	SIGL(2,K)	R4	
	RHOG(2,K)	R4	
	TQ(K + 1)	R4	Point in time until which the release phase K is to last; the end of the preceding release phase is taken as the time of commencement. For the first release phase the starting time of computation (SZEIT) automatically applies Remark: If instantaneous sources are used, the time difference TQ(K+1)-TQ(K), despite its insignificance in principle, should not be chosen too small because otherwise there is the danger that this aerosol source is not found but skipped through a time step greater than TQ(K+1)-TQ(K)

Card No.	Variable	Type	Explanation
3	NAMNUC(I)	C8	Name of the nuclide I; serves solely the purpose of nuclide identification Remark: The sequence and type of nuclides must be the same in each release.
	AKTIVI (1,K,I)	R4	Fraction of nuclide I in mode 1 in the release phase K, expressed in mass fractions
to	AKTIVI (2,K,I)	R4	Item for mode 2
NUKLID+2	I=1,NUKLID		
			The following cards define the time dependent rate of leakage from the containment; they are read in the TLEAKI subprogram (again count will restart here)
1	N	I4	Number of grid points of the leakage function; a linear interpolation is performed between the individual check points in the course of computation. In case N = 1 a constant leakage is assumed from time TL(1) onward, corresponding to the value RL(1). Even if the parameter LNOLK is set at .FALSE.,the cards must be available as dummy input for the leakage function.
2	TL(K),	R4	Time grid point of the leakage function [s]
	RL(K)	R4	Leakage rate at time TL(K) [vol.%/d]
to N	K=1, N		
			This input of the leakage function puts an end to the input, which is required in any case. Optionally, input of a measured mass distribution is still feasible as a source particle size distribution for each release mode. Input in the MWERT subroutine
1	NPH	I4	Index of release phase to which the input is to apply
	NMODE	I4	Index of release mode (1 or 2) to which the input is to apply With these two parameters the code examines whether the input is consistent with the statement of MESSI (NMODE,NPH) = .TRUE. If not, the computational run is discontinued by printout of an error message.
	WIEDER	L4	The distribution read in last is to be reused for the release mode defined by NPH and NMODE (=.TRUE.). In this case, a further input for this mode can be dispensed with.
2	N	I4	Number of grid points of the measured mass distribution
3	D(K)	R4	Diameter of the particles [µm]

Card No.	Variable	Type	Explanation
to N+2	BEL(K), K=1,N	R4	Mass of the particles with the diameter D(K), expressed in any unit (although, obviously, identical for all values of K). By spline interpolation a function is established to connect the grid points D(K) and BEL(K) in order to obtain grid points at the places defined by the parameters RMIN, RMAX and K2. Such a measured size distribution can be displayed twice for each release phase (i.e., up to 2 x NPHASE at the maximum). The input option is to facilitate above all the comparison with experiments.

All the following inputs are likewise but optional and required under defined conditions only. All data are read in unformatted which means that the individual records are defined by the WRITE statements making up the data file.

(b) Unit 3

Input of the correction factors taking into account removal by turbulence.

These data are included in the members of a partitioned data set (PDS), each member representing the data set belonging to a specific value of friction velocity u*. The points in time at which a new member each must be read in are determined by the input parameters TTURB(K), K = 1, NTURB. They are processed sequentially, e.g., a new member is read in every time the next point in time is attained. As information an appropriate message is printed out. However, the last point in time read in TTURB(NTURB) defines the end of removal by turbulence. If no data file is defined under unit 3 (i.e., a zero file is set for unit 3) reading in is suppressed within the code and no removal by turbulence is taken into account. A message to this effect is printed out. In this case, the statements with respect to the times TTURB are meaningless.

The following list shows the input variables arranged by sequence; they are identical for each member. Different members must be indicated in the desired sequence using the same unit number, but with the FORTRAN sequence number incremented by 1 each.

Record No.	Variable	Type	Explanation
1	USTERN	R4	Turbulent friction velocity [cm/s]
2 to K2+1	CORR(K), K = 1, K2	R4	Turbulence correction coefficient to take into account sedimentation ($C_T(r)$ in Eq. (5))
K2+2 to 2·K2+2	VVERTT(K) K = 1, K2	R4	Rate of turbulent removal towards vertical walls [cm/s] ($v_{VT}(r)$ in Eq. (3))
2·K2+2 to 3·K2+3	VCEILO(K), K = 1, K2	R4	Rate of turbulent removal towards the ceilings divided by the material density of the particles [$cm^4/s \cdot g$] ($v_{CT}(r)/\rho$ in Eq. (4))

(c) Unit 2

Read-in of leakage of an upstream compartment as the source of aerosols. The data file to be read must be established in a preceding PARDISEKO run (see output description for UNIT 8). Since the time steps are computed within the code, the PARDISEKO run to be established and the PARDISEKO run to be read are mostly not synchronous. Therefore, the current value for and size class is determined from the established size and time dependent leak rates by linear interpolation between the individual time grid points. With the exception of the first record, the entire data file is read in the READL subroutine

Record No.	Variable	Type	Explanation
1	VOL 1	R4	Volume of the upstream compartment [cm^3]
	NUKLID	I4	Number of the nuclides for which a balance has been established in the preceding compartment and for which a balance shall be established in the present run as well. This means overwriting of the input made before via unit 5.
	SOUTIM	R4	Duration of the aerosol source in the preceding computation [s]
	NAMNUC(K), K=1,NUKLID	C8	Names of the nuclides for which a balance shall be established
2 and ff.	ZEIT2	R4	Point in time of leak rate [s]
	RHO2	R4	Current material density of the particles flowing through the leak at that point in time [g/cm^3]
	RLPV2	R4	Integral leak rate at that point in time [$mg/m^3 \cdot s$]
	AKTIV2(K), K=1,NUKLID		Mass fraction of the individual nuclides in RLPV2
	Q2(K), K=1, K2		Leak rate of each particle size class at the time ZEIT2 [$1/cm^3 \cdot s$]

(d) Unit 19

Data file for restarting a run interrupted because the CPU time input (CPUZT) has been attained.

If this data file is to be read, the RESTRT parameter must be set to .TRUE.. This data file is established at the end of each run via unit 20. As this data file can be used only within the code, a detailed description of the individual variables can be dispensed with. It is possible by this restart option to break down each run into any number of single runs.

5. Code Output

The output by PARDISEKO IV is given to 5 units in all.

(a) Unit 6

Output printed in the usual way
This output is self-explanatory. It comprises as the first element the printout of all input variables, as the second

element a number of control printouts, and as the third element the printout of the results of computation grouped by the number of time steps defined by the input parameters NWRITE(1) and NWRITE(2). The printout following NWRITE(2) (large printout) differs from that following NWRITE(1) by the additional printout of the particle size distribution. In any case, a large printout is produced at the end of each computation.

(b) Unit 8

Output of the leak rate
This output corresponds to the input via unit 2 because it exclusively serves the purpose of being reread in a subsequent run. Thus, multi-compartment runs are feasible on the assumption that the individual compartments are interconnected by defined volume flows. The division into size categories defined by the parameters RMIN, RMAX and K2 must be identical for all compartments. For this reason, the listing below of outputs is identical in layout to the input list for unit 2 described in the preceding chapter.

Record No.	Variable	Type	Explanation
1	VOL	R4	Volume of the compartment [cm^3]
	NUKLID	I4	Number of the nuclides for which a balance should be established
	TQ(NPHASE+1)	R4	End point in time of aerosol source [s]
	NAMNUC(K), K = 1, NUKLID	C8	Names of the nuclides for which a balance should be established
2 and ff.	SZEIT	R4	Current point in time [s]
	RHOB	R4	Current material density of the aerosol particles [g/cm^3]
	RLPV	R4	Integral leak rate [mg/m^3s]
	AKTIV(K), K=1,NUKLID	R4	Present mass fractions of the individual nuclides
	ZLEAK(K), K=1, K2	R4	Leak rate of each individual size category [$1/cm^3s$] Since this record is written for each time step, the related data file may take a considerable volume. This should be considered when allocating the data file.

(c) Unit 20

Data file produced in order to enable restarting of a run discontinued because of attainment of the defined computer time (see also the input description for unit 19).

Remark on this restart option:

All the other data files which can be generated by the program such as the plot data files (unit 1 and unit 9) and the leakage data file (unit 8) have been designed in a way that by use of different data files, each generated by the restarted runs, these data files can be treated as one single data file by means of simple concatenation (evidently to be performed in the proper sequence).

(d) Unit 1

Data file to provide plots of different parameters as a function of the time

One record each of this data file is written after execution of NCARD time steps. Each record consists of 12 real* variables, the latest two values of them being dummy variables. This data structure was selected to achieve compatibility with the plot files established by the NAUAMOD4 code [11]. The following list gives the sequence of the variables which are contained in an identical manner in each record.

Record No.	Variable	Type	Explanation
1 and ff.	SZEIT	R4	Point in time [s]
	CON	R4	Particle number concentration [$1/cm^3$]
	SGEW	R4	Mass concentration of airborne substances [g/cm^3]
	R50M	R4	50% value of mass distribution [cm]
	DEPVER	R4	Cumulative surface loading on vertical surfaces [g/cm^2]
	DEPCEI	R4	" " " on ceiling surfaces [g/cm^2]
	DEPSED	R4	" " " on bottom surfaces [g/cm^2]
	SIGLB	R4	Geometric standard deviation of the current size distribution
	DEPTHD		Mean surface density on the thermophoretic removal surfaces [g/cm^2]
	SUMLK	R4	Cumulative leakage from the containment [g]
	DUMMY1	R4	Dummy variable, no significance
	DUMMY2	R4	

(e) Unit 9

Data file to provide plots of the aerosol size distribution At the points in time defined by TVGL(K), K = 1, NVGL (strictly speaking at the first point in time in the program sequence following these points in time) this data file is written on by the ordinate values required for plotting the size distributions. Since the size discretization remains unchanged during the computation, the values of the abscissa are written but once on a record at the beginning.

Record No.	Variable	Type	Explanation
1	K2	I4	Number of grid points of the size discretization
	X(K),K=1, K2	R4	Natural logarithm of particle radius R(K), K = 1, K2
	R(K), K=1, K2	R4	Mass equivalent radius of particle size class 1 to K2
2 and ff.	MZEIT	R4	Point in time [min]
	SGEW	R4	Mass concentration [mg/m^3]
	DVR(K), K=1, K2	R4	Sum distribution normalized to 100% related to aerosol mass
	GEW(K), K=1, K2	R4	Aerosol mass distribution [mg/m^3]

6. Summary and Discussion

PARDISEKO IV constitutes a program allowing to calculate the behavior of the aerosol type activity in any accident occurring in sodium cooled breeder reactors or, if special effects are left out of consideration such as steam condensation on the particles, permitting in more general terms to calculate the aerosol behavior in closed vessels. No restrictions must be imposed regarding the aerosol size distribution admitted and the release scenarios.

The major restricting assumptions underlying PARDISEKO IV are:

(a) The residence probability of particles of any size does not depend on the location in the containment (principle of homogeneous mixing).

This assumption relies on the presence of a mixing flow which can always be expected in a hypothetical accident because of the strong heat sources available.

(b) The properties of the particles can be described by one single parameter, in case of PARDISEKO IV by the mass equivalent radius.

This is by no means true a priori. For instance, it can be easily imagined that two particles, although having the same mass, possess different hydrodynamic properties on account of their completely different geometric shapes. This also implies that size distributions measured, e.g., for the aerodynamic radius, cannot be automatically converted to size distributions according to the mass equivalent radius. The transformation of the particle radii measured by different measuring techniques is performed using so-called shape factors which are defined in [12] (unfortunately not very consistently in some respects). The shape factors can be determined in practical application from measured mean values of specific particle properties for particle categories the classification of which is in turn determined by the properties of the measuring instrument. Therefore, the shape factors may not only differ for differing aerosols but they depend, moreover, on the particle sizes, size being understood to mean here a value correlated to the particle mass. In PARDISEKO IV, as in the former codes, only the input of the shape factors averaged over the entire size distribution is envisaged for the sake of simplicity. If this code is used for accident computations, the latter must be likewise varied over the range which is physically feasible so that their influence can be estimated. If appropriate data

on size dependent shape factors are available, they can be introduced in PARDISEKO IV after only minor modifications have been made to the code.

Regarding the formulae used to describe turbulent removal their semi-empirical nature must be taken into account. It is known in addition that turbulent flows cannot yet be computed for complicated geometries but only for a simple radially symmetric geometry [13]. The formulae implemented in PARDISEKO IV are therefore primarily intended for comparing computations with experiments because the test vessels in general are almost radially symmetric and thus the rate of variation u* can be determined approximately. At most, rough estimates on the influence of turbulent removal can be made for the accident computations proper. This is done to possess some measure of the additional safety margin available if turbulent removal is neglected.

7. Literature

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List of Symbols Used

r_i	: mass equivalent radius of the particles of category i	[µm]
V_i	: volume of particles of category i	[μm^3]
$n(r_i,t)$	: number of particles of category i at time t	[P/cm^3]
$S(r_i,t)$	: aerosol source	[$P/cm^3 \cdot s$]
N	: number of particle categories	
k	: Boltzmann constant	[erg/K]
T	: gas temperature	[K]
g	: gravitational acceleration	[cm/s^2]
η	: viscosity of carrier gas	[poise]
ρ_g	: density of carrier gas	[g/cm^2]
δ_D	: diffusion boundary layer	[cm]
δ_T	: thermophoretic boundary layer	[cm]
Kn	: Knudsen number λ/r with λ being the mean free path of the carrier gas	
ρ	: material density of the aerosol particle	[g/cm^3]
k_g,k_s	: thermal conductivity of the carrier gas and particles, respectively	[mW/cm·K]
C_t,C_m	: constants related to the kind of heat transfer and momentum transfer, respectively, between the carrier gas and the particle surface (see [6])	
A,Q,b	: empirical values for slip-flow correction according to Millikan [7] in connection with [8]	
f,$\mathscr{e}$	: shape factors of coagulation and mobility, respectively (see [2])	
V	: volume of the containment	[cm^3]
A_D	: surface of diffusive removal, in general the total internal surface area of the containment	[cm^2]
A_S	: bottom area of the containment	[cm^2]
A_{T_k}	: surface for thermophoretic removal, no. k	[cm^2]
ΔT_k	$= T - T_{W_k}$: temperature difference across the surface, no. k	[K]
Int(r)	: diffusive resistance integral associated with radius r (depends in addition on u*, on the angle of the removal surface with respect to gravity, and on a number of material variables)	
u*	: turbulent friction velocity	[cm/s]