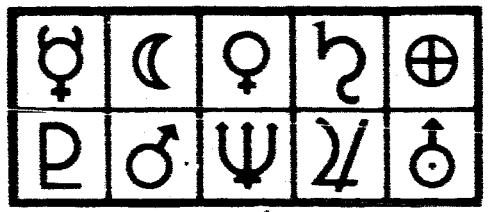SC-RR-66-421

July 1966

PLANETARY QUARANTINE

AN ASSEMBLY CONTAMINATION MODEL

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Planetary Quarantine Department
Sandia Laboratory, Albuquerque, New Mexico

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ABSTRACT

In this report, a model of biological contamination of a structure during assembly is developed. This model is stochastic in nature; treating both the amount of contamination and its surface distribution on the structure as random variables.

It is hoped that by using this model and subsequent refinements of it, one may be able to specify conditions under which the level of biological contamination of a structure may be predicted statistically with any desired degree of confidence.

Project No. 340.229.00

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INTRODUCTION

In this report, a stochastic model of contamination of structures during assembly is developed. This model is based on an underlying deterministic model developed by J. D. Johnson, formerly of Jet Propulsion Laboratories who kindly provided us with much information about his model and the problem in general.

In the way of a disclaimer, the model developed here is not intended to be, nor is it, a model guaranteed to handle all of the difficulties which arise in the problem of structural contamination. Rather, it is a model whose main virtues are the recognition that the problem is stochastic in nature and the inclusion of certain structural parameters which may be useful in engineering design.

In the first section of this report, the problem of contamination of a structure during assembly is discussed and analyzed from a point of view that will hopefully allow the mathematical model to be viewed intuitively. A rigorous abstract mathematical model is developed in the second section. This is done in order to present a precise axiomatic framework in which the problem may be further analyzed. There are a number of related areas in need of additional study, and we have attempted to point these out in the sequel. The third section treats some of these in detail.

Acknowledgement is due D. P. Peterson, M. S. Tierney and J. M. Worrell of Sandia Laboratory for their philosophical and technical assistance.

SECTION I - The Problem of Contamination

of a Structure During Assembly

References $\begin{bmatrix} 1 \end{bmatrix}$, $\begin{bmatrix} 2 \end{bmatrix}$, $\begin{bmatrix} 3 \end{bmatrix}$, give some indication of the current concern about the biological contamination of space vehicles which are to come in contact with other planets.

It is frequently proposed, that in order to obtain a sterile vehicle prior to launching, one first needs to obtain a completed structure whose level of microorganic contamination is less than some prescribed bound. If the prescribed bound is achieved in the completed structure, it is assumed to be possible to biologically sterilize the structure in a "reasonable" amount of time just prior to its use by subjecting it to heat of a "reasonable" temperature consistent with the ability of the structure's components to withstand heat.

J. D. Johnson of Jet Propulsion Laboratories has developed a deterministic model (see $\begin{bmatrix} 4 \end{bmatrix}$) in which the contamination is analyzed at each stage of assembly of the structure in order to predict the contamination remaining on the completed structure. In this model, he considers two types of contamination: internal and external. In a rough way, the physical distinction between these two concepts is that between microorganisms locked tightly into some inaccessible space (on the threads of a screw, for instance) and those on a surface exposed to the air in the work area. Theoretically, the distinction lies in the assumption that during a chemical decontamination cycle some <u>small</u> fraction, f, of the external contamination survives, while all, or essentially all, of the internal contamination survives. It is assumed that the survival factor, f, is that factor associated with the hardiest microorganism known.

In the model presented here, it is assumed that "survival" is not just a two-valued function, but that it varies with surface "type". Our concern lies in the possibility that in any given decontamination stage, some of the "least accessible" external contamination may survive in a higher proportion that the "more accessible" external contamination while, at the same time, have a higher probability of becoming internal contamination at the next assembly stage.

In order to make this more precise, let us define external contamination to be that contamination which is directly exposed to the surrounding air in the work area. This definition differs from that of Johnson's model, but it is more convenient for our purpose. This definition would seem to be a reasonable one, and it leads in a natural way to further inquiry about the notion of direct exposure. For example, it might be desirable to distinguish between exposure on a large flat surface and exposure in a tiny crevice since it is not unlikely that the latter "protected" contaminants would survive in a proportion different from that of the former "unprotected" contaminants during a given stage of decontamination. Making such a distinction leads to the uncomfortable possibility of having many degrees of contamination "protection".

For the same reason, one might wish to distinguish between contamination lying on a polished metal surface and a soft rubber surface, particularly when the decontamination mechanism is gas.

Such possibilities lead to the introduction of a stochastic element into the problem; namely, the distribution of contaminants on the external surface of the structure. This is clearly a matter of some concern if it is possible that the survival ratio of the external contamination depends on the location of the contamination upon the structure's external surface.

For example, in a complex structure possessing many surface "types", one possible distribution might be "all contaminants lie in screw hole A", although such a distribution of external contamination seems improbable. Another possible distribution might be "all contaminants lie on exposed flat surfaces", which again seems unlikely in a complex structure if "surface" is defined in some realistic manner.

The latter comment gives an indication of the first difficulty encountered in such an approach; namely, what should be regarded as a surface? As an example, consider the fact that geometrically most surfaces are locally flat, that is, nearly all of the points on the structure's external surface may be thought of as belonging to a small flat subsurface. Hence, it would seem that one should consider subsurfaces which are not, in general, just some small neighborhood of a point on the structure's external surface. In fact, at any given assembly stage, it would be desirable to divide the total external surface of the structure into subsurfaces in such a way that contamination distributed uniformly on the external surface of the structure has a fairly constant survival factor at all points of any given subsurface when decontaminant is applied uniformly on that subsurface.

Suppose for a moment that the external contamination at a given assembly stage is uniformly distributed over the external surface of the structure. Then we will assume that the survival factor, f, is a function of two surface parameters α and β. Here, α is assumed to be a parameter indicating the degree of "exposure" of the surface, and β is a parameter indicating the surface "type" at any given point of the external surface of the structure. Then the above states that, on the external surface, the survival factor

$$f = f(\alpha, \beta) \; ,$$

is a function of the two surface parameters α and β when the contamination is uniformly distributed on the total external area.

Two comments are in order. First, it is one thing to say "let α be a parameter indicating the degree of exposure of points on the external surface of the structure", and quite another thing to define such a parameter in physical terms. A similar comment may be made about β. Secondly, in keeping with the above discussion, one would like to define the parameters α and β in such a way that it is possible to divide the structure's external surface into subsurfaces on which both α and β are fairly constant. This would be convenient, since under such conditions, $f(\alpha, \beta)$ would be essentially a constant on each such subsurface.

Admittedly, it is not clear how the external surface of the structure can be parameterized in such a way. However, as a matter of convenience we will defer any further discussion about the definition of these parameters until Section III. For the moment, let us simply assume that at any stage of assembly, the external surface of the structure has associated with it two parameters α and β, with the property that: given a uniform distribution of contamination on the external surface of the structure, the survival factor

$$f = f(\alpha, \beta).$$

Making such an assumption allows us to proceed to make another. Let us suppose that the total external surface S of the structure in question is divided into subsurfaces $s_1, s_2, \ldots, s_n$ in such a way that:

    (1) the subsurfaces s_i together cover all of S,

    (2) the subsurfaces s_i do not overlap, and

(3)   there exists a small number ϵ such that for any

two points of s_i, with parameters (α,β), and (α',β')

$$|f(\alpha,\beta) - f(\alpha',\beta')| \leq \epsilon.$$

Several comments should be made about these conditions. The three conditions yield a total decomposition of the surface S into subsurfaces on each of which the survival factor is essentially a constant function of the surface parameters α, and β. Further, if the function $f(\alpha,\beta)$ were known, it would be theoretically possible to obtain such a decomposition of S into a finite number of subsurfaces satisfying (1), (2) and (3), provided f were a reasonably well behaved function (this can be made precise). This decomposition can be accomplished for any number ϵ prescribed in advance. That is to say, the function f can be made to vary as little as desired on the subsurfaces. For this reason, we will consider f to be, in fact, a constant f_i on each subsurface s_i. Finally, for a given ϵ, this decomposition cannot necessarily be accomplished in a unique way.

Thus, in reality, the assumption of a decomposition of S into subsurfaces satisfying (1), (2) and (3) is an assumption about knowledge of (and the nature of) the function, f, defined on S.

For the remainder of this section let us assume only that the contamination on any <u>subsurface</u> s_i is distributed uniformly and that the decontaminant is applied uniformly on any s_i (although the density may vary from one subsurface to another due to their varying degress of exposure). Suppose that the assembly at some stage has just been completed, and let us analyze the microbial loading within the framework developed above.

It seems improbable that the external contamination on the structure is known exactly. Thus in the model, the external contamination will be represented by a random variable, C. For convenience, and without loss of generality, we will assume that C is defined on the integers between 0 and b inclusive and that C assumes values on the integers in this same range. Here, the positive integer, b, represents a bound on the possible contamination. Clearly such a number exists although it may be extremely large.

In addition, the contamination is physically distributed among the subsurfaces s_i. That is, some portion of the contamination is on s_1, some portion on s_2, and so forth. This corresponds to the statement that the random variable C is decomposed into a sum of random variables C_1, $C_2, \ldots, C_n$ where C_i represents the contamination on the subsurface s_i, and each C_i is defined on the integers 0 thru b and assumes values in the same range. Now such a decomposition of C into the sum of random variables of this type is not unique, and indeed may generally be accomplished in many ways, although the number of such ways is clearly finite. The difficulty here is that, practically speaking, it is not known which of the many possible decompositions of C is the one which corresponds to the actual situation.

Since this point is critical, it seems desirable to elaborate some. In Figure 1, two possible decompositions of a random variable C are shown, where n = 2, b = 10 and that C is the identity function. In Figure 1(a), the graph represents C as the identity function mapping the integers from 0 thru 10 into themselves. Figure 1(b) shows one possible decomposition of C into two random variables $C_1^{(1)}$ and $C_2^{(1)}$. That is, in the usual functional way, $C = C_1^{(1)} + C_2^{(1)}$. Here, $C_1^{(1)}$ is the random variable rep-
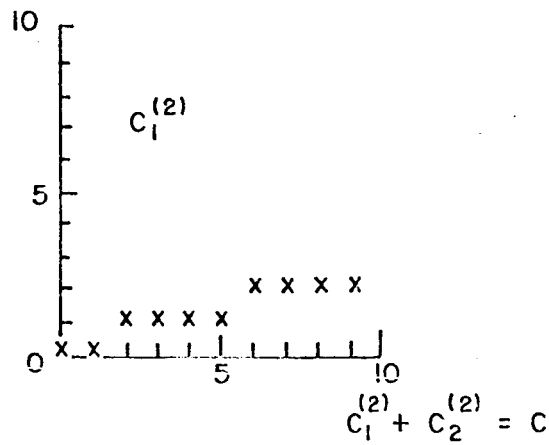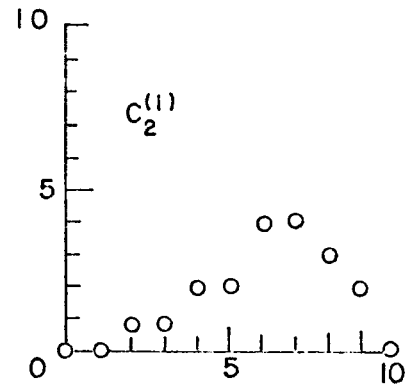
resenting the contamination on s_1, and $C_2^{(1)}$ represents the contamination on s_2. A similar example is shown in Figure 1(c).

THE RANDOM VARIABLE C

(a)

$C_1^{(1)}$

$C_2^{(1)}$

$C_1^{(1)} + C_2^{(2)} = C$

(b)

$C_1^{(2)}$

$C_2^{(2)}$

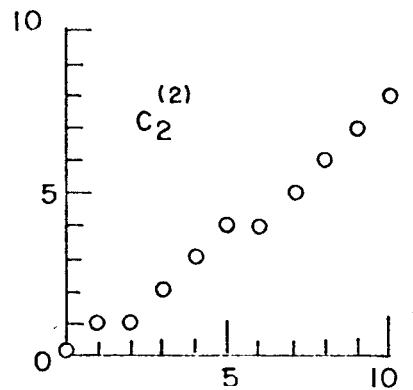$C_1^{(2)} + C_2^{(2)} = C$
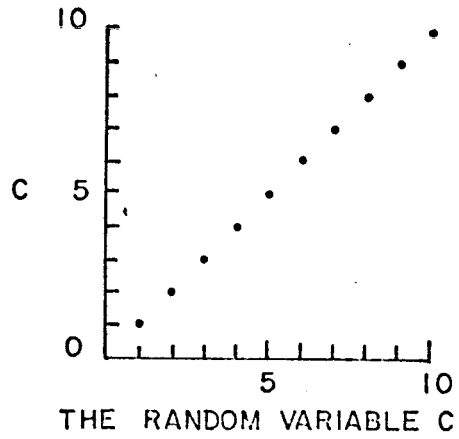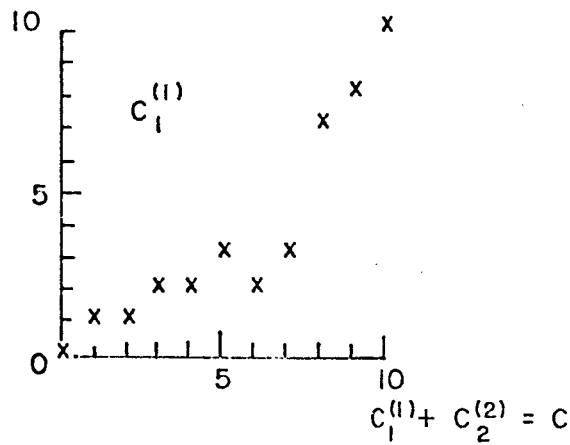
(c)

FIGURE 1

Without going into mathematical detail, one can intuitively sense that the two situations lead to quite different physical distributions of contamination on s_1 and s_2 for many values of C.

In the general case, it is obvious that there are many such possible physical distributions of the contamination among the subsurfaces s_1, s_2, ..., s_n. Let us denote any one such distribution, d, in the following way: $d = (C_1(d), C_2(d), ..., C_n(d))$, where $C_i(d)$ is the random variable representing the contamination on s_i, $i = 1,2,...,n$, for the particular physical distribution d.

Clearly many such d's will not represent anything which might reasonably be called a uniform distribution of contamination on the external surface of the structure. This fact leads us to reconsider our original ideas about the nature of the survival factor, f. We will still assume that the subsurfaces s_i satisfy the above conditions (1), (2) and (3) and that f is a constant function f_i of the parameters α and β on s_i. However, it seems to us that f_i cannot be treated as a function of the surface parameters α and β alone, but that it must also depend upon the amount of contamination present on the surface s_i. This contains the implicit assumption that the decontaminant is applied in a standard way, that is, no attempt is made to apply more decontaminant to those subsurfaces on which the contamination is greatest. This seems to be reasonable since the identity of these subsurfaces is not likely to be known in any given situation. Thus, for each physical distribution, $d = (C_1(d), C_2(d),...,C_n(d))$, the f_i are assumed to be functions of the random variable $C_i(d)$. That is

$$f_i = f_i(C_i(d)), \quad (i = 1,...,n),$$

and they become random variables because of their dependence on the random

variables $C_i(d)$. Of course, for this same reason, $f_i(C_i(d))$ is an implicit function of d.

In this context then, one obtains a new random variable,

$$C_i'(d) = f_i(C_i(d)) \cdot C_i(d),$$

representing the contamination which remains on the subsurface s_i after the decontaminant has been applied if $d = (C_1(d), C_2(d), \ldots, C_n(d))$ had been the physical distribution of C among the subsurfaces. Clearly $C_i'(d)$ is defined on the integers from 0 thru b. Also, by changing $f_i(C_i(d))$ slightly, $C_i'(d)$ will assume integral values in the same range without affecting its physical interpretation. As a matter of convenience, it will be assumed that this is the case.

Let us assume that there is associated with each possible physical distribution, d, a probability, P(d), that d will in fact represent the actual distribution of external contamination among the s_i's. This is an assumption with recognizable practical difficulties, but we will postpone discussion of these until Section III. We assume that the summation of the P(d) over all possible physical distributions, d, is unity.

This assumption allows one to calculate the random variable C_i' representing the expected contamination on s_i after decontamination in the usual manner:

$$C_i' = \sum_{\text{all } d} C_i'(d) P(d).$$

Once again, one may assume that C_i' is integral valued. This in turn leads to a random variable,

$$C' = \sum_{i=1}^{n} C_i' \, ,$$

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representing the expected contamination of the total external surface of the structure.

Due to the nature of the problem, it may be preferable to be pessimistic about the random variable representing the total external contamination, rather than rely on expected values as in the last equation. In this case, one might choose,

$$C'' = \max_{d} \sum_{i=1}^{n} f_i(C_i(d)) \cdot C_i(d)$$

to be the random variable representing the external contamination of the structure after decontamination. If this is done, let d_o be a distribution which maximizes the above sum. That is,

$$C'' = \sum_{i=1}^{n} f_i(C_i(d_o)) \cdot C_i(d_o) \ .$$

Then the ith term in the sum will be the random variable representing the contamination on the subsurface s_i after decontamination. Since d_o may not be unique, that has some disadvantages which will be discussed in Section III. However, in spite of the difficulties, this approach seems more reasonable than the former. Indeed the choice of a new random variable representing the external surface contamination after a decontamination cycle presents a decision making problem. This problem is discussed in somewhat more detail in Section III.

So far we have discussed only the external contamination problem associated with decontamination just after a given assembly stage of the structure. In general, the decontaminated structure, Σ_1, will be placed together with other decontaminated structures, Σ_j, $j = 2, \ldots, m$. to form a new structure, Σ, which is amenable to the above approach provided some means exists for obtaining the contamination random variable, C,

of Σ in terms of the random variables $c^{(j)}$ representing the external contamination of the Σ_j, $j = 1,2,\ldots,m$. Here of course, each of the $c^{(j)}$ correspond to the C' or C'' or some similarly derived random variable, on the structure Σ_j.

Returning to Johnson's model, we will assume, as he does, that the handling of the Σ_j prior to actual assembly into Σ imparts some external contamination, A_j, to Σ_j. This means that the total external contamination of Σ_j at the moment of assembly of Σ is $c^{(j)} + A_j$. Further, some portion of the external contamination will become internal contamination during the actual assembly of the Σ_j's into Σ, and following Johnson, we will denote this "fraction" by μ_j. Finally, during the actual assembly, some external contamination, B, will be added to Σ, and following Johnson's model, the total external contamination of Σ would be of the form:

$$C = B + \sum_{j=1}^{m} (c^{(j)} + A_j)(1 - \mu_j) \ .$$

Here it must be noted that we deviate from Johnson's model in that we assume that B, $c^{(j)}$, A_j are random variables defined on the integers 0 thru b and taking integral values in the same range.

Further, it seems reasonable that the fraction μ_j of external contamination on the structure Σ_j which becomes internal, is a function of the physical distribution of the random variable $c^{(j)} + A_j$ on the external surface of the structure Σ_j. Thus, μ_j is also a random variable. This arises from reasoning along the following lines. If the actual physical distribution of $c^{(j)} + A_j$ on Σ_j is

$$d^{(j)} = (c_1^{(j)}(d^{(j)}),\ldots,\ c_{n_j}^{(j)}(d^{(j)}))$$

defined by

$$\text{i)} \quad c_1^{(j)}(d^{(j)}) = c^{(j)} + A_j, \text{ and}$$

$$\text{ii)} \quad c_k^{(j)}(d^{(j)}) = 0, \ k = 2,\ldots,n_j$$

(where n_j is the number of subsurfaces on Σ_j), then it is possible that <u>all</u> the contamination $c^{(j)} + A_j$ be internal or external if the subsurface $s_1^{(j)}$ of Σ_j should become entirely internal or external during the assembly of Σ. This is an extreme situation, but one can easily see from it how μ_j depends on the physical distribution, $d^{(j)}$, of the external contamination $c^{(j)} + A_j$ among the subsurfaces $s_1^{(j)}$, $s_2^{(j)}$,..., $s_{n_j}^{(j)}$ of the structure Σ_j.

When one allows this possibility, the external contamination contributed by Σ_j to Σ takes the form:

$$E_j(d^{(j)}) = \sum_{k=1}^{n_j} \left[c_k^{(j)}(d^{(j)}) \right] \left[1 - \mu_k^{(j)}(c_k^{(j)}(d^{(j)})) \right] \qquad (*)$$

where $c_k^{(j)}(d^{(j)})$ and $\mu_k^{(j)}(c_k^{(j)}(d^{(j)}))$ are random variables which, in addition, possess a dependence on the physical distribution, $d^{(j)}$, of $c^{(j)} + A_j$ on Σ_j.

In these terms, the random variable representing the external contamination of Σ takes the form:

$$C(d^{(1)}, d^{(2)},\ldots,d^{(m)}) = B + \sum_{j=1}^{m} E_j(d^{(j)}).$$

Again taking a pessimistic view of external contamination, one may wish to consider the external contamination of Σ to be given by the expression $C = \max\limits_{d^{(1)}} \ \max\limits_{d^{(2)}} \ \ldots \ \max\limits_{d^{(m)}} \ C(d^{(1)}, d^{(2)},\ldots, d^{(m)}),$

or he may wish to use an expected value model

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$$C = \sum C(d^{(1)}, \ldots, d^{(m)}) P(d^{(1)}, \ldots, d^{(m)})$$

where the sum is taken over all m-tuples $(d^{(1)}, \ldots, d^{(m)})$, and of course, it is assumed that the probability, $P(d^{(1)}, \ldots, d^{(m)})$, of the occurrence of these m-tuples exists and is known.

In either case, the practical difficulties which exist are much the same as those arising in the previous analysis of the decontamination mechanism, and these are discussed in Section III.

Nonetheless, depending upon one's decision criterion, either of the above expressions for C yield a random variable which may be viewed as representing the external contamination of the structure Σ in terms of the subsurface contaminations $C_k^{(j)}(d^{(j)})$ of its immediate substructures and the external contamination variable, B, added during assembly.

This approach allows the relations between surface type, physical distribution of contamination, and decontamination to be taken into account.

One can carry this analysis a step further to investigate the "critical" subsurfaces only. That is, one can extract information pertaining to those external subsurfaces parts of which are to become internal at the next stage of assembly by simply summing equation (*), above, over the indices of such subsurfaces only. For the remaining indices, k, in the range 1 to n_j one has $\mu_k^{(j)} = 0$.

Without going into detail, it should be clear that internal contamination can be treated using this same approach.

SECTION II - Mathematical Model

In this section, the definitions necessary for the construction of an abstract mathematical model of the situation described in Section I are given. A few salient propositions are stated without proof. It is our intent to rigorously build the foundation from which the problem can be studied further, and as such, this section is generally devoid of new ideas about the problem itself. We urge any reader interested only in expository treatment to advance to Section III. For further elaboration of Definitions 1 through 9, the reader is referred to $\lfloor 5 \rfloor$, while for Definitions 10 through 12, $\lfloor 6 \rfloor$ may prove helpful.

Contamination Space:

Definition 1. Let I_b denote the set of integers from 0 to b (> 0) inclusive. A probability space of the form $(I_b, 2^{I_b}, p)$ will be called a contamination space, P. A random variable, C, defined on this space having as its range a subset of I_b will be called a contamination variable, and the number b is called the contamination bound. Let $\mathcal{C}(P)$ be the set of all contamination variables on the contamination space $P = (I_b, 2^{I_b}, p)$.

M-Parameter Survival Factor:

Definition 2. If f is a continuous function of bounded variation mapping $\lfloor 0, 1)^m$ into $\lfloor 0, 1 \rfloor$ it will be called an m-parameter survival factor. Note that $\lfloor 0, 1)^m$ contains half closed and half open sets. This is done in order to guarantee that the R_j to be defined in "Proposition 1" be non-overlapping.

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Proposition 1. If f is an m-parameter survival factor and $\epsilon > 0$ is any real number, then there exist m-by-n matrices $\|a_{ij}\|$ and $\|\delta_{ij}\|$ defined over $[0, 1)$ with the properties:

(i) in the region R_j of $[0, 1)^m$ defined by

$$|a_{ij} - x_i| < \delta_{ij}, \quad (i = 1, \ldots, m),$$

$$|f(x_1, \ldots, x_m) - f(a_{1j}, \ldots, a_{mj})| < \epsilon, \text{ and}$$

(ii) $\displaystyle\bigcup_{j=1}^{n} R_j = [0, 1)^m$ and $R_i \cap R_j = \emptyset$ if $i \neq j$.

"Proposition 1" (a well known theorem on continuous functions) will yield a method of breaking the surface of any component into n subsurfaces on which the m-parameter survival factor, f, is nearly equal to its representative value $f(a_{1j}, \ldots, a_{mj})$ $(j = 1, \ldots, n)$.

ϵ-Decomposition $[0,1)^m$ Relative to f.

Definition 3. Such a decomposition of $[0, 1)^m$ into $R_1, \ldots, R_n$ as given in Proposition 1 is called a <u>ϵ-decomposition</u> <u>of</u> $[0, 1)^m$ <u>relative</u> <u>to</u> <u>f</u>. For a given ϵ-decomposition, we define

$$f_j(\epsilon) = f(a_{1j}, \ldots, a_{mj}), \quad (j = 1, \ldots, n).$$

The Set $\mathcal{C}(P,C)$:

Definition 4. For a given contamination variable, C, in $\mathcal{C}(P)$, we define the <u>set</u> <u>$\mathcal{C}(P,C)$</u> to be that set of random variables $X: I_b \dashrightarrow [0, 1]$ with the additional property that $X \cdot C$ is in $\mathcal{C}(P)$.

Proposition 2. For a given contamination space P and contamination variable C in $\mathcal{C}(P)$, the set $\mathcal{C}(P,C)$ is a finite non-empty set.

ε-Survival Functions:

Definition 5. Given an m-parameter survival factor, f, a number ε > 0, a ε-decomposition $R_1,\ldots,R_n$ of $[0,1)^m$ relative to f, an n-tuple $(f_1,\ldots, f_n)$ is called a set of ε-survival functions if:

(i) f_j is defined on $\mathcal{C}(P)$ and $f_j(C,\epsilon)$ is in $\mathcal{C}(P,C)$ for all C in $\mathcal{C}(P)$ and all $j = 1,\ldots,n$, and

(ii) for the contamination variable Θ in $\mathcal{C}(P)$ defined by $\Theta(i) = 0$, $i = 0,1,\ldots,b$, one has $f_j(\Theta,\epsilon) = f_j(\epsilon)$, the latter being defined in Definition 3 above.

m-Parameter Surface:

Definition 6. An ordered pair (S, g) is called an **m-parameter** surface if S is a surface in E^3 and g is a function mapping the points of S into $[0, 1)^m$.

Proposition 3. Let an m-parameter survival factor, f, an m-parameter surface (S, g), $\epsilon > 0$, and an ε-decomposition $R_1,\ldots,R_n$ of $[0, 1)^m$ relative to f be given. Then the relation ~ among the points of S defined by $p_1 \sim p_2$ if and only if $f(g(p_1))$ and $f(g(p_2))$ belong to the same R_i, is an equivalence relation.

ε-Subsurfaces of S:

Definition 7. The ~ equivalence classes of S, under the conditions of Proposition 3, are denoted $s_1,\ldots,s_n$ and are called ε-subsurfaces of S.

Contaminated Surface:

Definition 8.   An ordered triple (S, g, C) is called a <u>contaminated</u> <u>surface</u> if (S, g) is an m-parameter surface for some m, and C is a contamination variable defined on some contamination space.

Physical Decomposition of C:

Definition 9.   Given a contamination space, P, and C in $\mathcal{C}(P)$, an n-tuple $(C_1, \ldots, C_n)$ is called a <u>physical</u> <u>decomposition</u> <u>of</u> $\underline{C}$ if:

(i) C_i is in $\mathcal{C}(P)$, $i = 1, \ldots, n$, and

(ii) $C = C_1 + C_2 + \ldots + C_n$.

We let $\Delta(C)$ denote the set of such n-tuples.

Proposition 4.   The set $\underset{\sim}{\Delta}(C)$ is a finite nonempty set.

An Assembly Network:

Definition 10.   A digraph is an ordered pair $D = (V, X)$ where V is a finite nonempty set called the set of points of D and $X \subset V \times V$ is called the set of <u>lines</u> of D. An <u>assembly</u> <u>network</u> is a digraph, $N = (V, X)$ satisfying:

(i)   there is exactly one point of N for which the outdegree at that point is zero (we denote this point v_T), and every other point has outdegree one, and
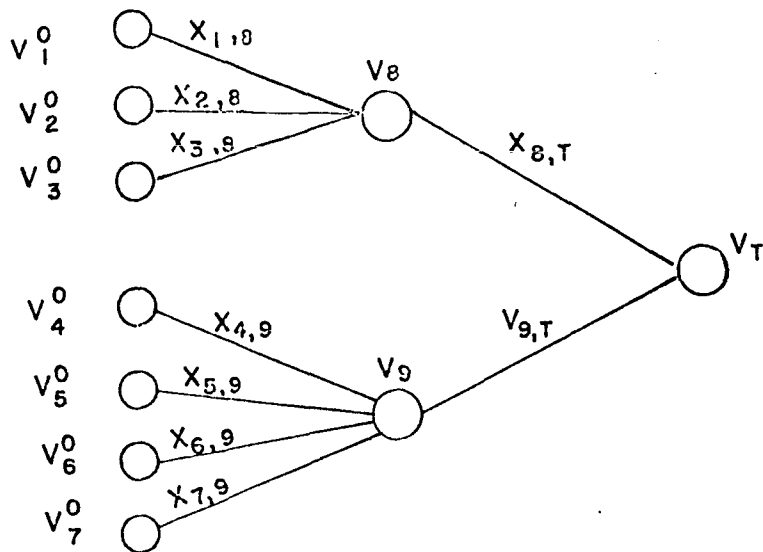
(ii) N contains no directed cycles.

FIGURE 2. AN ASSEMBLY NETWORK

Proposition 5. In any assembly network there exists a nonempty set of points, $I = \{v_1^o, \ldots, v_r^o\}$ such that each point v_i^o has indegree zero, $i = 1, \ldots, r$, and all other points have a non-zero indegree.

Proposition 6. Let N be an assembly network, $I = \{v_i^o, \ldots, v_r^o\}$ as in Proposition 5, and v any point in N. Then there exists a directed path from some point in I to v_T which contains v. Thus in particular, N is weakly connected.

Proposition 7. Let v be any point of an assembly network, N. Then there exists a unique path from v to v_T. The relation * defined on V by v * v' if and only if the $v \dashrightarrow v_T$ path and the $v' \dashrightarrow v_T$ path are the same length, is an equivalence relation.

Assembly Stages:

Definition 11. The * equivalence classes defined on V in Proposition 7

in an assembly network N are called <u>assembly</u> <u>stages</u>; the point v_T is called the sth assembly stage, where s is the length of the longest directed path in N. In general, any other point v belongs to the rth stage if it belongs to a line $\langle v, v' \rangle$ with v' in the $r + 1^{st}$ assembly stage.

<u>A Contaminated Structure Assembly Network:</u>

<u>Definition 12.</u> A contaminated structure assembly network is an ordered 12-tuple whose entries are:

(1) an assembly network, N = (V, X), with the number of vertices = t and $v_T = v_t$,

(2) a contamination space, P

(3) a set $\{\Sigma_i : i = 1,\ldots,t\}$ where each Σ_i is an m-parameter surface,

(4) a set $\{A_i : i = 1,\ldots,t-1 \text{ and } A_i \text{ is in } \mathcal{C}(P)\}$ where each A_i represents the additional external contamination imparted to Σ_i prior to actual assembly.

(5) a set $\{C_i : i \text{ such that indegree } (v_i) = 0, C_i \text{ in } \mathcal{C}(P)\}$,

(6) a set $\{B_i : i \text{ such that indegree } (v_i) \neq 0, B_i \text{ in } \mathcal{C}(P)\}$, where each B_i represents the external contamination that may be added during actual assembly.

(7) an m-parameter survival factor, f,

(8) a real number $\epsilon > 0$,

(9) a set $\{R_j : j = 1,\ldots,n\}$ whose elements constitute a ϵ-decomposition of $[0, 1)^m$ relative to f,

(10) a set $\{s_{ij} : s_{1j},\ldots,s_{nj} \text{ are the } \epsilon\text{-subsurfaces of } \Sigma_j, \, j = 1,\ldots,t\}$,

(11) a set $(f_{i1}, f_{i2},\ldots, f_{in})$ of ϵ-survival functions

for each $i = 1,\ldots,t$, and

(12) a set $(\eta_{i1},\eta_{i2},\ldots,\eta_{in})$ of ϵ-survival functions

for each $i = 1,\ldots,t$, where each η_{ij} represents

that fraction of the external contamination on the

j^{th} subsurface of the $\Sigma_i{}^{th}$ m-parameter surface that

remains external after decontamination and assembly.

In Section I,

$$\eta_{ij} = (1 - \mu_{ij})$$

Definition 13. Given a contaminated structure assembly, the <u>contamination</u>

of a point v_i in N is defined in terms of its indegree

as follows:

(i) if indegree $(v_i) = 0$

$\quad c^{(i)} = C_i' + A_i$ where

$$C_i' = \max_{d^{(i)}} \sum_{j=1}^{n} f_{ij} \left[C_{ij}(d^{(i)}) \right] \cdot C_{ij}(d^{(i)}), \text{ and}$$

$$d^{(i)} = \left\{ C_{i1}(d^{(i)}),\ldots,C_{in}(d^{(i)}) \right\} \text{ is in } \Delta(C_i), \text{ or}$$

(ii) if indegree $(v_i) \neq 0$,

$$c^{(i)} = B_i + \sum_{j \to i} \max_{d^{(j)}} \left\{ E_{jk}(d^{(j)}) \cdot \eta_{jk} \left[E_{jk}(d^{(j)}) \right] \right\} \text{ where}$$

$$E_{jk}(d^{(j)}) = f_{jk} \left[C_{jk}(d^{(j)}) \right] \cdot C_{jk}(d^{(j)}) + A_{jk}(d^{(j)}) \text{ and}$$

$$\left\{ C_{j1}(d^{(j)}),\ldots, C_{jn}(d^{(j)}) \right\} \text{ is in } \Delta(c^{(j)}), \text{ and}$$

$$\left\{ A_{j1}(d^{(j)}),\ldots, A_{jn}(d^{(j)}) \right\} \text{ is in } \Delta(A_j) .$$

SECTION III - Practical Aspects of the Model

In this section, the practical features of the model will be discussed. In general, our remarks will be confined to the intuitive presentation of the model in Section I. The development depended heavily upon one's ability to parameterize the external surface of the structure in such a way that the survival factor was completely specified as a function of these parameters alone if the variations in amount of contamination were ignored. In Section I, we chose only two parameters, while the abstract model was developed for an arbitrary finite integer, m. The reasoning in Section I was the following: if the kill mechanism is gas, then the survival factor will depend, in all probability, upon the ability of the gas to reach the contamination (a) and upon the ability of the surface to "adsorb" gas, once the gas has reached it. Thus, the parameter, a, was envisioned as the degree of "exposure", while the parameter, β, was envisioned as being related to the "adsorptivity" of the surface. Both parameters seem capable of precise definition within the realm of present technology.

On the other hand, only one relatively satisfactory means of defining a has occurred to us. The practical difficulties arising from this definition are formidable. However, if the behavior of f as a function of a could be determined experimentally under laboratory conditions on surfaces designed to have specific a values, the results might lead to surface design criteria for the structure in question. We would now like to formulate a rigorous definition for degree of exposure, a.

We will call a surface S in 3-space a $P_0 \rightarrow P_1$ <u>snake</u>, where P_0 and P_1 are points in 3-space, if:

(1) there exists a simple differentiable rectifiable arc,

$A(t) = (x_1(t), x_2(t), x_3(t))$, $0 \leq t \leq 1$, in 3-space with $(x_1(i), x_2(i), x_3(i)) = P_i$, $i = 0,1$, such that every point on S belongs to a circle $z(t)$ whose plane is perpendicular to $A(t)$ and whose center is $(x_1(t), x_2(t), x_3(t))$,

(2) the radius of $z(t_1) \leq$ radius of $z(t_2)$ for $t_2 \leq t_1$, and

(3) there exists t', $0 \leq t' < 1$ such that the surface for $t \leq t'$ is a right cone having as its base the disc enclosed by $z(t')$ and as its vertex, the point P_1. Let t_0 be the first such t'.

The <u>value</u> of the snake S is defined to be $v(s) = $ radius $z(t_0)$.

For any given external point P_1 on the structure, we consider the set

$T(P_1) = \{$S: S is a $P_0 \rightarrow P_1$ snake whose interior does not intersect any portion of the structure, and P_0 is a point from which gas is to be dispensed$\}$.

Thus, the set $T(P_1)$ is a mathematical description of the set of all paths a gaseous decontaminant might take entering the decontamination chamber at P_0 and finally reaching the point P_1 on the surface to be decontaminated.

The <u>value</u> of any subset $T'(P_1)$ of $T(P_1)$ is defined to be,

$$v(T'(P_1)) = \sum_{S \in T'(P_1)} v(S).$$

A subset $T'(P_1)$ of $T(P_1)$ is called <u>independent</u> if for any two elements S_1 and S_2 of $T'(P_1)$, S_1 and S_2 have <u>no</u> interior points in common.

Then the <u>value</u> of P_1 is defined to be

$$v(P_1) = \max v(T'(P_1))$$

where the maximum is taken over all independent subsets $T'(P_1)$ of $T(P_1)$.

When the values of all points P_1 are known, they can clearly be normalized to lie in the interval $[0,1)$ and these normalized values are considered to be the <u>exposure parameter values, a</u>.

The practical problems inherent in such a definition are obvious, but it <u>is</u> possible to <u>design</u> surfaces on which the parameter values, in the above sense, can be evaluated. Hence, it would be possible to experimentally determine the dependence of f on a if the problems of control and measurement of contamination could be overcome. If this could be done, the results would certainly provide design criteria for surfaces of the structure which would be directly related to the problem of contamination.

It would be difficult to determine <u>a priori</u> whether such criteria would conflict with others designed for the same purpose. We are thinking particularly of design criteria which would maximize the decontamination due to assembly of the structure in a clean room environment.

At this point it seems appropriate to mention the major fault of the model, that is, its independence of <u>time.</u> In any clean room situation, the amount of contamination on a surface, whether viewed as a random variable or otherwise, should be considered a function of time. Also, the amount of contamination on a surface should be regarded as a function of time in a completely different sense, namely, in terms of the ability of many microorganisms to multiply rapidly. Certainly any model which can be considered "good" must take these things into account. It is our opinion that the analysis of clean room effects upon complex contaminated structures would involve a great deal of time and effort.

Another point which we promised to discuss is the problem of determining with what probability the various possible physical distributions of contamination occur. Given a static situation, this would seem

to be almost impossible on an a priori basis because of the unknown way in which the additive contamination, A_j, is introduced at each assembly stage. On the other hand, it would not seem unreasonable to expect that a thorough analysis of the effect upon contamination by the air flow in a clean room would help determine the probable location of contamination on the surface as a function of time, surface characteristics, and structure orientation.

Another notion whose discussion was deferred until this section deals with decision criteria for choosing a random variable to represent the contamination remaining after decontamination has occurred.

It will be recalled that we suggested the choice

$$C'' = \max_{d} \sum_{i=1}^{n} f_i\left[c_i(d)\right] \cdot c_i(d)$$

and suggested that the distribution d_0 which maximizes the above sum would not generally be unique. This causes certain theoretical difficulties at this stage in the event one would like to analyze only those particular subsurfaces which are to become interior at the next stage. That is, the sum of the

$$f_i\left[c_i(d_0)\right] \cdot c_i(d_0)$$

taken over indices, i, corresponding to surfaces, parts of which are to become interior, does truly depend on the choice of distribution d_0 maximizing the sum over all indices.

However, if one desires to be pessimistic about internal contamination, the following decision criterion seems most desirable.

Let $D_0 = \{d \mid d \text{ maximizes } \sum_{i=1}^{n} f_i\left[c_i(d)\right] \cdot c_i(d)\}$ and let

$I = \{i \mid \text{a portion of } s_i \text{ becomes interior in the next stage of assembly}\}$.
Then choose $d_0' \in D_0$ which maximizes

$$\sum_{i \in I} f_i\left[c_i(d)\right] \cdot c_i(d).$$

Again, d_0' might not be unique, but the original objection has been overcome in the sense that

$$C'' = \sum_{i=1}^{n} f_i\left[c_i(d_0')\right] c_i(d_0')$$

represents the maximum possible external contamination remaining and, subject to this condition, yields maximal interior contamination at the next stage.

There are other philosophical and practical problems associated with any attempt to make such a decision. From a predictive point of view, it seems that one would like to make decisions that yield a maximum total contamination remaining on the structure after decontamination following the last stage of assembly. If such contamination was less than the prescribed bound (with the desired probability) then surely the true amount of contamination would also be. At least two difficulties arise in attempting to do this. The first is that, even in the above framework, the mathematical problem may prove too difficult to be solved, principally because the quantity to be maximized is a random variable. Secondly, such an approach is severely limited as long as the dependence of the problem upon time is not included.

Three further comments. First, this model is based upon the assumption that by obtaining a completed structure with a known amount of biological

contamination, one can proceed to sterilize the structure by heating it.
This is probably not unreasonable, but we feel that the usual law of
logarithmic kill should be investigated further since there seems to be
evidence (see $[7]$) that it may not be valid in all situations.

Secondly, the assembly analysis is sequential in nature, moving from
one assembly stage to the next. This has great advantages in large calcu-
lations involving a computer.

Thirdly, any attempt to obtain the random variables representing
the total external and internal contamination at the last stage of
assembly in closed form is probably doomed to failure. Finally, because
of the mathematical complexities involved in any such an attempt, we would
recommend a Monte Carlo approach.

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