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SOLUBILITY PARAMETER TECHNOLOGY
AND EVAPORATIVE RATE ANALYSIS USED
TO EVALUATE CONTAMINANTS

EP 04067100, Topical Report

L. C. Jackson, Project Leader

Project Team:
E. T. Walsh

May 1973

MASTER

Prepared for the
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**Kansas City
Division**

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Prepared by L. C. Jackson, D/814, under EP 04067100

Solubility parameter technology is used to evaluate the general nature of contaminants detected by evaporative rate analysis. Descriptions of the evaporative rate technique and solubility parameter principle are given. The combination of these two technologies has been shown to indicate potential in distinguishing differences between contaminants.

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THE BENDIX CORPORATION

KANSAS CITY DIVISION

KANSAS CITY, MISSOURI

A prime contractor for the
Atomic Energy Commission

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SUMMARY

Contaminants on solid surfaces can be detected by using solubility parameter technology combined with the principle of evaporative rate analysis. This combination of technologies is being used to detect particles larger than 0.5 micron and organic residues smaller than 0.5 micron. Any material that causes unwanted adhesion or electrical surface leakage is considered a contaminant.

Solubility parameter technology has been used previously in the paint industry to predict solubility and solvent sensitivity of polymers. NASA has used evaporative rate analysis to monitor contaminant levels. However, the two technologies have not been used together to characterize contaminants.

Similar materials are more mutually soluble than dissimilar materials because the attraction between molecules of similar materials is greater. If the solubility parameter values of two solvents, or a solvent and a plastic (or organic residue), are reasonably close together, solution is easily achieved. On the other hand, if the solubility parameter values are far apart, then the compatibility of two materials is reduced. This system of matching solubility parameter numbers as close as possible is more valid for non-polar molecules than for polar or hydrogen bonded molecules.

It is important that the polar and non-polar molecules approximate each other as well as having matching solubility parameter numbers. Hydrocarbons, for example, have no polarity; esters have a relative polarity function or contribution of less than 20 percent; ketones range from 30 to 60 percent; and nitriles vary from 50 to 80 percent. Thus, non-polar plastics (or contaminants) would be expected to be affected less by polar solvents than non-polar solvents, even though solubility parameters are equal.

The other class of intermolecular bonds involves hydrogen. These are not chemical bonds but are a result of the sharing of electrons. The hydrogen atom may be considered a bridge between the two molecules. Solubility prediction problems develop when hydrogen bonding occurs.

The accuracy of predicting compatibility of organic materials is 50 percent if hydrogen bonding factors are not taken into consideration. An increase to 95 percent reliability is possible when a classification of solvents is used according to poor, moderate, or strong hydrogen bonding tendencies.*

*Harry Burrell, "The Challenge of the Solubility Parameter," Journal of Paint Technology, Volume 520, May, 1968.

DISCUSSION

SCOPE AND PURPOSE

A unique capability is being established to distinguish between contaminants. This technique utilizes a contamination detection method (evaporative rate analysis) combined with interpretive solubility parameter technology.

PRIOR WORK

No attempt had ever been made to use solubility parameter technology to distinguish between contaminants detected by evaporative rate analysis.

ACTIVITY

Degree of Contamination

Cleanliness is relative: a level of acceptable cleanliness must be established before contamination removal can be effective. However, since the capability to detect and identify organic residues on surfaces is extremely limited, the presence and degree of contamination has always been a matter of speculation.

A contaminant is any unwanted material that coats a surface to cause adhesion or electrical surface leakage problems. For convenience, contaminants may be classified as particles larger than 0.5 micron or as organic residues smaller than 0.5 micron.*

Evaporative Rate Analysis

Evaporative rate analysis is a technique used for evaluating surface conditions. It involves measuring the rate of evaporation of a radioactive chemical from a surface. The degree of retention of the radioactive solvent is a measure of contamination. Carbon-14 tagged solvents having varying solubility capabilities can be used. The Meseran Surface Analyser manufactured by Ametek Technical Products employs the principle of evaporative rate analysis and was used in this work. The lower limit of contaminant detection reported for this equipment is 0.1 microgram per square centimeter.

*Contamination Control Handbook, NASA N70-13566, 1969, V-5.

Solubility Parameter Technology

Solubility parameter technology involves the principle of matching molecules of a solid and a liquid to achieve solution. When materials with dissimilar molecules are mixed, the attraction between the molecules is not as great as when similar molecules are mixed. The solubility parameter value of a material is a function of its attraction forces or intermolecular interactions. These may be identified in terms of the van der Waal's forces (polar and non-polar forces) and hydrogen bonding. Solubility parameter technology can be used to predict compatibility between a solid and a solvent.

Contaminant Evaluation

Contaminants may be considered in terms of their chemical structure or class (such as aliphatic hydrocarbon, aromatic hydrocarbon, chlorinated hydrocarbon, esters, ethers, ketones, alcohols, amines) and, therefore, provide the opportunity of utilizing solubility parameter technology.

Similar type molecules will tend to be compatible with each other. Unlike materials on the other hand, will be less attracted to each other and less soluble. Selected Carbon-14 tagged solvents (tridecane, diethylsuccinate, and beta cyclohexylethanol) can be used with the Meseran Surface Analyzer to detect whether a contaminant is non-polar, polar, or possibly hydrogen bonded. An evaluation of several contaminants is given in Table 1. The larger numbers indicate more compatibility of a radioactive solvent with a specific contaminant than do lower radioactive counts. Comparison of a contaminant with the three radioactive solvents will indicate similarity or lack of similarity.

The following is an analysis of the data given in Table 1.

The fingerprint is primarily aliphatic or aromatic in nature with little hydrogen bonding capability since it yielded a high count with the radioactive non-polar tridecane and low count with high hydrogen bonded β -cyclohexylethanol.

The Kaydry soaked in isopropyl alcohol is a residue which has no polarity (low diethylsuccinate radioactive count) but is more indicative of an aromatic or aliphatic molecule (tridecane count is higher).

The fingercot leaves a residue that has a very high hydrogen bonding tendency as determined by the large radioactive count with β -cyclohexylethanol.

The SBS-61 lotion soap appears to be a formulation of several materials which provide high values with each radioactive solvent and, therefore, must be a composition of non-polar, polar, and hydrogen bonding materials.

Table 1. Detection of Contaminants by Radioactivity Count

Radioactive Solvent: Contaminant	Radioactivity Counts		
	Meseran Number of Tridecane*	Meseran Number of Diethyl Succinate**	Meseran Number of β -Cyclohexyl Ethanol***
Fingerprint	451	116	41
Kaydry Soaked in Isopropyl Alcohol	38	3	15
Fingercot	0	43	107
SBS-61 Lotion Soap	372	310	566
*Solubility Parameter 7.69 joules/cubic meter **Solubility Parameter 9.65 joules/cubic meter ***Solubility Parameter 10.47 joules/cubic meter			

ACCOMPLISHMENTS

Several select contaminants have been detected by the Meseran Surface Analyzer and analyzed by using solubility parameter technology. The technique of combining the technology of solubility parameters and evaporative analysis had been shown, in this preliminary analysis, to have potential in distinguishing between contaminants.

FUTURE WORK

A more detailed characterization of many potential contaminants and their effective removal will be performed in another project. In addition to effective contaminant removal by solvents, gas plasma will also be used to achieve contaminant removal from a variety of metal and plastic surfaces.