

**FEASIBILITY INVESTIGATION OF VISCOUS
SOLVENT REMOVAL OF TRACE CONTAMINANTS**

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FOREWORD

This study was initiated by the Biomedical Laboratory of the Aerospace Medical Research Laboratories, Wright-Patterson Air Force Base, Ohio. The research was conducted by the Denver Research Institute, University of Denver, under Contract AF 33(615)-1463. The work was performed in support of Project No. 6373, "Equipment for Life Support in Aerospace," Task No. 637302, "Respiratory Support Equipment." Mr. W. H. Toliver, Sr., of the Respiratory Equipment Branch, was the contract monitor for the Aerospace Medical Research Laboratories.

This report covers work performed between March 1964 and March 1965.

The work at the Denver Research Institute was performed by Dr. John A. Krimmel and Dr. Thomas D. Nevens, Co-Project Supervisors, Mr. David R. Jordan, Mr. Nicholas J. Bourg, and Mr. George E. Bohner.

This technical report has been reviewed and is approved.

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ABSTRACT

Twenty-three compounds were studied as potential solvents for the removal of trace contaminants from the atmosphere of a space capsule. The contaminants to be removed included a wide variety of chemical types such as aliphatic (both saturated and unsaturated), alicyclic, and aromatic hydrocarbons, chlorinated hydrocarbons, Freons, alcohols, aldehydes, acids, ketones, acetates, ethers, and other miscellaneous compounds. In an effort to dissolve as many of the contaminants as possible, solvents which contained a number of different chemical structures were synthesized. Most of the solvents were esters derived from the reaction of a polyhydric alcohol such as pentaerythritol, trimethylolpropane, or isorbide with a mixture of organic acids. Esters of sebacic and isosebacic acids also were considered. The solubilities of representative contaminants in each of the solvents were determined. Calculations based on these data showed that the best solvent was much less efficient than charcoal for the removal of the contaminants.

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SECTION I

INTRODUCTION

This study was carried out to determine the feasibility of removing volatile organic trace contaminants from manned cabin atmospheres by absorption in a solvent. Since the cabin atmosphere must be recirculated, the solvent must have a very low vapor pressure, and the solvent vapors must be non-toxic. For the solvent to be useful in a zero-gravity field without a complicated mechanical system to contain the solvent, it must have a high viscosity for incorporation in a simple static system, such as a solvent coated fiberglass mat. Also, the solvent must be noncorrosive, stable, and preferably should have a relatively high surface tension. Finally, the trace contaminants should be highly soluble in the solvent.

Table I shows the contaminants detected in the atmospheres of the Mercury spacecraft and the Evaluator Flight 90 (3-30)MD-1 and considered in the study.

TABLE I

CONTAMINANTS DETECTED IN SPACE CRAFT ATMOSPHERES

Methanol	Carbon dioxide	<u>trans</u> -2-Butene
Hexamethylcyclotrisiloxane	Freon-114	<u>cis</u> -2-Butene
2, 2-Dimethylbutane	Toluene	Acetylene
1-Propanol	Freon-11	<u>p</u> -Dioxane
Freon-114, unsym.	<u>m</u> -Xylene	Sulfur dioxide
Methyl isopropyl ketone	<u>o</u> -Xylene	Allyl alcohol
Carbon disulfide	Benzene	Isobutylene
<u>trans</u> -1, 2-Dimethylcyclohexane	Acetone	Isoprene
Tetrachloroethylene	Ethylene	Acetic acid
1, 1, 3-Trimethylcyclohexane	Freon-22	Propionic acid
1, 1-Dimethylcyclohexane	Freon-23	Butyric acid
Ethylene dichloride	Freon-12	Toluene
1-Butanol	Freon-125	3-Methylpentane
Vinylidene chloride	Hexene-1	Ethyl formate
2-Propanol	Propylene	Vinyl chloride
<u>n</u> -Propyl acetate	<u>n</u> -Butane	Ethyl alcohol
1-Chloropropane	1-Butene	Ethyl acetate
Acetaldehyde	Isopentane	1, 4-Dioxane
Methylchloroform	<u>n</u> -Pentane	Cyclohexane
Formaldehyde	Propane	<u>n</u> -Hexane
2-Butanol	Methylene chloride	Trichloroethylene
Methyl ethyl ketone	<u>p</u> -Xylene	

In addition to the above list, hydrogen and methane also were considered.

Solubility studies were carried out with a selected member of the solutes in 23 different solvents. From the solubility data and assumed set of conditions, calculations were then made for design of an absorber.

SECTION II

DESCRIPTION OF APPARATUS AND PROCEDURE

SOLUBILITY APPARATUS

The apparatus used for determination of the solubility of gases in various liquids was a variation of that used by Young (ref 1). The solvent being studied was confined over mercury in a closed-end tube. A syringe was used to inject a known quantity of solute into a known quantity of solvent, through a serum cap in the bottom of the tube, and the pressure in the tube was adjusted to the desired value by a mercury leg. After equilibrium had been established by mixing, the volume of solute in the vapor phase was determined, and the amount of solute in the solvent was determined by difference. From this data, the Henry's law constant was calculated.

Figure 1 shows a sketch of the apparatus used for the determination of the solubility of gases in liquids. The apparatus was contained in an 18 by 20 by 28 cm plywood box containing a window for observation. The internal temperature control system consisted of a cooling coil, a heating coil, an air-circulating fan contained in a circulating duct, and a mercury temperature controller capable of maintaining the temperature within $\pm 0.2^\circ$ C. The sample tube, 10 mm ID by 18 cm long, was connected to a mercury leg and leveling bulb near the bottom. Just above the middle of the sample tube, a side arm was connected so that the volume of the sample tube above the side arm was approximately 6 ml while the volume below was approximately 8 ml.

To change a solvent sample to the sample tube, the apparatus was tilted approximately 45° counterclockwise, the plug of the stopcock was removed, and the level of the mercury in the sample tube was adjusted so that it was just above the lower side arm. A known amount of solvent (approximately 4 ml) was introduced into the sample tube. At this time, a 6-mm diameter steel ball for stirring was added to the tube. The stopcock was then replaced and the apparatus returned to the vertical position. The sample was degassed through the stopcock at a pressure of approximately 0.02 mm for a 4- to 16-hour period. During the degassing, the temperature was maintained at 25° C and the sample was continuously stirred. The steel ball stirrer was actuated by a magnet which slid up and down the outside of the sample tube. The magnet was connected to one end of a rod while the other end of the rod was connected to an eccentric on a 10-rpm motor.

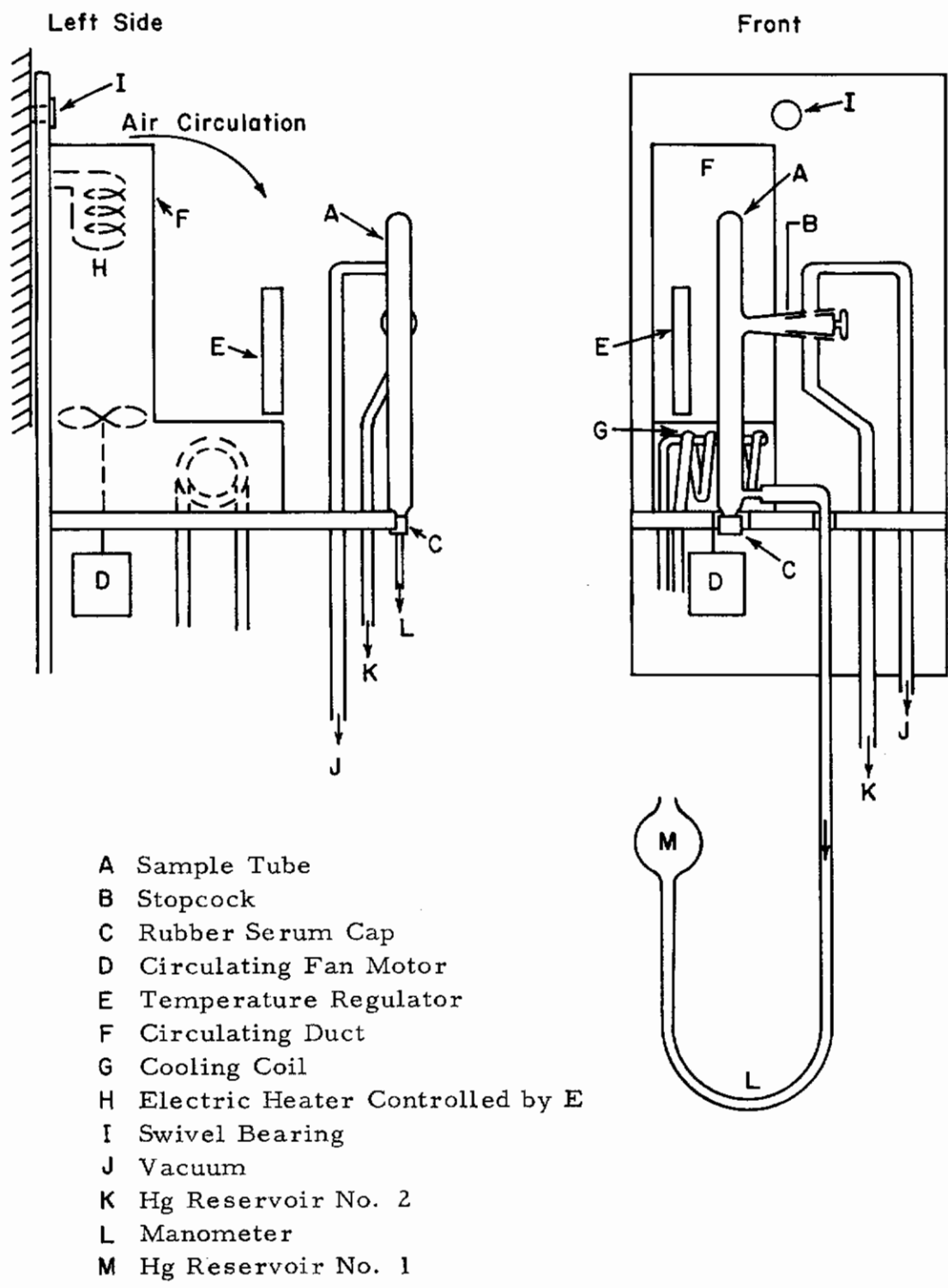


Figure 1. Apparatus for Determining Solubility of Contaminants in Solvents

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After degassing, the apparatus was tilted approximately 45° clockwise. The stopcock was then regulated so that mercury from reservoir No. 2 was allowed to fill the stopcock and the side arm up to the side arm entrance to the sample tube so that none of the solvent sample would enter the sidearm. The mercury reservoir No. 1 was raised so that the mercury meniscus in the sample tube was raised above the side arm. The stopcock was then closed and the apparatus returned to the vertical position.

Because solvent-degassing only approaches completeness, a "blank" determination of vapor pressure above the solvent was made prior to each run to determine the degree of completeness. The blank was made by setting the mercury reservoir M so the absolute pressure above the solvent in the sample tube was between 0 and 1 mm pressure. The partial pressure of the air in the solvent was calculated and later subtracted from the partial pressure of the contaminant gas or liquid solute.

A known quantity of solute (usually 0.5 ml if the solute was a gas, or 0.01 ml if the solvent was a liquid) was next introduced into the solvent by means of a long needle syringe inserted through the serum cap. The pressure on the solvent was then reduced until the volume of solute in the vapor phase was approximately 1 ml. The mixture was then agitated for approximately one-half hour and the height of the mercury meniscus in the sample tube noted. Stirring was continued for another one-half hour and the mercury level noted. This was repeated until the mercury level did not change over a one-half hour period. When equilibrium had been established, the following readings were taken:

- (a) Barometric pressure
- (b) Height of reference line on sample tube
- (c) Height of solvent meniscus
- (d) Height of solvent-mercury interface meniscus
- (e) Height of mercury meniscus in reservoir No. 1

All height measurements were made with a cathetometer accurate to within ± 0.005 cm. From the above data, the partial pressure above the solvent was calculated. The weight of solvent in the sample tube was obtained by multiplying the volume added by the solvent density. The amount of solute gas or liquid injected into the sample tube was measured directly, and the amount of gas or liquid absorbed by the solvent was calculated as the difference between that injected and that calculated to

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be in the vapor. The total volume of solute and residual air in the vapor phase was determined from a plot of sample tube volume versus distance from a reference line on the top of the tube to the solvent-vapor interface. The volume of residual air as determined in the blank run was subtracted from the total volume of solute and residual air to obtain the volume of solute in the vapor phase. The weight of solute in the vapor phase was then calculated by applying the ideal gas law. Finally, the Henry's law constant was calculated by dividing the partial pressure in mm of Hg by the concentration of the solute in the solvent in weight percent.

After a few determinations with the above apparatus, the sample tube was modified as shown in figure 2 and a second apparatus constructed. Figures 3 and 4 show the apparatus with and without the cover. The new apparatus functioned essentially in the same manner; however, the following changes in operation were required:

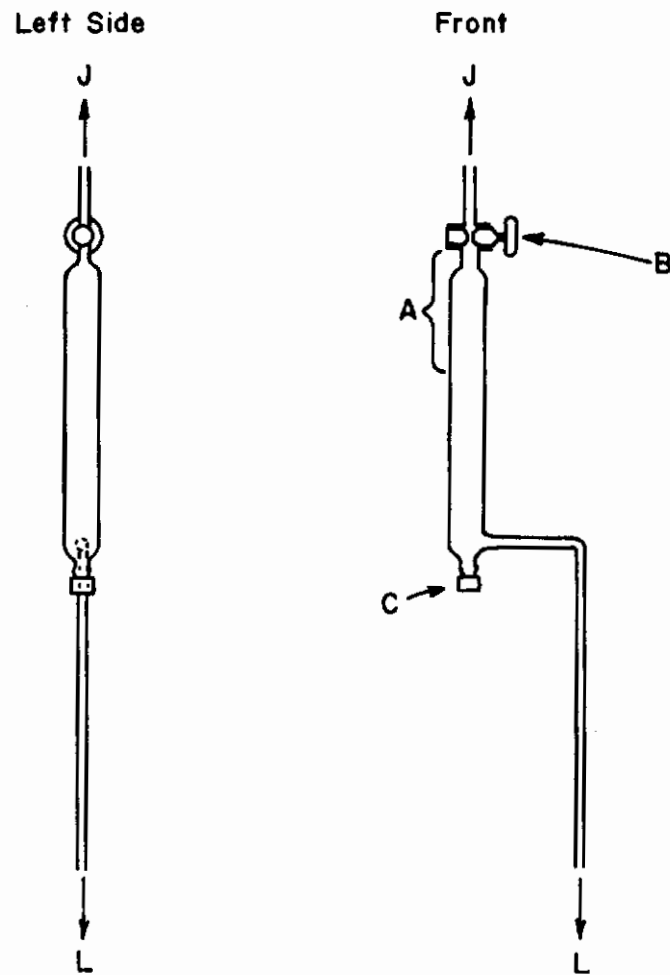
- (a) The steel stirring ball was inserted through the opening, which was subsequently sealed by the serum cap.
- (b) The apparatus did not have to be tilted during any phase of its operation.
- (c) The sample of solvent was introduced through the stopcock by means of a syringe fitted with a needle of sufficient length to extend into the sample tube.
- (d) By placing the stopcock at the top of the sample tube instead of on the side, the No. 2 mercury reservoir was eliminated.

VAPOR PRESSURE

The vapor pressure of a selected number of the solvents used in the study was determined with an isotenscope which was essentially the same as that described by S. A. Greene (ref 2).

VISCOSITY

The viscosity procedure followed was "Test for Kinematic Viscosity" ASTM D445-53T (Appendix A) using the Cannon-Fenske viscometer.



- A Sample Tube
- B Stopcock, Straight Bore
- C Rubber Serum Cap
- J Vacuum
- L Manometer and Hg Reservoir

Figure 2. Modified Sample Tube

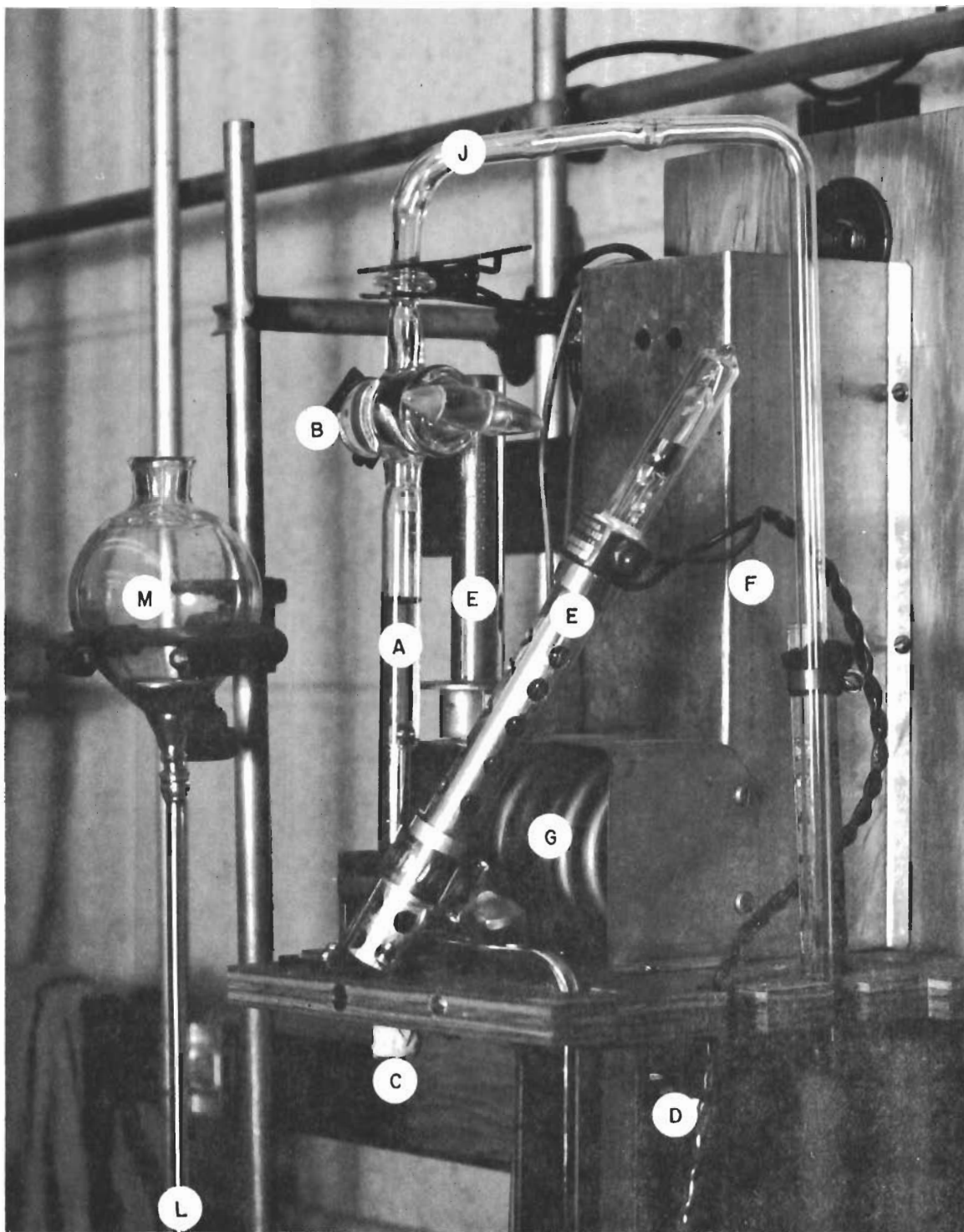


Figure 3. Apparatus for Determining Solubility of Contaminants in Solvents, Modified Sample Tube, Cover Removed

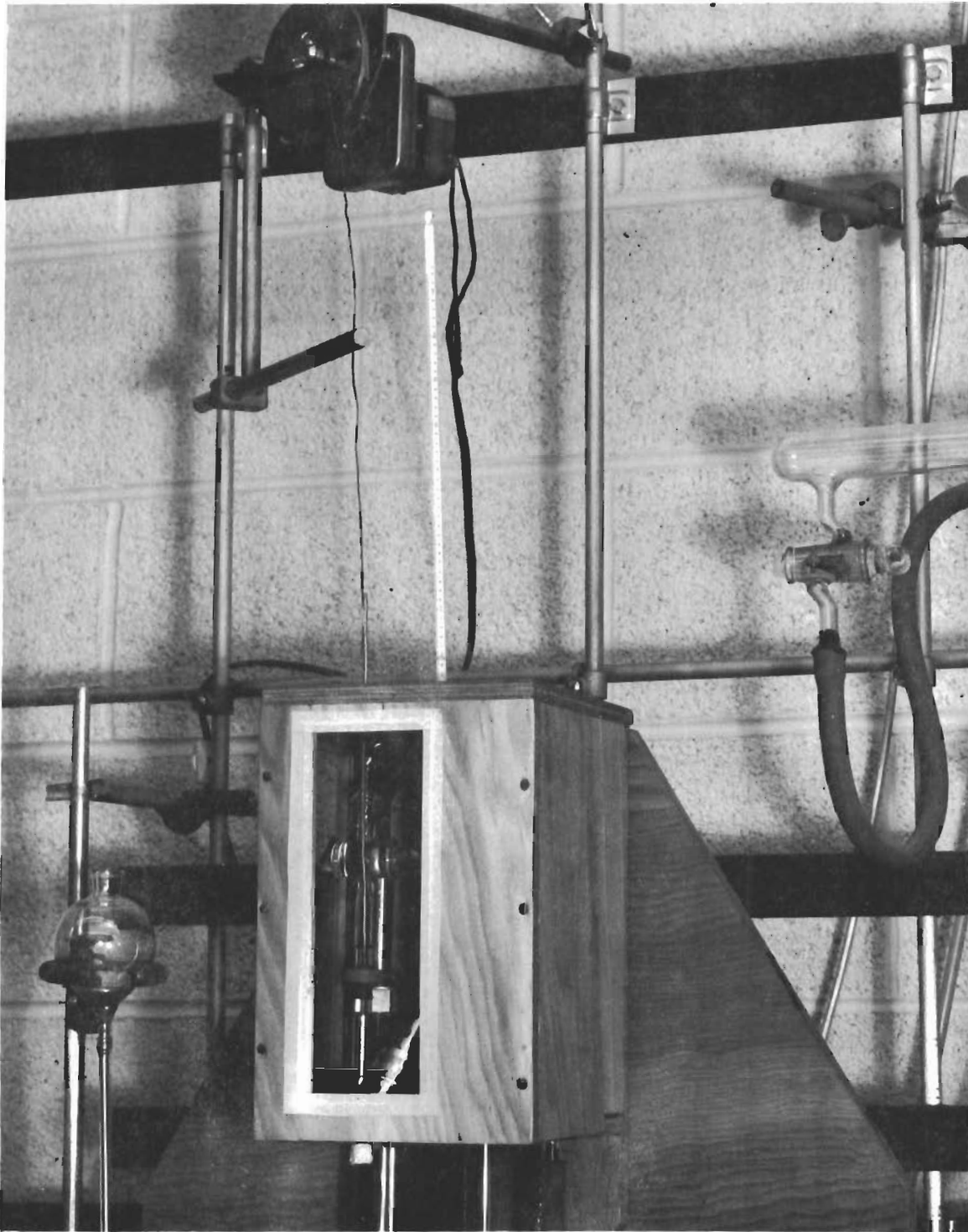


Figure 4. Apparatus for Determining Solubility of Contaminants in Solvents, Modified Sample Tube, Cover in Place

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SECTION III

SYNTHESIS OF SOLVENTS

Most of the solvents used in this study were synthesized at Denver Research Institute. However, several commercial compounds were used.

The selection of solvents to be synthesized was guided by the well-known concept that a substance is most soluble in a solvent to which it is closely related in molecular structure. Solvents were desired which contained several different molecular structures such as a paraffin portion to dissolve aliphatic hydrocarbons, an aromatic portion to dissolve aromatic compounds, etc. Our approach was to prepare esters from polyhydric alcohols, such as pentaerythritol or trimethylolpropane, and different kinds of acids, or from polybasic acids and different kinds of alcohols. In this way, many different molecular structures could be incorporated into the molecule.

The possibility of removing the contaminants either through a chemical reaction or by hydrogen bonding was considered. For example, the incorporation of an amino group into the solvent might provide a means of removing an acidic contaminant through the formation of an amine salt. However, many of the expected contaminants, such as the Freons and hydrocarbons, are too unreactive to be removed through a chemical reaction. Similarly for hydrogen bond formation, various contaminants contain either proton or electron donating groups and thus might be amenable for hydrogen bond formation through the use of an appropriate electron or proton donor in the solvent. However, many of the contaminants would not enter into a hydrogen bonding reaction.

The esters were prepared by refluxing stoichiometric quantities of a polyhydric alcohol (or a polybasic acid) with one or more acids (or alcohols) in the presence of a small amount of *p*-toluenesulfonic acid and a suitable solvent (xylene). For example, to prepare compound No. 1, 34 g (0.25 mole) of pentaerythritol (a tetrahydroxy compound), was reacted with a mixture of 34 g (0.25 mole) of *m*-toluic acid, 32 g (0.25 mole) of cyclohexanecarboxylic acid, 28 g (0.25 mole) of furoic acid, and 36 g (0.25 mole) of 2-ethylisohexanoic acid.

For all preparations of the esters, the water formed during the reaction was removed azeotropically and measured. The esterification was

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considered complete when the collected water equaled the theoretical expected amount. In some preparations, less than the theoretical amount of water was collected. These were considered complete when the amount of collected water did not increase during several hours of refluxing. The reaction mixture was washed with water, aqueous sodium bicarbonate, and again with water. Sometimes, during washing, emulsions formed. Whenever this occurred, benzene was added to aid in breaking the emulsion. The solution of the ester was dried with anhydrous sodium sulfate. The solvents were removed under reduced pressure. The residue was heated from 200 to 250° C at 1 mm Hg to remove small amounts of volatile materials. The crude ester was stirred with a mixture of decolorizing charcoal (1 part) and chromatographic grade alumina (2 parts) at 40° to 80° C for several hours. Filtration of the mixture through a fritted glass plate gave the product used for subsequent solubility tests. All products were clear and slightly colored.

Table II describes the esters synthesized and other solvents studied. Each ester is assigned an arbitrary number rather than a chemical name. Those esters which were prepared from a single alcohol and a single acid could be assigned a definite chemical structure. However, those prepared from a polyhydric alcohol, such as pentaerythritol, and two (or more) different acids can not be assigned a definite chemical structure, as they may be a mixture of a number of compounds in which one of the acids has esterified one, two, three, or four of the hydroxyl groups, and another acid has esterified the remaining groups. Such a mixture is highly desirable in this work, as it tends to give the synthesized solvent a lower melting point.

Some of the solvents synthesized (Nos. 1, 3, 4, 6, and 8) were not sufficiently fluid at 45° C (the maximum test temperature used) to permit stirring and accordingly solubilities of contaminants were not determined in these compounds. Some of these compounds were prepared with the thought that they might be blended with other compounds to produce low-melting mixtures; however, this approach was not explored.

Pour points and viscosities were determined for some of the compounds. These data are not needed for the determination of Henry's law constants

TABLE II
SOLVENTS FOR TRACE CONTAMINANT REMOVAL

Compd. No.	<u>Esters of Polyhydric Alcohols</u>		Molar Ratio <u>Acid/Polyol</u>
	<u>Polyhydric Alcohol</u>	<u>Acids used to Esterify Polyhydric Alcohol</u>	
1	Pentaerythritol	<u>m</u> -Toluic	1
		Cyclohexanecarboxylic	1
		2-Furoic	1
		2-Ethylisohexanoic	1
2	Pentaerythritol	2-Ethylisohexanoic	4
3	Trimethylolpropane	2-Furoic	3
4	Trimethylolpropane	<u>m</u> -Toluic	3
5	Trimethylolpropane	Benzoic	1
		Trichloroacetic	1
		Nonanoic	1
6	Trimethylolpropane	(4-Chloro-2-methylphenoxy)acetic	3
7	Trimethylolpropane	(4-Chloro-2-methylphenoxy)acetic	1
		Nonanoic	1
		Benzoic	1
8	Isosorbide	(4-chloro-2-methylphenoxy)acetic	2
9	Pentaerythritol	Benzoic	1
		Nonanoic	1
		Trichloroacetic	1
		(4-Chloro-2-methylphenoxy)acetic	1
10	Pentaerythritol	Benzoic	1
		Nonanoic	1
		Trichloroacetic	1
		Cyclohexanecarboxylic	1
11	Pentaerythritol	Benzoic	2
		2-Ethylisohexanoic	2
12	Pentaerythritol	Benzoic	1
		<u>o</u> -Chlorobenzoic	1
		2-Ethylisohexanoic	2

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TABLE II (continued)

Compd. No.	<u>Polyhydric Alcohol</u>	<u>Acids used to Esterify Polyhydric Alcohol</u>	<u>Molar Ratio Acid/Polyol</u>
13	Pentaerythritol	Benzoic Oleic Propanoic Picolinic	1 1 1 1
14	Pentaerythritol	Benzoic Oleic Propanoic Cyclohexanecarboxylic	1 1 1 1
17	Isosorbide	Benzoic Oleic	1 1
18	Pentaerythritol	Oleic Linoleic	2 2
19	Trimethylolpropane	Oleic Linoleic	1.5 1.5
20	Isosorbide	Oleic Linoleic	1 1
22	1, 10-Decanediol	Oleic Linoleic	1 1

Esters of Dibasic Acids

Compd. No.	<u>Dibasic Acid</u>	<u>Alcohol (s) Used to Esterify Acid</u>	<u>Molar Ratio Alcohol/Acid</u>
15	Isosebacic	Tridecanol (mixed primary isomers)	2
16	Sebacic	1-Methylcyclohexylmethanol Isodecanol	1 1
21	Sebacic	1-Methylcyclohexylmethanol	2
23	Isosebacic	Tridecanol (mixed primary isomers)	1
24	Half ester No. 23	Trimethylolpropane	0.33

TABLE II (continued)

Other Solvents

<u>Compd. No.</u>	<u>Name</u>
25	Octoil-S
26	Dow Corning 705 Fluid
27	Vegetable oil (Mazola)
28	4'- <u>n</u> -Heptyl- <u>m</u> -tercyclohexyl

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and serve only to describe the compound. These properties were determined for the following compounds:

Compound No.	Pour Point		Viscosity (centistokes)	
	$^{\circ}$ F	$^{\circ}$ C	100 $^{\circ}$ F (37.78 $^{\circ}$ C)	210 $^{\circ}$ F (98.89 $^{\circ}$ C)
2	5	-15.00	189	10.7
5	-15	-26.12	85.3	7.7
7	25	- 3.89	302	12.7
9	55	12.78	1640	26.4
10	25	- 3.89	425	17.7

Vapor pressures were determined for compounds Nos. 2, 11, and 18. For each compound, vapor pressures were measured at three or more different temperatures in the range from 110 to 150 $^{\circ}$ C. A plot of $1/T^{\circ}$ K vs the logarithm of the vapor pressure gave a straight line which was extrapolated to obtain a vapor pressure value at 25 $^{\circ}$ C. The following values were determined.

<u>Compound No.</u>	<u>Vapor Pressure, mm Hg/25$^{\circ}$ C</u>
2	0.03
11	0.02
18	0.04

Two commercially available esters were used in this study, namely Mazola corn oil (largely a glyceride of linoleic and oleic acids) and Octoil-S (specially purified di(2-ethylhexyl sebacate). In addition, two compounds which were not esters were examined, namely, Dow Corning 705 fluid, a silicone, and 4'-n-heptyl-m-tercyclohexyl. The latter compound was available from other work at the Denver Research Institute and its synthesis is described in reference 3. For ease in comparison, these four compounds have been assigned Nos. 25 through 28 (See table II).

SECTION IV

RESULTS

The experimental results are shown in tables III, IV, and V. Table III shows the experimentally determined Henry's law constants for a selected number of contaminants in 23 different solvents. Table IV compares the Ideal Henry's law constant and the Henry's law constant experimentally determined for a selected number of contaminants in solvent compound No. 18. Table V compares the absorption capacity of compound No. 18 and the corresponding adsorption capacity of activated charcoal for a selected number of contaminants. Design calculations for a solvent absorber are also included in the results.

TABLE III
EXPERIMENTAL VALUES OF HENRY'S LAW CONSTANT

Contaminant	Henry's Law Constant, mm Hg/wt %, at 25° C																
	Compound No. ^a																
	2	5	7	9	10	11 ^b	12 ^b	13	14	15	16	17					
Methane	120,000	170,000	300,000	150,000	120,000	550,000	160,000	240,000	160,000	32,000	24,000	39,000					
Ethane	4,500	8,100	27,000	28,000	18,000	11,000	11,000	5,100	4,600	3,600	3,800	5,200					
n-Butane	-	-	3,000	-	4,400	-	-	-	-	-	-	-					
n-Hexane	-	-	29	-	50	-	-	-	-	-	-	-					
Acetylene	3,200	2,300	4,500	5,200	4,600	17,000	6,500	4,500	3,100	3,000	2,100	2,400					
Benzene	-	-	10	-	4.8	-	-	-	-	-	-	-					
Toluene	-	-	3.9	-	-	-	-	-	-	-	-	-					
p-Xylene	-	-	2.3	-	-	-	-	-	-	-	-	-					
1-Butene	4,800	1,300	29,000	1,700	7,000	5,700	7,600	6,400	4,100	1,700	800	1,300					
Methanol	33	20	79	40	69	140	7.2	26	46	65	47	37					
Acetaldehyde	16,000	1,700	16,000	6,900	36,000	12,000	10,000	15,000	17,000	1,100	700	330					
1-Butanol	-	-	4.0	-	-	-	-	-	-	-	-	-					
Cyclohexane	-	-	10	-	-	-	-	-	-	-	-	-					
p-Dioxane	-	-	5.4	-	-	-	-	-	-	-	-	-					
Carbon disulfide	-	-	17	-	-	-	-	-	-	-	-	-					
Ethyl acetate	-	-	9.7	-	-	-	-	-	-	-	-	-					
Sulfur dioxide	-	-	4,000	-	1,200	-	-	-	-	-	-	-					
Acetone	-	-	25	-	-	-	-	-	-	-	-	-					
Freon 23	-	-	5,700	-	3,500	-	-	-	-	-	-	-					
1-Chloropropane	-	-	27	-	-	-	-	-	-	-	-	-					
Freon 114	-	-	2,800	-	3,200	-	-	-	-	-	-	-					
Acetic acid	-	-	2.0	-	-	-	-	-	-	-	-	-					
Vinyl chloride	-	-	6,100	-	6,100	-	-	-	-	-	-	-					

^aThe compositions of the solvents are described in table II.

^bThe values in this column were determined at 45° C.

TABLE III (continued)

Contaminant	Compound No. ^a												
	18	19	20	21	22	23	24	25	26	27	28		
Methane	35,000	19,000	24,000	37,000	28,000	37,000	39,000	38,000	150,000	47,000	62,000		
Ethane	3,600	3,000	3,200	5,500	3,800	2,800	3,600	3,900	6,600	8,800	2,700		
n-Butane	290	-	-	-	-	-	-	-	-	1,700	-		
n-Hexane	13	-	-	-	-	-	-	-	-	-	-		
Acetylene	2,700	3,300	2,600	1,500	2,200	2,800	2,900	2,900	4,900	3,900	-		
Benzene	5.6	-	-	-	-	-	-	-	-	6.0	-		
Toluene	3.5	-	-	-	-	-	-	-	-	-	-		
p-Xylene	1.9	-	-	-	-	-	-	-	-	-	-		
1-Butene	1,400	630	460	1,100	500	930	360	130	500	6,300	330		
Methanol	90	72	56	56	70	29	30	51	170	95	440		
Acetaldehyde	370	290	690	3,900	370	470	320	450	1,000	24,000	580		
1-Butanol	8.3	-	-	-	-	-	-	-	-	-	-		
Cyclohexane	8.6	-	-	-	-	-	-	-	-	12	-		
p-Dioxane	15	-	-	-	-	-	-	-	-	-	-		
Carbon disulfide	14	-	-	-	-	-	-	-	-	-	-		
Ethyl acetate	15	-	-	-	-	-	-	-	-	-	-		
Sulfur dioxide	770	-	-	-	-	-	-	-	-	600	-		
Acetone	36	-	-	-	-	-	-	-	-	-	-		
Freon 23	1,900	-	-	-	-	-	-	-	-	2,400	-		
1-Chloropropane	18	-	-	-	-	-	-	-	-	-	-		
Freon 114	210	-	-	-	-	-	-	-	-	2,900	-		
Acetic acid	5.3	-	-	-	-	-	-	-	-	-	-		
Vinyl Chloride	590	-	-	-	-	-	-	-	-	2,900	-		
Hydrogen	1,600,000	-	-	-	-	-	-	-	-	-	-		

TABLE IV

IDEAL AND EXPERIMENTAL VALUES OF HENRY'S LAW CONSTANT
FOR COMPOUND NO. 18

<u>Solute</u>	<u>Ideal Henry's Law Constant mm Hg/wt %</u>	<u>Experimental Henry's Law Constant mm Hg/wt %</u>
<u>Chlorinated Hydrocarbons</u>		
Vinyl chloride	637	590
Vinylidene chloride	75.7	
Methylene chloride	58.9	
1-Chloropropane	51.4	18
Ethylene dichloride	10.1	
Methylchloroform	9.2	
Trichloroethylene	7.0	
Tetrachloroethylene	1.4	
<u>Freons</u>		
Freon-23	5,950	1,900
Freon-22	1,080	
Freon-125	858	
Freon-12	479	
Freon-114 unsym.	123	
Freon-114	117	210
Freon-11	69.3	
<u>Alcohols</u>		
Methanol	47.5	90
Ethanol	14.7	
2-Propanol	8.6	
Allyl alcohol	5.2	
1-Propanol	3.6	
2-Butanol	2.9	
1-Butanol	1.2	8.3
<u>Aldehydes</u>		
Formaldehyde	1,970	370
Acetaldehyde	256	

TABLE IV (continued)

<u>Solute</u>	Ideal Henry's Law Constant <u>mm Hg/wt %</u>	Experimental Henry's Law Constant <u>mm Hg/wt %</u>
<u>Paraffins</u>		
Methane	175, 000	35, 000
Ethane	12, 600	3, 600
Propane	1, 950	(1, 000) ^a
<u>n</u> -Butane	402	300
Isopentane	116	(90) ^a
<u>n</u> -Pentane	86	(66) ^a
2, 2-Dimethylbutane	46	(34) ^a
3-Methylpentane	26	(16) ^a
<u>n</u> -Hexane	22	13
<u>Acids</u>		
Acetic Acid	3. 2	5. 3
Propionic acid	0. 64	
Butyric acid	0. 12	
<u>Olefins</u>		
Ethylene	21, 600	
Propylene	2, 530	
1-Butene	510	1, 400
Isobutylene	488	
<u>trans</u> -2-butene	276	
<u>cis</u> -2-butene	254	
Isoprene	105	
Hexene	25	
<u>Aromatics</u>		
Benzene	15	5. 6
Toluene	3. 8	3. 5
<u>p</u> -Xylene	1. 0	1. 9
<u>m</u> -Xylene	0. 96	(1. 8) ^a
<u>o</u> -Xylene	0. 80	(1. 4) ^a
<u>Alkynes</u>		
Acetylene	16, 600	2, 700

TABLE IV (continued)

<u>Solute</u>	<u>Ideal Henry's Law Constant mm Hg/wt %</u>	<u>Experimental Henry's Law Constant mm Hg/wt %</u>
<u>Cyclic Aliphatics</u>		
Cyclohexane	14	8.6
1,1-dimethylcyclohexane	2.4	
<u>trans</u> -1,2-dimethylcyclohexane	2.1	
1,1,3-Trimethylcyclohexane	1.2	
<u>trans</u> -1-Methyl-3-ethylcyclohexane	0.94	
<u>Ketones</u>		
Acetone	47	36
Methyl ethyl ketone	17	
Methyl isopropyl ketone	4.4	
<u>Acetates</u>		
Ethyl formate	42	
Ethyl acetate	12	15
<u>n</u> -Propyl acetate	4.0	
<u>Ethers</u>		
1,4-Dioxane	5.4	15
<u>Miscellaneous</u>		
Hydrogen	5,650,000	1,600,000
Carbon dioxide	13,000	
Sulfur dioxide	440	770
Carbon disulfide	57	14
Hexamethylcyclotrisiloxane	1.1	

^a Extrapolated values

TABLE V
COMPARISON OF ABSORPTION CAPACITY
OF COMPOUND NO. 18 AND CHARCOAL

	Wt. of Contaminant absorbed (g) ^a <u>1000 g Solvent No. 18</u>	Wt. of Contaminant absorbed (g) ^a <u>1000 g Charcoal</u>
Methane	0.000020	0.0026 ^b
Acetylene	0.00016	0.017 ^b
Ethylene	0.000018	0.016 ^b
Ethane	0.00010	0.017 ^b
Propane	0.00025	0.044 ^b
Isobutane	0.00064	0.087 ^b
1-Butene	0.00014	0.090 ^b
Methanol	0.0039	24 ^c
Benzene	0.025	150 ^c

^a Contaminant concentration = 50 ppm at 1 atm total pressure and 25°C.

^b Reference 4.

^c Reference 5.

DESIGN OF ABSORBER

To gage the feasibility of using a low volatile, viscous solvent for removal of trace contaminants, a design of a possible absorber showing size and weight is desirable. To make a specific design calculation, a number of assumptions are necessary:

ASSUMPTIONS

Space cabin volume = 1000 ft³

Cabin atmosphere = air at 25° C and 760 mm pressure

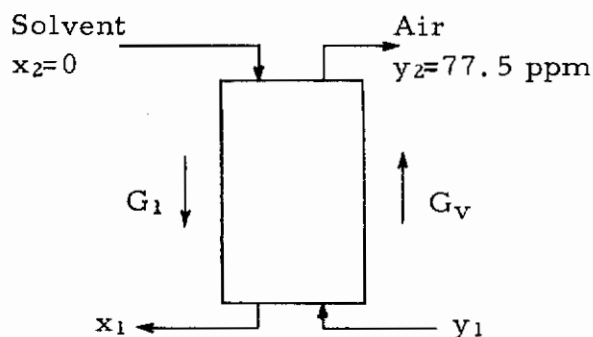
Solvent used in absorber = No. 18

Air Rate through absorber = 300 ft³/min.

Contaminant generation rate = 6.5 g/day

Allowable contaminant concentration = 77.5 ppm

To facilitate the calculation of the height of a transfer unit and the number of transfer units, the absorber will be assumed to consist of a, more or less, standard packed absorber in which gas is passed counter-current to solvent flowing over the packing as shown at the right.



Assuming a contaminant generation rate of 6.5 g/day the concentration to be removed from the atmosphere as it passes through the column is calculated as:

$$\frac{6.5 \text{ g}}{\text{day}} \times \frac{1}{300 \frac{\text{ft}^3}{\text{min}}} \times \frac{1}{0.074 \frac{\text{lb}}{\text{ft}^3}} \times \frac{1}{454 \frac{\text{g}}{\text{lb}}} \times \frac{1}{1440 \frac{\text{min}}{\text{day}}} \times \frac{1}{10^6} \quad (1)$$

= 0.45 g contaminant/million g air (ppm) where 0.074 is the density of air at 1 atm and 25° C.

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Assuming that the gas enters the column at 0.45 ppm above the toxic limit of 77.5, then

$$\begin{aligned}y_1 &= 77.95 \text{ ppm} \\y_2 &= 77.5 \text{ ppm}\end{aligned}\tag{2}$$

To determine the gas flow rate, a flooding velocity correlation by Lobo, et al (ref 6) is used. The mass velocity for flooding in a column packed with 1/2-inch Berl saddles or equivalent is given by:

$$\begin{aligned}G_V &= \sqrt{\frac{g_c^1 \epsilon^3 \rho_V \rho_l}{4 a_V (\mu_l)^{0.2}}} \\G_V &= \frac{537 \text{ lb}}{\text{ft}^2 \text{ hr}}\end{aligned}\tag{3}$$

The cross-sectional area of the column can be determined as:

$$\begin{aligned}A &= \frac{W}{G_V} = \frac{300 \text{ ft}^3}{\text{min}} \times \frac{0.074 \text{ lb}}{\text{ft}^3} \times \frac{\text{ft}^2 \text{ hr}}{537 \text{ lb}} \times \frac{60 \text{ min}}{\text{hr}} \\A &= 2.5 \text{ ft}^2\end{aligned}\tag{4}$$

Considering a circular column

$$\frac{\pi}{4} d^2 = 2.5 \quad d = \frac{4 \times 2.5}{\pi} = 1.78 \text{ ft. column}\tag{5}$$

Since y_1 , y_2 and G_V are known, the minimum liquid flow rate can be determined. This minimum liquid flow rate exists when x_1 is in equilibrium with y_1 . It is first necessary to calculate the average Henry's law constant. From the list of 21 compounds for which Henry's law constant was experimentally determined, excluding methane and hydrogen:

$$H = \frac{553 \text{ mm Hg}}{\text{wt } \%}\tag{6}$$

To convert this to ppm units it is necessary to divide by the total cabin pressure and multiply by the ratio of molecular wt. of contaminants/molecular weight of air, and multiply by 100.

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Average molecular weight of contaminants is = 72

Molecular wt of air = 29

$$H = \frac{553 \times 72 \times 100}{760 \times 29} = 180 \text{ in ppm units} \quad (7)$$

$$X_1 \text{ minimum} = \frac{77.95}{180} = 0.431 \text{ ppm}$$

From a material balance

$$G_1 \text{ minimum} = \frac{537.0 (0.45)}{0.431} = \frac{560 \text{ lb}}{\text{ft}^2 \text{ hr}} \quad (8)$$

This flow rate will give a pinch at the bottom of the column and will result in an infinite height to effect the necessary separation.

If twice the minimum solvent flow rate is assumed:

$$G_1 = \frac{1120 \text{ lb}}{\text{ft}^2 \text{ hr}} \quad (9)$$

The final liquid concentration can now be set from a material balance

$$\begin{aligned} x_1 &= \frac{537 (0.45)}{1120.0} = 0.216 \text{ ppm} \\ x_2 &= 0 \\ y_1 &= 77.95 \\ y_2 &= 77.50 \end{aligned} \quad (10)$$

To find the height of the column, it is necessary to find the height of a transfer unit and the number of transfer units. The height of a transfer unit will be calculated from a correlation by Sherwood (ref 7) for 1/2-inch Berl saddle packing or equivalent as follows:

$$H_1 = 0.00666 \left(\frac{G_1}{\mu_1} \right)^{0.28} \left(N_{SC_1} \right)^{0.5} \quad (11)$$

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To calculate the liquid phase Schmidt number, it is necessary to calculate the diffusivity of the contaminants in the liquid phase. From a correlation by Wilke (ref 8) by assuming the solvent property $\phi = 0.9$ and using the average molecular volume as calculated from Foust, et al (ref 9, p 555):

$$\begin{aligned}V_{AVG} &= 82.97 \text{ cm}^3/\text{g mole} \\D_{ab_1} &= 4.06 \times 10^{-7} \frac{\text{ft}^2}{\text{hr}}\end{aligned}\quad (12)$$

The liquid phase Schmidt number is

$$N_{sc_1} = \frac{\mu_1}{\rho_1 D_{ab_1}} = 11.75 \times 10^6 \quad (13)$$

This number is very high due to the high viscosity of the solvent, 106.9 cp. (258 lb/hr ft) as compared to 1.0 cp. for water.

$$\begin{aligned}H_1 &= 0.00666 \left(\frac{1120}{258} \right)^{0.28} (11.75 \times 10^6)^{0.5} \\&= 34.4 \text{ ft}\end{aligned}\quad (14)$$

The liquid phase mass transfer coefficient is given by

$$k_{1a} = \frac{G_1}{H_1} = \frac{1120}{34.4} = 32.6 \quad (15)$$

To calculate the gas phase mass transfer coefficient a correlation by Treybal (ref 10) which relates the gas phase mass transfer coefficient of a unknown system to that of the $\text{NH}_3 - \text{H}_2\text{O}$ system with the same flow rates and column conditions as follows:

$$k_{va} = k_{va\text{NH}_3} \left(\frac{(N_{sc})_{\text{NH}_3}}{N_{scv}} \right)^{2/3} \quad (16)$$

The gas phase mass transfer coefficient for the NH_3 - H_2O system is calculated from a correlation by Dwyer (ref 11):

$$\begin{aligned}k_{va_{\text{NH}_3}} &= 0.0065 (G_v)^{0.9} (G_l)^{0.39} \\ &= 0.0065 (537)^{0.9} (1120)^{0.39} \\ &= 29.0\end{aligned}\tag{17}$$

The gas phase Schmidt number for NH_3 in Air at 1/3 atmosphere pressure calculated from a Lennard - Jones calculation as shown by Foust, et al (ref 9, p 106):

$$N_{sc_{\text{NH}_3}} = 0.663\tag{18}$$

The gas phase Schmidt number for the contaminants is obtained from a similar calculation using the average molecular volume, molecular weight and boiling point of 38.5°C giving:

$$N_{sc_v} = 1.717\tag{19}$$

The gas phase mass transfer coefficient becomes

$$k_{va} = 29.0 \left(\frac{0.663}{1.717} \right)^{2/3} = 15.35\tag{20}$$

The calculation of the number of transfer units as reviewed by Foust, et al (ref 9, p 276) involves the integration of

$$N_1 = \int_{x_1}^{x_2} \frac{dx}{x - x_i}\tag{21}$$

where x_i is the interfacial concentration and is determined by a line connecting the operating line with the equilibrium curve and having a slope of

$$-k_{1a}/k_{va} = \frac{32.6}{15.35} = -2.12\tag{22}$$

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The graph in figure 5 is the determination of the interfacial concentration and the graphical integration of

$$N_1 = \int_{x_1}^{x_2} \frac{dx}{x - x_i} \quad (23)$$

The height of the column required is given by

$$Z = N_1 H_1 \quad (24)$$

From the following graphs

$$\begin{aligned} N_1 &= 0.703 \\ Z &= 34.4 \times 0.703 = 24.2 \text{ ft} \end{aligned} \quad (25)$$

SUMMARY

To effect the separation it will be necessary to have a column:

$$\begin{aligned} \text{diameter} &= 1.78 \text{ ft} \\ \text{height} &= 24.2 \text{ ft} \end{aligned}$$

The liquid flow rate through this column is so slow it can be assumed to be a stagnant film. Therefore, it will be required to place on the packing $1120 \times 2.5 = 2800$ lb of fresh solvent for each hr of operation. If the column could operate with minimum solvent and perfect equilibrium conditions, it would be required to carry $560 \times 2.5 = 1400$ lb of solvent for each hr of operation.

NOMENCLATURE

A	= cross sectional area - ft ²
A _v	= specific surface area of packing - ft ² /ft ³
d	= diameter - ft
D _{ab1}	= diffusivity of contaminant in solvent - ft ² /hr
g _c ¹	= acceleration due to gravity - ft/hr ²
G _v	= gas flow rate - lb/ft ² hr

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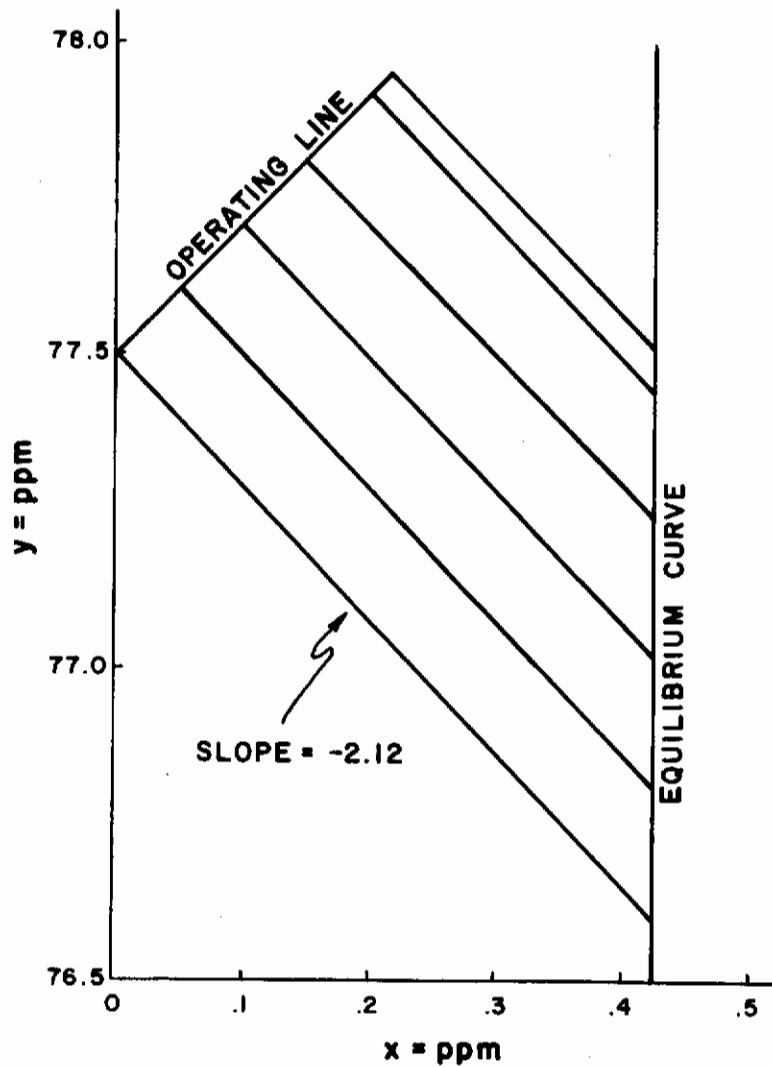
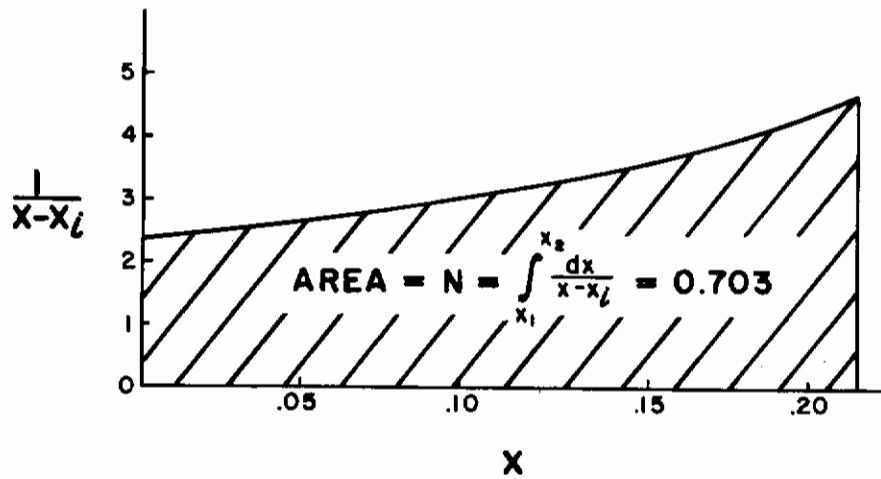


Figure 5. Graphical Evaluation of the Number of Transfer Units

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G_1	= solvent flow rate - lb/ft ² hr
H	= Henry's law constant
H_1	= height of liquid-phase transfer unit - ft
k_{1a}	= liquid-film transfer coefficient - lb/hr ft ³ (unit concentration difference).
k_{va}	= gas-film transfer coefficient - lb/hr ft ³ (atm)
N	= number of transfer units
N_{sc1}	= dimensionless Schmidt No. - $\mu/\rho D_{ab1}$
W	= mass flow rate - lb/hr
X_1	= concentration of solvent leaving column - ppm
X_2	= concentration of solvent entering column - ppm
y_1	= concentration of gas entering column - ppm
y_2	= concentration of gas leaving column - ppm
ρ_v	= density of gas - lb/ft ³
ρ_1	= density of solvent - lb/ft ³
μ_1	= viscosity of solvent - lb/hr ft

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SECTION V

DISCUSSION OF RESULTS

Table III shows the experimental values of Henry's law constant in terms of mm of mercury per weight percent of contaminant dissolved in solvent at 25° C. The data on compounds Nos. 11 and 12 were determined at 45° C as they were too viscous at 25° C to stir and thus reach equilibrium in a reasonable length of time. The usual units of Henry's law constant, mm of mercury per mole fraction were not used as the precise molecular weight of the solvent was not known for some compounds. The Henry's law constant was determined at contaminant concentrations in the solvent which varied from 0.0010 to 0.50 weight percent, which should be at a sufficiently low concentration that the partial pressure versus composition curve is essentially a straight line from the concentrations studied down to zero concentration. Table III shows a fairly wide variation in Henry's law constant for any given contaminant in various solvents; for example, methane varies from 550,000 mm Hg/wt percent in compound No. 11 to 19,000 in compound No. 19; ethane varies from 28,000 in compound No. 9 to 2700 in compound No. 28; and methanol varies from 440 in compound No. 28 to 7.2 in compound No. 12. Generally, the Henry's law constants for the various contaminants in compound No. 18 were as low or lower than the other solvents tested; thus, compound No. 18 was used for comparison purposes.

Table IV compares the ideal and experimental values of Henry's law constant for compound No. 18. The ideal solubility may readily be calculated from the vapor pressure and the molecular weight (which was 1190 for compound No. 18) of the solute as shown by Glasstone (ref 12). Since the vapor pressure of compound No. 18 was only 0.04 mm at 25° C, its vapor pressure in both the ideal solubility calculations and experimental study was neglected.

Generally, the experimentally determined Henry's law constants for the more volatile contaminants are in the range of one-third to one-fifth of the ideal values; whereas, for the less volatile compounds, the experimentally determined and the ideal values are of the same order of magnitude. This is a considerable improvement over what might be predicted. The values shown in parentheses in table IV were extrapolated from a plot of the ideal versus the experimentally determined Henry's law constant. The data were found to correlate very well for

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homologues within a particular class of contaminants; however, the correlation was not satisfactory for interpolation between different classes of contaminants.

To check the Henry's law constant of a mixture, two experimental determinations of solubility in compound No. 18 were made using approximately equimolar concentrations containing methane, ethane, Freon 23, acetylene, *n*-butane, Freon 114, 1-butene, 1-chloropropane, methanol, benzene, ethyl acetate, 1-butanol, and acetone. The runs were made in an apparatus similar to that shown in figure 2, with the exception that the sample tube was approximately 50 ml in volume. The gas sample was transferred to an evacuated gas sample tube containing a serum cap, and was compressed from approximately 30 mm Hg pressure to atmospheric pressure over mercury. A gas sample was removed from the tube with a syringe and analyzed by gas chromatography. Since the gas samples available after compression to atmospheric pressure were very small, on the order of 0.25 ml, and it was not known for sure whether some of the higher boiling point compounds might have partially condensed during compression, the analyses were somewhat questionable. However, the results indicated that the Henry's law constant for the seven contaminants which are gaseous at normal conditions were in the range of 30% less than those found individually and the six contaminants which are liquids at normal conditions were in the range of 50% greater than those found individually.

In table V a comparison is made between the absorption capacity of compound No. 18 and the adsorption capacity of charcoal for a select number of contaminants. The adsorption capacity on a weight basis of the individual contaminants in charcoal is between 100 and 6000 times as great as their respective solubility in compound No. 18. Although the data in table V include only five classes of compounds, the same relative absorption or adsorption capacities would be expected for other classes such as Freons, ketones, ethers, acetates, etc.

To determine the relative size of equipment required for trace contaminant removal by a solvent, a given set of conditions were assumed as shown in the absorber design calculations. Although the assumed conditions are undoubtedly not optimum, the size of the absorber and the quantity of liquid required are so large as to render the consideration of a solvent impractical. In the design calculations, the film coefficients were based on correlations for Berl saddle packing, which has a surface area of $150 \text{ ft}^2/\text{ft}^3$ of volume. Obviously, because of the high weight per unit volume for Berl saddles, they would be impractical to

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consider. If however, fiber glass packing (similar to a furnace filter) with a bulk density of 1.25 lb/ft^3 and a liquid surface area of approximately $1200 \text{ ft}^2/\text{ft}^3$ were considered, an absorber approximately 6 ft in height and 1.78 ft in diameter instead of 24.2 ft in height and 1.78 ft in diameter might be considered.

The design calculations were based on an average Henry's law constant of 553 mm/wt %, which did not include methane or hydrogen. Even if a solvent could be found with a Henry's law constant of 50, the absorber height would not be decreased more than approximately 25%. For example, if the space cabin atmospheric pressure and absorber were operated at $1/3$ atmosphere, the absorber height would be increased by approximately 20%.

For convenience the design calculations were based on a more or less conventional absorber having a continuous flow of solvent over the packing, counter-current to the flow of gas. If a static system is considered in which the viscous solvent is impregnated on a packing such as fiber glass and if equilibrium might be approached, it would require approximately 1400 lbs of fresh solvent per hour for 6.5 g/day of contaminants to be removed if a Henry's law constant of 553 is realized. A lesser quantity of solvent could be used if the solvent were regenerated more frequently than once per hour. It would be impossible to impregnate fiber glass or any similar packing with more than 4 to 5 lbs/ft^3 of packing, even with a solvent two or three times as viscous as solvent No. 18 which was assumed as the model in the calculations. In any case, the more viscous the solvent, the larger the absorber must be, as the height of the absorber is a function of the Schmidt number of the contaminants in the solvent which, in turn, is directly proportional to the viscosity of the solvent. The absorber diameter could be reduced if the air circulation rate were reduced; however, either the assumed trace contaminant concentration of 77.5 ppm would be surpassed or a higher absorber would be required.

Another problem which would be difficult to solve with a solvent absorbent would be regeneration. If the solvent were impregnated on a packing and the solvent regenerated by exposure to vacuum, there would be an appreciable loss of the cabin atmosphere because of the large voidage in the absorber, and the rate of evacuation of the solvent would necessarily be slow, in order to avoid frothing resulting from flashing of the absorbed contaminants.

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SECTION VI

CONCLUSIONS

From the study of twenty-three solvents of various chemical structures it was found that Henry's law constant of the various contaminants studied was in general lower in compound No. 18, which was an ester formed from pentaerythritol and oleic and linoleic acids, than any of the other compounds.

It was found that the contaminants were up to five times as soluble in compound No. 18 than would be predicted from ideal behavior and that in general the low vapor pressure contaminants approached ideal solubility and that the higher the vapor pressure of the contaminant the further it deviated from ideality.

Although the solubilities of the contaminants tested were as much as five times as soluble as might be predicted for compound No. 18, for a solvent to absorb the same quantities of contaminants per unit of weight as activated charcoal, it would be necessary to have a solvent which deviated from ideality by a factor of approximately one-hundred.

To remove 6.5 g/day of contaminants having a Henry's law constant of 550 mm Hg/wt % with compound No. 18 (if the maximum allowable concentration were 77.5 ppm) would require the use of the equivalent of 1400 lb per hour of freshly regenerated solvent. Also, if a more or less conventional type absorption column were used, it would have to be approximately 2 ft in diameter and 6 ft high.

Because of the low absorption rates and the low solubility of trace contaminants in the solvents studied, thus requiring a large sized absorber, regeneration of the solvent would be a most difficult task.

Even though some solvents were found which had an appreciable higher solubility for contaminants than would be predicted, because of the extremely high volatility and the relative inertness of the sixty-five contaminants considered, it is unlikely that any solvent can be found which would either react with or have suitable solubility to be considered. Thus, it is concluded that trace contaminant removal from space cabin atmospheres by the use of solvents is not feasible.

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13. ABSTRACT Twenty-three compounds were studied as potential solvents for the removal of trace contaminants from the atmosphere of a space capsule. The contaminants to be removed included a wide variety of chemical types such as aliphatic (both saturated and unsaturated), alicyclic, and aromatic hydrocarbons, chlorinated hydrocarbons, Freons, alcohols, aldehydes, acids, ketones, acetates, ethers, and other miscellaneous compounds. In an effort to dissolve as many of the contaminants as possible, solvents which contained a number of different chemical structures were synthesized. Most of the solvents were esters derived from the reaction of a polyhydric alcohol such as pentaerythritol, trimethylolpropane, or isorbide with a mixture of organic acids. Esters of sebacic and isosebacic acids also were considered. The solubilities of representative contaminants in each of the solvents were determined. Calculations based on these data showed that the best solvent was much less efficient than charcoal for the removal of the contaminants.		

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