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DEVELOPMENT OF A PREPROTOTYPE TRACE CONTAMINANT CONTROL SYSTEM

MARCH 31, 1977

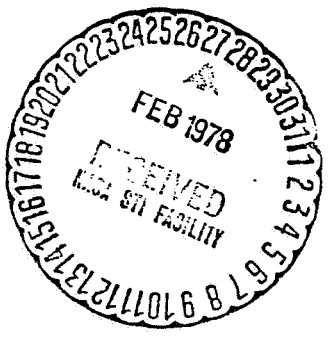
Prepared Under Contract NAS 9-14897

by

BIOTECHNOLOGY
LOCKHEED MISSILES & SPACE COMPANY, INC.
SUNNYVALE, CALIFORNIA

for

NATIONAL AERONAUTICS & SPACE ADMINISTRATION
JOHNSON SPACE CENTER



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INTRODUCTION

Previous development efforts have advanced the state of the art of contaminant control systems providing data on sorbent and catalytic oxidizer performance, hardware improvements, and system design methodology. The previous efforts have been directed toward providing basic design tools, so that as the contaminant load models are better defined, contaminant removal systems can be easily designed to meet spacecraft requirements.

Contract NAS 1-11526 covered the design, fabrication and testing of a trace contaminant control system designed to meet Space Station Prototype (SSP) requirements. The system included a fixed charcoal canister, regenerable charcoal canister, catalytic oxidizer, pre and post sorbent beds, high and low flow fans, electronic controller and supporting structure, valves, and ducting. The SSP system design was based on a contaminant load model that had evolved over the years, based largely on manned chamber testing results. The system embodied the most up-to-date system components and operating conditions.

The effort described in this report was based on these previous developments and covered the following major tasks:

- Revision of the steady state contaminant load model based on Shuttle equipment and material test programs and on the current Space Station studies.
- Definition of an emergency upset contaminant load model based on anticipated emergency upsets that could occur in an operational Space Station.
- Establishment by test, of control methods for the contaminants generated by the emergency upsets.
- Preliminary design of both steady state and emergency contaminant control systems for the Space Station application.

CONTAMINANT LOAD MODELS

Both steady state and emergency upset contaminant load models were generated to support preliminary design of a trace contaminant control system for an earth orbiting Space Station. At the time of this study effort, Space Station studies were directed more toward establishing mission objectives and overall vehicle size and configuration, and thus detailed information that would allow contaminant load model definition was not available. Therefore, the steady state model was based on an extrapolation of Spacelab data generated during a previous NASA contract effort (Ref. 1). The emergency load model was developed based on a review of the type of emergencies that could present themselves and a model upset condition.

Steady State Model

The Space Station steady state contaminant load model was based on data obtained from equipment and materials testing for the Space Shuttle program. In principle, contaminant generation rate can be determined by combining knowledge of the generation rate for the various organic materials used in the spacecraft and the amounts of materials present. Instead of using this approach, past programs such as Apollo relied upon a combination of material qualification testing, spacecraft testing, and animal exposure testing of groups of materials to obtain the successful result of no gross atmospheric contaminant problems. Spacecraft qualified materials were those that emitted less than 25 microgram/gm of CO, and less than 100 microgram/gm of TO (total organics) when tested according to a prescribed test procedure. Materials qualification testing was performed at the NASA White Sands Test Facility (WSTF), and additional requirements for approved materials, such as odor and flammability, were imposed. Only materials passing these test requirements were allowed in contact with the spacecraft habitable atmosphere.

Strict material screening requirements will probably not be applied to Space Station payload equipment in order to obtain the economic advantage of using "off-the-shelf" commercial equipment. To determine the contaminant generation rates for this type of equipment, the following logic has been used: Tests of commercial equipment off-gassing and of spacecraft components not fabricated using only approved materials were analyzed and contaminant generation rates per unit equipment weight were determined. This, combined with the estimated payload weight, gives the estimated payload contaminant generation rate. In addition, materials off-gassing tests were analyzed to determine contaminant generation rates for additional contaminants not detected in the equipment tests. Contaminants detected in the atmosphere of Skylab or Apollo, in flight or in ground testing were also added to the contaminant source list. In establishing contaminant generation rates from atmosphere tests, it was assumed that generation rates were directly proportional to cabin atmosphere concentrations. A number of contaminants were detected, but not quantified during previous manned space flight ground simulation tests. These contaminants were added to the source listing without estimating a production rate.

The subsystem contaminant generation rates not established by approved materials test results, were determined based on the payload generation rates. This was done by applying ratios of approved materials test results to equipment test results. In determining the ratios, it was assumed that equipment test results were representative of payload contaminant generation rates and that approved material test results were representation of subsystem contaminant generation rates. Ratios were determined by dividing equipment contaminant generation rates by material contaminant generation rates.

It is necessary to assume that the available contaminant test data is representative of the average composition of the payload and subsystem equipment contaminant off-gassing behavior. The items used in the analysis are equipment items tested for the Shuttle, Apollo-Soyuz, or Apollo in WSTF tests, or selected as representative Spacelab instrumentation in the Marshall Space Flight Center Component Verification Test program.

Payload Equipment Tests

Equipment items which are not fabricated under strict non-metallic materials controls are tested as "configuration tests" by the NASA WSTF. A total of 29 "configuration test" results were available and were analyzed. These tests were performed in dry air at 322^{o}K and 85 KPa. Each item was exposed for 72 hours according to the requirements of NHB 8060.1A Test 7 (Ref. 2). The chemical analysis techniques are well-developed and reliable, and are based on combination gas chromatography-mass spectroscopy, supplemented by infra-red analysis. Table 1 gives a list of the 29 configuration test items, which have a total weight of 48.7 kg. Off-gassing rate for each compound is reported as microgram per gm after the 72 hour exposure. Carbon monoxide (CO) and total organics (TO) expressed as pentane equivalents are also reported. The data was analyzed by multiplying the compound yield by 1000 to obtain milligram/1000 kg and dividing by 3 to obtain milligram/1000 kg-day. These values were then weight averaged for the 29 items.

Component Verification Test (CVT) results were available from the Marshall Space Flight Center. These tests were performed in moist air at atmospheric pressure. The test item surface temperature was held at 322^{o}K, and where appropriate, the test item was powered. The similarity between the WSTF and CVT test conditions was judged to be close enough, so that, for contaminants reported in common from both tests, the compound generation rate was averaged. Table 2 gives the 10 CVT Test items used, which weigh 113.6 kg. Data handling for the CVT data was similar to that used for the WSTF data.

A third source of component off-gassing data is contained in tests performed by Analytical Research Laboratory as part of a study of the suitability of commercial instrumentation for Spacelab (Ref. 3). The Analytical Research Laboratory off-gassing tests were performed in an open looped, continuously purged, nitrogen atmosphere, at atmospheric pressure and at the equilibrium temperature reached under normal powered operation with the exposure chamber at room temperature. These conditions would be expected to result in low off-gassing rates for the equipment items, and a comparison of off-gassing rate for contaminants found

Table 1 WSTF Configuration Test Items

WSTF No.	Description	Weight
4726	Intercom Set - Andrea Radio Corp.	2.65 kg
4743	TACAN	12.2
4774	Edge Lighted Panel - Acrylic/Epoxy/Vinyl/Glass Coastal Dynamics	.012
4840	Power Supply UPM - 15/100 - Datel Systems	.140
5120	UHF Transceiver P/N RT-1051/AVC 150	3.67
5144	Seals-Silicone-Nylon Nomex HT 2002	.019
5188	Binocular 20x60 S/N 1005	1.33
5189	Inertial Measurement Unit Singer-Kearfott	3.06
5227	Battery, Dry Chromalloy Electronics	.402
5228	Radio Transmitter ACR RT-10 ACR Electronics	.690
5232	Circuit Board Connectors Armel Electronics	.043
5235	Annunciator Korry Manufacturing Co.	.101
5251	Battery, Dry Mallory and Co.	.140
5252	Apollo Swimmer Radio Sylvania Electric Inc.	.528
5253	Radio Set AN/PRC-90 Oklahoma Aerotronics	.627
5255	Zoom Viewing Device	.950
5273	Edge Lighted Panel Acrylic/Epoxy/Vinyl Coastal Dynamics	.076
5274	Edge Lighted Panel Acrylic/Epoxy/Polyimide	.049
5275	Edge Lighted Panel Acrylic/Epoxy/Vinyl	.086
5334	MIB Board Page Circuit Boards IBM	.587
5349	Mars 1400 Recorder Bell and Howell	20.2
5361	Color Wheel Assembly S/N 1001	.166
5403	Patch Board - Dially Phthalate AMP Inc.	.206
5405	DAP/Glass 1280 Contact Board Virginia Panel Corp.	.020
5406	Edge Lighted Panel Polycarbonate/Epoxy/Vinyl	.122
5407	Edge Lighted Panel Acrylic/Epoxy/Vinyl/Fire Retardent - Coastal Dynamics	.125
5447	Film, Polaroid, B&W Type 107 Polaroid Corp.	.141
5466	E. L. Panel Acrylic/Vinyl/Flame Crete Coastal Dynamics	.134
5666	Hose, Altitude Oxygen, Silicone	.229
	Total Weight	48.70

Table 2 CVT Test Items

	Item Description	Weight
1.	Brush Strip Chart Recorder	29.5 kg
2.	Gulton Strip Chart Recorder	29.5
3.	USI Model 30 Elec. Hematocrit	1.45
4.	Fluke Model 8120A Dia. Multimeter	3.63
5.	Crimron Mod. DMM40 Dig. Multimeter	3.63
6.	Fluke Model 1952A Timer-Counter	3.63
7.	Newport Model 700 Timer-Counter	4.99
8.	H. P. Mod. 180E Oscilloscope	14.1
9.	Tektronix Mod. 7603 Oscilloscope	13.6
10.	Tektronix Mod. 485 Oscilloscope	9.53
	Total	113.56 kg

in the Analytical Research Lab equipment tests with either the WSTF or CVT results verifies this expectation. Carbon monoxide was not detectable by the instrumentation used, and none was reported. Lower limit of detectability for some contaminants appears to be lower for these tests than the WSTF or CVT tests, as some contaminants are reported only in the Analytical Research Lab testing. Thus, the Analytical Research Lab contaminant yield was not used, except if it was the only data available on a contaminant, in which case it was used as the contaminant generation rate. The rates were calculated at the maximum off-gassing rate reported for a single 12 hour period during the 10 day test of each equipment item. The rates were averaged to give milligram per 1000 kg of equipment per day.

Table 3 gives the data calculated using the methods just described. There are 64 compounds on this list. As the equipment test results are considered the best data source, these were used as the final payload rates for the contaminants detected.

Materials Tests

WSTF has tested thousands of non-metallic materials for possible use in the Apollo or Shuttle programs. A selected group of materials tested for the Shuttle program was analyzed. These were tested according to NHB 8060.1A Test 7 at 322^{O}K, using air as the test atmosphere. These materials were submitted for test by NASA-JSC or the Shuttle prime contractors, and are judged to be representative of the materials used in Shuttle or Spacelab subsystem fabrication. A total of 85 materials tests were examined, in which a total weight of 2.4 kg of materials was tested. Only materials that pass the requirements of less than 100 microgm/gm TO and 25 microgm/gm of CO were analyzed. Table 5 of Reference 1 lists the material WSTF identification numbers and the contaminant generation rates in mg/kg/day.

There were 56 compounds off-gassed by these tested materials, of which 14 had not been detected as off-gas products from the equipment tests. Materials test data was analyzed using a simple computer program, and the weight averaged yield of each compound determined, using the same method previously discussed. Table 4 gives the data calculated from the materials tests.

Table 3 Payload Contaminant Generation Rates as Determined by Equipment Test Data

	Contaminant Generation Rate (mg/1000 kg-day)			
	WSTF	CVT	ARL	Average
Total Organics	5003*		137	5000
Alcohols				
Iso-Butyl Alcohol		9		9
n-Butyl Alcohol	28	69.6	9.09	49
Cyclo Hexanol	82.3			82
Ethyl Alcohol	25.3	58	.84	42
Methyl Alcohol	1167	57	.32	612
Phenol	8.4		4.5	8.4
Iso-Propyl Alcohol	348	4.0	.55	180
n-Propyl Alcohol	15.4			15
Aldehydes				
Acetaldehyde	3.81			3.8
Butyraldehyde	82.1			82
Propionaldehyde	.647			.65
Aromatics				
Iso-Propyl Benzene	.0906			.091
Benzene	2.62	22	.084	12
Ethyl Benzene		44		44
Ethyl Methyl Benzene			.87	.87
Mesitylene	1.79		3.5	2.7
Styrene	1.09		7.5	1.1
Toluene	1115	80	2.5	598
Xylenes	148	102	19	125
Esters				
Butyl Acetate		28		28
Ethoxy Ethyl Acetate	26.8			27
Methyl Butyrate			.11	.11
Methyl Methacrylate	3.16			3.2
Propyl Acetate		8		8

Table 3 (continued)

	Contaminant Generation Rate (mg/1000 kg-day)			
	WSTF	CVT	ARL	Average
Ethers				
1,4 Dioxane	.403		.45	.40
Furan	.0428			.043
Tetrahydro furan	.	6		6
Chlorocarbons				
Chloro Benzene		9	5.0	9
Chloro Butane	19.0			19
Chloroform	6.32			6.3
Dichloro Ethane	11.8			12
Methyl Chloride	.144			.14
Methyl Chloroform	250		25	250
Methylene Chloride	658	13	.06	336
Tetrachloro Ethylene	8.05			8.1
Trichloro Ethylene	17.0		2.45	17
Chlorofluorocarbons				
F-113	584		17.4	580
Hydrocarbons				
Butane	6.02			6
Butene-1	3.77		.61	3.8
Cyclo Hexane		120	.75	120
Decane	.166			.17
Dimethyl Cyclohexane	.22		.09	.22
Heptene	7.82		.065	7.8
Hexane			17.5	18
Methane		26		26
Methyl Cyclohexane			.76	.76
3-Methyl Pentane			.09	.09
Octane	4.63		5.0	4.6
Octene	4.54			4.5
Nonane	.153			.15
Pentane	4.54			4.5
Propane	3.12			3.1
Propylene	4.42			4.4

Table 3 (continued)

	Contaminant Generation Rate (mg/1000 kg-day)			
	WSTF	CVT	ARL	Average
Ketones				
Acetone	125	277	1.6	201
Methyl Butyl Ketone	.475			.48
Methyl Ethyl Ketone	46		55	46
Methyl Iso-Butyl Ketone	48.1	17	2.8	32
Methyl Vinyl Ketone	.166			.17
Miscellaneous				
Ammonia	1.94			1.9
Carbon Monoxide	410	88		249
Dimethyl Sulfide			.16	.16
Siloxane Dimer	16.5			17
Siloxane Trimer	23.4			23
Siloxane Tetramer	76.6			77

*Total Organic Response reported from WSTF data was 2224, which is lower than the sum of the individual generation rates because of the lower response of the detection method to the individual contaminants, e.g. Freon-113 response of factor of three lower than pentane.

Table 4 Materials Offgassing Results

	Contaminant Production Rate mg/1000 kg (non-metallic)-day
Alcohols	
Butyl	4.4
Ethyl	144
Cyclohexanol	71
Methyl	460
Propyl	263
Aldehydes	
Acetaldehyde	270
Acrolein	29
Butyraldehyde	15
Propionaldehyde	22
Aromatics	
Benzene	56
Ethyl Methyl Benzene	3.7
Mesitylene	9.7
Methyl Styrene	18.0
Styrene	23.9
Toluene	307
Xylene	298
Esters	
Ethoxy Ethyl Acetate	5.5
Ethers	
Dioxane	19.5
Furan	2.1

Table 4 (continued)

	Contaminant Production Rate mg/1000 kg (non-metallic)-day
Chlorocarbons	
Chloro Benzene	4.9
Chloro Ethane	22.7
Chloro Propylene	1.4
Dichloro Ethane	14.2
Dichloro Methane	9.4
Methyl Chloride	7.9
Trichloro Ethylene	6.0
Chlorofluorocarbons	
Freon 11	26.9
Freon 113	384
Hydrocarbons	
Butadiene	7.7
Butane	0.04
Butene	30.1
Decane	8.0
Ethane	0.05
Heptane	0.19
Hexane	0.19
Methane	251
Octane	2.9
Octene	13.4
Pentane	1.6
Propane	2.2
Propylene	9.6
Ketones	
Acetone	717
Cyclohexanone	14.7
Mesityene Oxide	3.7
Methyl Butyl Ketone	38.1
Methyl Ethyl Ketone	110
Methyl Isobutyl Ketone	144

Table 4 (continued)

	Contaminant Production Rate mg/1000 kg (non-metallic)-day
Miscellaneous	
Siloxane	13.8
Siloxane Dimer	16.3
Siloxane Trimer	35.1
Siloxane Tetramer	82.1
Ammonia	265.
Acetophenone	9.6
Acetonitrile	6.7
Nitromethane	0.54
Carbon Monoxide	452.0

Materials offgas production rates were assumed to be characteristic of subsystems, so were factored upward to account for the increased off-gassing rate anticipated for unapproved materials as contrasted to approved materials in order to determine payload rates. A factor was derived for each class of compounds (alcohols, aldehydes, etc.) by comparing materials rates and equipment off-gassing rates for the compounds for which simultaneous data existed. These ratios are shown below:

	$\frac{\text{Payload Materials Yield}}{\text{Approved Materials Yield}}$
Alcohols	5.6
Aldehydes	5.6
Aromatics	2.4
Esters	5.6
Ethers	1.0
Chlorocarbons	10.8
Chlorofluorocarbons	9.7
Hydrocarbons	8.8
Ketones	2.1
Miscellaneous	5.6

To perform this calculation, it is necessary to have a factor for the amount of non-metallic material per unit of total equipment weight. Examination of this factor for the Apollo spacecraft and for Skylab gives a value of 0.16 for the fraction of non-metallics in spacecraft equipment and systems. Materials testing added 14 contaminants to the list and gave the above ratios that would later be used to determine subsystem rates once payload rates were known.

Skylab/Apollo Atmospheric Contaminants

Sixty-two additional contaminants were added to the model using the atmospheric monitoring results obtained from Skylab ground and flight monitoring, and from the Apollo atmosphere ground tests. The rule was applied that if a contaminant had been detected in a previous spacecraft it was added

to the list. The assumption was made that the generation rates are proportional to the reported concentrations. Production rates for contaminants not observed in equipment or materials tests were thus determined by ratioing as follows:

$$\text{Unknown Production Rate} = \text{Reference Production Rate} \times \frac{\text{Test Conc. of Unkn. Cont.}}{\text{Test Conc. of Ref. Cont.}}$$

For each unknown production rate, the reference contaminant was a member of the same chemical family e.g. (alcohol, aromatic, ester, chlorocarbon, halocarbon, hydrocarbon, ketone, or miscellaneous).

A priority of information was established, and compound production rates were calculated using the first appearance of the compound in the following list:

1. Skylab AM/MDA ground test - cryogenic trapping results (Ref. 4).
2. Skylab AM/MDA ground test - atmospheric grab sample results (Ref. 4)
3. Skylab flight data (Ref. 4)
4. Apollo ground test atmospheric monitoring data (Ref. 6)
5. Skylab AM/MDA ground test - charcoal desorption data (Ref. 4)

A number of other contaminants have been previously detected, but not quantified, during spacecraft ground simulator tests. Forty-four such contaminants were included in the listing, without production rates. Final payload contaminant generation rates were calculated by multiplying off-gassing rates of mg/1000 kg of non-metallic/day by a total source weight of 1634 kg, as determined from Spacelab Mass Properties Status Reports (Ref. 7, 8).

Subsystem Contaminant Generation Rates

To determine the rate of contaminant generation by Spacelab subsystems, the payload generation rate was factored downward to account for the use of approved materials in subsystem construction. The ratios developed earlier for the difference between approved and unapproved materials were used to derive subsystem generation rates. Payload generation rate per unit payload weight multiplied by these ratios gives the generation rate per unit subsystem weight. The subsystem weight that contributes to off-gassing was determined in a manner similar to that used to obtain payload contributing weight.

Subsystem source weights were determined by subtracting structure and other all-metallic parts from the total subsystems weight. Spacelab Mass Properties Status Reports (Ref. 7, 8) were used, and the listing for each subsystem examined to make the determination. The resulting contributing subsystem weight was 1433 kg. Because subsystem generation rates were determined from payload values, no new contaminants were added to the list from subsystem rate studies.

Metabolic Contaminants

Metabolically generated contaminants added eleven compounds to the list. In developing the metabolic contaminant load, production rates were defined only for contaminants where documented experimental evidence existed to define the rate or allow the rate to be calculated. The only source considered for metabolic contaminants were off-gassing from breath, sweat and flatus. Off-gassing from urine and feces were not considered, since it was assumed that the Orbiter waste management collection system would essentially eliminate these as a source of atmospheric contaminants. Tests involving man in closed chambers were also not considered, because it is impossible to separate contaminants generated by man from those generated by equipment. Eleven metabolically generated contaminants are listed with no production rates cited. These represent situations where contaminants were observed as metabolic products but not quantified. It can probably be assumed that these are at relatively low production rates since they were generally only observed in trace quantities. The basis of production rate for the individual contaminants follows:

n-butyl Alcohol, Ethyl Alcohol, Methyl Alcohol, Acetaldehyde, Acetone

The production rates for these contaminants are based on the average value cited by R. A. Dora (R. A. Dora, et. al. "Monitoring of the Bioeffluent of Man to Establish Space Vehicle Environmental Control Requirements", Aerospace Medical Association Preprint 36th Annual Meeting, April 1965, New York). In these tests a number of subjects were enclosed in bags and the contaminant build-up rates were monitored. Pyruvic acid (reported by Dora) was not included in the model. No other investigators have detected pyruvic acid. In addition, testing, at LMSC, in which pyruvic acid was introduced as a liquid at the rate defined by Dora, established that pyruvic acid could not exist as a vapor in the atmosphere at a level near its maximum allowable concentration.

Methane

The production rate for methane was based on data presented on the generation and composition of flatus in the Bioastronautics Data Book (Bioastronautics Data Book, NASA SP 3006, P. Webb M.D. 1964). The data book cites a range of flatus production from 100 to 2800 ml/day and a range of methane composition in flatus of 0 to 30%. An average value of 1500 ml/day of flatus and an average value of 15% methane composition was assumed.

Hydrogen

The production rate for hydrogen was based on data presented in the Bioastronautics Data Book for hydrogen in flatus. The data book shows a range of hydrogen composition in flatus of 3 to 34%. An average value of 18% was assumed. The value of 1500 ml/day for flatus production was also used.

Hydrogen Sulfide

The production rate for hydrogen sulfide was based on data presented in the Bioastraonutics Data Book for hydrogen sulfide in flatus. The data book shows a range of hydrogen sulfide composition in flatus of 0 to 0.0017%. An average value of 0.0009% was assumed with a flatus production rate of 1500 ml/day.

Ammonia

The production rate for ammonia was based on data presented in the Bioastronautics Data Book for ammonia in sweat. The data book shows a range of 2.5 to 35.0 mg of ammonia per 100 ml of sweat. An average value of 19 ml/100 ml was assumed. A sweat production rate of 2500 ml/day was also assumed.

Carbon Monoxide

The production rate for carbon monoxide was based on the results of a comprehensive literature survey. (Lockheed IDC to T. M. Olcott from R. J. Jaffe, Carbon Monoxide Production Rate, dated 20 October 1975). In the reference document, average values from seven tests were presented. Adjustments were made to account for metabolic activity and experimental variability. The

study concluded with a recommendation of 23 mg/man-day as the average value for the production rate of carbon monoxide.

Integrated Steady State Model

Table 5 presents the steady state contaminant load model established for the preliminary design of a Space Station contaminant control system. The model was derived from the Spacelab model by multiplying all payload and subsystem generation rates by a factor of 4, based on the estimated relative sizes of the two space cabins. The resultant rates are shown under the heading equipment rates on Table 5. Metabolic rates are shown as mg/man-day.

Emergency Upset Model

A review of the planned activities on-board a Space Station as currently under study by NASA, resulted in selection of three areas of potential emergency upset.

- Fire in the Space Station
- Accidents relating to experimental operations or scientific experiments
- Failures of life support equipment

Each of these areas was studied and a model situation was established from which emergency upset contaminant loads were derived.

Contaminants Generated by a Fire

To estimate the contaminants generated by a fire in a Space Station, a model involving spacecraft electronic equipment was developed. The model established the amounts and identity of the material consumed in the postulated fire. Also it was assumed that the fire was extinguished using a system similar to that of the Shuttle Orbiter and Spacelab which according to data obtained early in the study utilized Halon 1301 and Freon 14 as the estinguishing agents. These chemicals are converted to other species in the process of fire extinguishment, which are included in the contaminant load. The established contaminant load was compared to data obtained in the Apollo Command Module

Table 5 Preliminary Space Station Contaminant Generation Rates for Steady State Conditions

Contaminant	Equipment Rates (mg/day)	Metabolic mg/man-day
Alcohols		
Iso Amyl Alcohol	9.2	
n-Amyl Alcohol	14.0	
Allyl Alcohol	18.8	
Iso Butyl Alcohol	68	1.2
Sec Butyl Alcohol	52	
n-Butyl Alcohol	372	
Capryl Alcohol	4.8	
Cyclo Hexanol	624	
Ethylene Glycol	4.8	
Ethyl Alcohol	320	4
Methyl Alcohol	4660	1.5
2 Hexyl Alcohol	9.2	
Iso Propyl Alcohol	1372	*
n-Propyl Alcohol	116	*
Phenol	48	
Aldehydes		
Acetaldehyde	28	0.09
Acrolein	4.8	
Butyraldehyde	624	
Formaldehyde	*	
Propionaldehyde	4	
Benzaldehyde	292	
Valeraldehyde		*
Aromatics		
Benzene	112	
Iso Propyl Benzene	2.4	
n-Propyl Benzene	116	
Ethyl Benzene	400	
Ethyl Methyl Benzene	7.6	
1,2,4 Tri Methyl Benzene	420	
Decahydro Naphthalene	*	
Indene	60	
Mesitylene	22.4	
Naphthalene	*	
Methyl Styrene	60	
Styrene	11.2	
C-2 Styrene	96	
Xylene	1132	
Toluene	5240	

Table 5 (continued)

Contaminants	Equipment Rates (mg/day)	Metabolic mg/man-day
Esters		
Iso Butyl Acetate	380	
Butyl Acetate	216	
Ethoxy Ethyl Acetate	204	
Methyl Acetate	52	
Methyl Butyrate	0.8	
Methyl Methacrylate	23.2	
Ethyl Acetate	556	
Ethyl Lactate	104	
Propyl Acetate	60	
Iso Propyl Acetate	888	
Butyl Lactate	104	
Ethers		
1,4 Dioxane	5.2	
Furan	0.8	
Methyl Furan	*	
Tetrahydro Furan	76	
Chlorocarbons		
Carbon Tetrachloride	36	
Chloro Benzene	64	
Chloro Butane	136	
Chloroform	43.6	
Chloro Ethane	276	
Chloro Propylene	172	
Chloro Propane	*	
Chloro Acetylene	*	
Dichloro Benzene	30.4	
Dichloro Ethane	88	
Dichloro Ethylene	*	
Ethylene Dichloride	*	
Methyl Chloride	0.8	
Methyl Chloroform	1780	
Methylene Chloride	4780	
Tetrachloro Ethylene	56	
Trichloro Ethane	740	
Trichloro Ethylene	120	
Vinylidene Chloride	8.8	
Vinyl Chloride	*	

Table 5 (continued)

Contaminant	Equipment Rate (mg/day)	Metabolic mg/man-day
Chlorofluorocarbon		
Freon 11	292	
Freon 12	17.6	
Freon 13	*	
Freon 21	2.8	
Freon 22	4740	
Freon 113	4140	
Freon 114	92	
Freon 124	380	
Freon 112	52	
Trifluorochloroethylene	920	
Chlorodifluoroethylene	0.1	
Dichlorodifluoroethylene	192	
Fluoro Chloro Ethylene	17.6	
Fluorocarbons		
Difluoroethylene	*	
Ethyl Fluoride	*	
Fluoropropane	*	
Fluoroethane	*	
Pentafluoroethane	*	
Tetrafluoroethylene	*	
Hexafluoroethane	*	
Trifluoropropene	*	
Trifluoro Propane	*	
Trifluoro Methane	*	
Octafluorobutane	*	
Octafluoropropane	*	
Hexafluoropropene	*	
Vinylidene Fluoride	*	
Trifluoroethylene	*	
Hydrocarbons		
Butadiene	80	
Acetylene	13.2	
Butane	44	
Iso Butane	40	
Butene-1	26.4	
Cyclo Hexane	864	
Cyclo Hexene	17.6	
Cyclo Pentane	*	
Cyclo Propane	*	
Cyclo Pentene	66	
Decane	1.2	
Dimethyl Butane	57.2	
Dimethyl Cyclo Hexane	1.6	
Dimethyl Pentane	*	

Table 5 (continued)

Contaminants	Equipment Rate (mg/day)	Metabolic mg/man-day
Hydrocarbons (continued)		
Ethane	83.6	
Ethylene	1.2	
Ethyl Acetylene	*	
Heptane	15.6	
Heptene	57.2	
Hexane	132	
Limonene	84	
Methane	190	160
Isoprene	75	
Hexene	8.8	
Methyl Cyclohexane	5.2	
Methyl Acetylene	4.4	
2 Methyl Pentane	*	
3 Methyl Pentane	0.8	
Methyl Cyclopentane	418	
Methyl Cyclohexene	128	
Octane	35.2	
Octene	30.8	
Octyne	*	
Nonane	1.2	
Nonene	64	
Iso Pentane	8.8	
Pentene 1	17.6	
Propane	22	
Propadiene	189	
Propylene	30.8	
Pentene 2	*	
C-11 Alkane	8.8	
C-12 Alkane	30.8	
C-13 Alkane	2.8	
C-14 Alkane	8.8	
Pentane	30.8	
Dodecane	2.8	
Trimethyl Hexane	8	
Trimethyl Butane	*	
Ketones		
Acetone	1890	0.2
Methyl Butyl Ketone	56	
Di Isobutyl Ketone	360	
Methyl Ethyl Ketone	432	
Methyl Iso Butyl Ketone	552	
Methyl Iso Propyl Ketone	*	
Methyl Propyl Ketone	116	

Table 5 (continued)

Contaminant	Equipment Rate (mg/day)	Metabolic mg/man-day
Ketones (continued)		
Methyl Vinyl Ketone	2.0	
2 Octanone	18	
Cyclohexanone	48	
Mesityl Oxide	56	
Hydroxy Ketone+	132	
Mercaptans		
Ethyl Mercaptan		*
Methyl Mercaptan		*
Propyl Mercaptan		*
Organic Acids		
Acetic Acid		*
Butyric Acid		*
Caprylic Acid		*
Lactic Acid		*
Valeric Acid		*
Miscellaneous		
Ammonia	316	475
Acetophenone	64	
Acetonitrile	42	
Benzonitrile	*	
Carbon Monoxide	1890	23
Cyanamide	*	
Di Ethyl Sulfide	*	
Di Methyl Sulfide	1.2	
Di Ethyl Disulfide	*	
Di Methyl Disulfide	*	
Hydrogen		26
Hydrogen Sulfide		0.09
Methoxy Acetic Acid	*	
Nitromethane	3.6	
Trimethyl Silanol	88	
Hexamethyl Disiloxane	224	
Hexamethyl Cyclo Trisiloxane	316	
Octamethyl Cyclo Tetrasiloxane	616	
Decamethyl Cyclo Pentasiloxane	160	
Dodecamethyl Cyclo Hexasiloxane	233	
Tetradecamethyl Cyclo Heptasiloxane	180	
Hexadecamethyl Cyclo Octasiloxane	65.2	

+Compound detected in Skylab 4 atmosphere, structure and identity not presently known.

Table 5 (continued)

Contaminants	Equipment Rate (mg/day)	Metabolic mg/man-day
Miscellaneous (continued)		
Di Methyl Difluorosilane	*	
Tri Methyl Fluorosilane	*	
Sulfur Dioxide	*	
Trifluoroacetonitride	*	

*Indicates that the contaminant has been found in spacecraft or ground simulator test, but data does not allow a rate to be calculated.

Boilerplate Model test program, in which fires were ignited in the spacecraft and the resulting contaminants monitored. The agreement is surprisingly good for the contaminants detected in the test and predicted by the analysis.

It was assumed that 530 gm (1.17 lb) of organic material was consumed in the fire based on an estimated quantity of non-metallics in a "typical" electronic black box. The identity and mass of the material is given in Table 6. The selection was made based on the usual materials used in spacecraft electronic systems and in commercial instrumentation. The fire was assumed to involve commercial instrumentation in a Space Station Common Operational Research Equipment (CORE) rack. Contaminants involved were determined from reference 9 and from results previously obtained in the Lockheed Missiles & Space Company, Biotechnology Laboratory, for Teflon, silicone, and epoxy combustion. Table 7 shows the contaminants evolved in the reference fire. DuPont Bulletin S-35A was the source of the data which was averaged to estimate the yields of those contaminants generated by Halon 1301 and Freon 14; i.e., COF_2, $COBr_2$, HF, and HBr. The total amount of extinguishing agent released was estimated from Celesco Proposal AO-140, Oct. 1974, as the amount released to stop a fire in a 6.8 m^3 equipment rack.

Additional study of the fire model and additional discussions with NASA personnel following establishment of the data in Table 7 revealed that revised plans called for use of only Halon 1301 as a fire extinguishing agent, instead of both Halon 1301 and Freon 14. The contaminants evolved using 1301 only were established by analysis and review of the available literature which resulted in the following conclusions. Each extinguisher discharges 1.6 kg of 1301 upon actuation. The system uses two extinguishers which provide a total of 3.2 kg of Halon 1301 as the source. Decomposition product information is contained in DuPont Bulletin S35A, which reproduced tests by J. F. Treon of Kettering Labs, and by the Underwriters Laboratory. The Treon tests were conducted at 700°C and 1100°C, by passing 1301 in air thru an Inconel tube. The products formed were HF, HBr, Br_2 and carbonyl halide (expressed as $COBr_2$). The Underwriters tests were performed by analyzing the gases resulting from extinguishing a gasoline-on-wood fire. The same products were observed. Haun (AMRL-TR-66-240) burned 1301 in an oxygen-hydrogen

Table 6 Materials Consumed in Reference Fire

Polymer	Amount Burned (gm)
Silicone	110
Epoxy	110
Polypropylene	80
Polycarbonate	46
Teflon	32
Polyimide	30
Polyvinyl chloride	30
Polyurethane	26
Polyphenylene Oxide	26
Phenol-formaldehyde	20
Polysulfone	10
Polyester	10

Table 7 Contaminants Generated by Model Fire
(Halon 1301 + F14 as Extinguishing Agents)

	Weight (mg)			
	Polymers	Fire Exting.	Total Source	Apollo Burn Tests
CO_2	283,000		283,000	410,000
CO	154,000		154,000	920
Methane	8,800		8,800	
Alkane (ethane)	1,200		1,200	
Alkene (propylene)	12,100		12,100	
Methanol	800		800	
Butanol	1,100		1,100	
Acetaldehyde	120		120	
Propionaldehyde	62		62	
Acetone	320		320	
Benzene	1,680		1,680	
Toluene	700		700	
Ethyl Benzene	320		320	
Styrene	560		560	
Vinyl Chloride	40		40	
COF_2	320	15,800	16,100	10,900
CF_4	3,200		3,200	2,000
Tetrafluoroethylene	6,400		6,400	
$COBr_2$		8,200	8,200	
NO	14		14	
NO_2	21		21	
N_2O	3,000		3,000	
SO_2	1,500		1,500	
NH_3	150		150	
SiF_4				2,900
HCN	1,600		1,600	
HCl	9,100		9,100	
HF	320	80,200	80,500	
HBr		1,640	1,640	
Unchanged Fire Extinguishment Agent				
CF_4		1.5 kg	1.5 kg	
$CBrF_3$		1.6 kg	1.6 kg	

flame, at 800°C. The products he observed were HF, HBr, and Br_2. He reported a probable identification for a comound $CF_3O\text{-}CH_2CH(OCF_3)_2$. The amount of HF produced varied widely for these three decomposition tests. (The Underwriters Lab work does not cite the amount of 1301 used, so that yields of the compounds cannot be calculated).

Experimenter	Temperature	HF Yield
Treon	700°C	23.1 gm
Treon	1100°C	429 gm
Haun	800°C	1918 gm

Another study of this problem was conducted by E. T. McHale (Fire Technology Vol. 10, 15, 1974). His correlation is ppm/sec of HF formed in applying 1301 to a 0.093 m^2 fire, inside a 28.3 m^3 enclosure. 6.8 gm of HF were produced by a 0.093 m^2 fire burning for 60 seconds. Considering these data sources, an engineering judgement was made that the Treon 700°C decomposition data is appropriate for the products formed in extinguishing a fire using Halon 1301. There is no data on the relative distribution of COF_2 and $COBr_2$, so a 50-50 split was assumed. Table 8 presents the contaminant load model for a fire using Halon 1301 only as a fire extinguishing agent.

Experimental Operations or Scientific Experiment Upsets

Typical operations expected to be conducted onboard a Space Station were studied to determine the type of contaminants that would be released in the event of malfunctions. A number of documents were consulted (references 10 thru 16). One of the studies selected three candidate space manufacturing operations and a set of scientific experiments as the basis for Space Station design (Ref. 10). This set was used in the analysis.

Manufacturing

Three representative manufacturing processes were selected: biological, crystal growth and solidification processing. The biological manufacturing

Table 8 Contaminants Generated by Model Fire
(Halon 1301 as Extinguishing Agent)

	Weight (mg)			Apollo Burn
	Polymers	Fire Exting.	Total Source	Tests
CO_2	283,000		283,000	410,000
CO	154,000		154,000	920
Methane	8,800		8,800	
Alkane (ethane)	1,200		1,200	
Alkene (propylene)	12,100		12,100	
Methanol	800		800	
Butanol	1,100		1,100	
Acetaldehyde	120		120	
Propionaldehyde	62		62	
Acetone	320		320	
Benzene	1,680		1,680	
Toluene	700		700	
Ethyl Benzene	320		320	
Styrene	560		560	
Vinyl Chloride	40		40	
COF_2	320	3,000	3,300	10,900
CF_4	3,200		3,200	2,000
Tetrafluoroethylene	6,400		6,400	
$COBr_2$		3,000	3,000	
Br_2		5,400	5,400	
NO	14		14	
NO_2	21		21	
N_2O	3,000		3,000	
SO_2	1,500		1,500	
NH_3	150		150	
SiF_4				2,900
HCN	1,600		1,600	
HCl	9,100		9,100	
HF	320	23,000	23,000	
HBr		3,400	3,400	
Unchanged Fire Extinguishment Agent				
CBr_2F_3 Halon 1301		3,150 gm	3,150 gm	

operation consists of tissue culturing to produce valuable materials followed by electrophoresis to separate the desired product. The major possible source of Space Station contaminant is the gas storage and handling equipment used with the tissue culturing-fermentation tank. It has been assumed that carbon dioxide is the gas used, to maintain the proper growth pH, as for earth-based culturing units. We assume that because of equipment malfunction or human error that 10% of the tank contents are released to the Space Station atmosphere. This amounts to 2270 gm of CO_2.

Both the crystal growth and solidification processing operations are concerned with reforming materials brought from earth, not with producing the materials on board by chemical synthesis. Both operations seek to take advantage of crystal growth in zero g, and involve remelting the material at high temperature. An inert gas atmosphere is used for both processes. Making the same assumption of 10% loss of gas tank contents because of equipment malfunction or human errors, we calculate that 13,000 gm of helium may be released.

Further refinements in producing solar cells from the silicon ribbon produced in crystal growth may occur subsequently. These involve etching the silicon ribbon with HF, and doping the silicon using chemical gases. These might present major toxicological problems if released. However, the solar cell fabrication operation is not an early Space Station type of operation and need not be considered at present.

Many other Space Station manufacturing operations, such as large structure fabrication (beam welding, beam extrusion) or antenna construction are EVA. They have no impact on the trace contaminant control system.

Scientific Research

The following life science missions were extracted from reference 10.

- Body Fluid-Blood Volume Dist. & Electrolyte Metabolism
- Cardiovascular Function, Hemodynamics & Hematology
- Vestibular Neurological Function
- Pulmonary, Musculo-Skeletal Metabolic Function

- o Microbiological, Immunological Functions and Genetics
- o Zero-G Effects on Life Processes and Cell Tissues

Other scientific research missions, such as the radio telescope, solar observatory, and the space power development article (SPDA) antenna involve electronic instrumentation, and extra vehicular operations, and have no new impact as emergency conditions for the trace contaminant control system. To evaluate possible contaminants from Life Sciences Laboratory operations aboard Space Station, a preliminary equipment item specification catalog prepared in December 1975 was used (Ref. 11). Table 9 is a summary of the possible contaminants and the estimated yields. For several contaminants, multiple possible sources exist. In those cases, the largest yield is the one tabulated. Individual sources are discussed below. In some cases, such as Polaroid film usage, contaminants will be released as a result of normal operations. Suitable provisions to handle these contaminants, such as an "exhaust duct" direct to the contaminant control system inlet are recommended.

Invertebrate Anesthetizer (E.U. 70) - The anesthetizer uses CO_2. For a 30 day mission, the total mass of CO_2 stored is 354 gm, using supercritical storage. It is assumed that 10% may be vented to the atmosphere, or 35 gm.

Polaroid Film (E.I. 75F) - Film for the Polaroid SX70 camera has a weight of 0.11 kg for 10 frames. Similar film (B&W Type 107) was tested by NASA White Sands Test Facility (item No. 5447) in use conditions simulating Space Shuttle operations. The resultant off-gassing was mostly toluene and methyl isobutyl ketone. It is estimated that 1 mg each are released.

Cardiopulmonary Analyzer (E.U. 31) - This analyzer includes storage for oxygen, carbon dioxide, nitrous oxide, argon, and carbon-18 labeled carbon monoxide. Storage is in six 975 liter high pressure bottles. The gases of interest are nitrous oxide and carbon monoxide. For 10% leakage, the amounts that are released are 184 and 142 gm respectively.

Table 9 Contaminants Released During Scientific Research Operations

Contaminant	Amount Released (grams)
Ammonia	3
Carbon Dioxide	35
Carbon Monoxide	142
Nitrous Oxide	184
Nitric Acid (20% solution)	10
Formaldehyde (formalin solution)	10
Ethyl Alcohol	10
Isopropyl Alcohol	1.5
Chloral Hydrate	2.5
Gram Stain	14
Wright Stain	7
Recorder Ink	2.8

Chemicals (E.I. 44) - The preparation and preservation unit includes miscellaneous prepackaged and premeasured chemicals for life sciences research. The requirements are equipment-specific and no definition is now available. It was estimated that 500 gm of chemicals and containers would be required for a 7-day mission. These would be contained in a chemical storage unit which cushions and holds down the containers. For the sake of estimating leakage, we assume that misoperation results in the release of 10 gm each of nitric acid and formaldehyde.

Hemotology and Urology Unit (E.I. 105) - This kit is provided to collect, transfer, process and analyze blood and urine. It includes two 100 gm containers of ethyl alcohol. At 10% release to the atmosphere thru mishap, the contaminant released is 10 gm of the ethyl alcohol. If alcohol swabs are used to prepare the skin for taking blood samples, it is likely that much of the contained alcohol will enter the atmosphere. A typical commercial foil packaged gauze swab was tested and contained 1.5 gm of isopropyl alcohol.

Histology Kit (E.I. 108) - This kit is provided for preparation and preservation of small tissue samples. It includes 100 gm each of ethanol and formalin fixative, and 200 gm of assorted staining agents. The leakage source is estimated at 10 gm of ethyl alcohol and 10 gm of formaldehyde.

Microbiology Kit (E.I. 110) - The microbiology kit contains the material needed to facilitate growing and analyzing microbial organisms. It includes 50 gm of ethyl alcohol, leading to a 5 gm source in case of accidental spillage.

Dissection Kit (E.I. 114A) - The dissection kit contains the equipment needed for performing surgical procedures on vertebrates. It includes 25 gm of chloral hydrate. The estimated release in case of misoperation is 2.5 gm.

Vertebrate Physiology Kit (E.I. 114C) - The materials in this kit are used to perform physiological measurements on rats or macqaue monkeys. They include two-100 gm packages of ethyl alcohol and 25 gm of chloral hydrate. The leakage sources are 10 gm of ethyl alcohol and 2.5 gm of chloral hydrate.

Strip Chart Recorder (E.I. 150A) - The strip chart recorder discussed for Spacelab experiments is the Brush 222. It has two lead/lead dioxide batteries that are sealed. The pressurized fluid marking system contains a 28 gm ink cartridge. Leakage of 2.8 gm of recorder ink is assumed, in case of misoperation. In the event of battery malfunction, hydrogen gas may be released on recharge. Contaminants that may be released in case of an explosion are not presently quantified.

Staining System (E.I. 159) - The staining system is designed for zero-gravity slide staining. It contains an estimated 2 kg of Gram stain and Wright stain reagent, in the ratio of 2 to 1 in syringe dispensers. Provisions are made to route waste liquids to a disposable bag filled with an absorbent material. As the staining agents are contained to some extent, it is assumed that misoperation results in leakage of 1% of the contents, or 14 gm of Gram stain and 7 gm of Wright stain.

Thermocouple Indicator (E.I. 178B) - The thermocouple indicator is portable, and contains a 1.8 kg, 12v, rechargable nickel-cadmium battery. In the event of battery malfunction, hydrogen gas may be released on recharge. Contaminants that may be released in case of an explosion are not presently quantified.

Biological Specimen Holding Facility - Contaminants from the Biological Specimen Holding Facility (BSHF) were derived from the LMSC study of this facility completed in June 1976 and reported in reference 12. The environmental control system for the BSHF is a process loop which continually exchanges Spacelab air. The loop provides for removal of CO_2 and CO generated by the biological specimens. Urine and feces are air dried within the BSHF. Ammonia is absorbed using a chemically treated wicking mat. The estimated production rate for the reference design capacity of 4 Rhesus monkeys plus 24 rodents is 3 gm per day of ammonia. The emergency condition assumed is the release of 3 gm of ammonia to the Space Station atmosphere. Other contaminants such as hydrogen (69 mg/day) and methane (4630 mg/day) are not of interest as emergency condition hazardous contaminants.

EMERGENCY UPSET CONTROL METHODS

The investigation of emergency upset control methods was accomplished by identifying those contaminants that would exceed emergency allowable concentrations, establishing the contaminants for which there is little or no removal data and conducting laboratory testing to evaluate various control methods.

Identification of Problem Contaminants

The first step in the study of emergency upset control methods was to calculate the contaminant concentrations that would result from the instantaneous injection into the Space Station cabin of the contaminant quantities specified in the upset load model. The resultant concentrations were compared with 10 minute and 60 minute Emergency Exposure Limits (EEL) and 30 day Spacecraft Maximum Allowable Concentrations (SMAC) in order to assess the degree of the emergency removal problem. Three categories of severity were considered:

- Contaminants that exceed EEL would require immediate isolation of the crew from the space cabin atmosphere (face mask or equivalent) and rapid emergency removal.
- Contaminants that exceed SMAC, but are below EEL would require rapid removal from the cabin atmosphere, but would not require crew isolation.
- Contaminants that do not exceed SMAC do not require any action other than normal contaminant system operation.

The upset contaminant concentration calculations were based on a Space Station cabin volume of 300 m^3, which is approximately equivalent to 4 Spacelab modules.

For several compounds, 60 minute Emergency Exposure Limits (EEL) have been established by the National Academy of Science/National Research Council Panel on Air Quality in Manned Spacecraft (Ref. 17). These EEL values "are designed to avoid significant degradation in crew performance in emergencies and to avoid permanent health injury. They contain essentially no safety factor, and transitory effects may result." Similarly "10 minute special area" limits have been proposed for allowable repeated exposures that may be obtained in a spacecraft sanitary commode. There is no connotation of emergency exposure in their formulation or use.

Table 10 presents the results of the emergency upset contaminant concentration calculation. A comparison of the calculated cabin concentrations and the EELs and SMACs show those contaminants that require crew isolation and/or emergency removal. The following contaminants require crew isolation and emergency removal, i.e., they exceed EEL and SMAC.

- Carbon Monoxide
- Formaldehyde
- Hydrogen Chloride
- Hydrogen Fluoride
- Hydrogen Bromide
- Hydrogen Cyanide
- Carbonyl Fluoride
- Carbonyl Bromide
- Bromo Trifluoromethane (Halon 1301)
- Bromine

The following compounds require emergency removal, but not crew isolation; i.e., they exceed SMAC, but not EEL:

- Benzene
- Carbon Dioxide
- Sulfur Dioxide

The contaminants listed above formed the basis for the next step in the program, i.e., contaminant removal testing. Test data on the removal of benzene by charcoal and the removal of carbon dioxide and sulfur dioxide on lithium hydroxide are readily available, so that additional tests are not needed for the compounds in the second category. Removal data for the con-

Table 10 Comparison of Contaminant Concentrations, EEL and SMAC Emergency Upset Conditions

Contaminants	Production Rate (gm) Mfg	Sci. Exp.	Fire	Step Change in Cabin mg/m^3 Conc.	EEL mg/m^3	SMAC mg/m^3
Carbon Dioxide	2270	35	283	943	58,200	9,822
Carbon Monoxide	-	142	154	513	125	29
Halon 1301	-	-	3150	10,500	6,100	610
Nitrous Oxide	-	184	3	10	-	44
Ammonia	-	3	0.15	10	70	17
Formaldehyde	-	10	-	33	1	0.1
Ethyl Alcohol	-	10	-	33	3,800	95
Isopropyl Alcohol	-	1.5	-	5	500	100
Hydrogen Cyanide	-	-	1.6	5.3	-	1.0
Hydrogen Chloride	-	-	9.1	30	15	0.7
Hydrogen Fluoride	-	-	23	77	4	0.1
Hydrogen Bromide	-	-	3.4	11	-	0.1
Methane	-	4.6	8.8	29	-	1720
Ethane	-	-	1.2	4	-	184
Propylene	-	-	12.1	40	-	859
Methyl Alcohol	-	-	0.8	2.7	260	52
Butanol	-	-	1.1	3.7	600	30
Acetaldehyde	-	-	0.12	0.4	90	18
Propionaldehyde	-	-	0.062	0.2	-	119
Acetone	-	-	0.32	1.0	2400	240
Benzene	-	-	1.68	5.6	320	3
Toluene	-	-	0.7	2.3	760	75
Ethylene Benzene	-	-	0.32	1.0	860	87
Styrene	-	-	0.56	1.9	215	86
Vinyl Chloride	-	-	0.04	0.13	-	0.3
Carbonyl Fluoride	-	-	3.3	11	0.2	0.04
Freon 14 (CF_4)	-	-	3.2	11	2040	410
Tetrafluoroethylene	-	-	6.4	21	-	200
Carbonyl Bromide	-	-	3.0	10	4	0.08
Bromine	-	-	5.4	18	0.2	0.07
Nitrogen Oxide	-	-	0.014	0.05	-	1.2
Nitrogen Dioxide	-	-	0.021	0.07	4	0.9
Sulfur Dioxide	-	-	1.5	5	13	3

taminants in the first category is not available with perhaps the exception of hydrogen chloride, so they formed the basis for the test program.

Contaminant Removal Test Program

In order to test the removal of the contaminants generated during an emergency upset, a closed loop flow system, simulating a Space Station cabin, was designed and constructed. Figure 1 presents a schematic of the test setup which consisted of a 1.13 m^3 tank, sorbent canister, fan, humidifier and contaminant introduction system. In operation, the contaminants were injected into the mixing tank loop through one of two syringes. The syringes were charged with a known quantity of gas which was forced into the mixing tank loop by mechanically operating the syringe. Air was drawn through the flowmeter and sorbent canister by a fan located in the flow loop. A humidifier and shutoff valve allowed mixing tank humidity to be maintained within reasonable limits. Contaminant injection quantities were calculated to produce contaminant levels anticipated by the upset condition established by the load model. The decay of a contaminant was monitored during the test period as the sorbent or catalyst removed the contaminant from the mixing tank loop. Humidity and contaminant levels were monitored from the sample lines at the inlet and outlet of the sorbent canister.

Because most all of the contaminants to be tested are extremely toxic, the test setup was placed in a specially constructed room, built around a large exhaust hood. The room was sealed except for a six inch space around the floor which allowed the flow of air to enter around the floor area and sweep upward across the test apparatus, so that leakage, if there was any, would be swept up into the hood and out of the building. The test operator and sample taker wore a fireman's air breather at any time that toxic contaminants were handled, introduced into the system, or sampled. An observer was stationed at the test room door to insure the safety of the test operator. The observer also wore an air breather, ready for activation if needed.

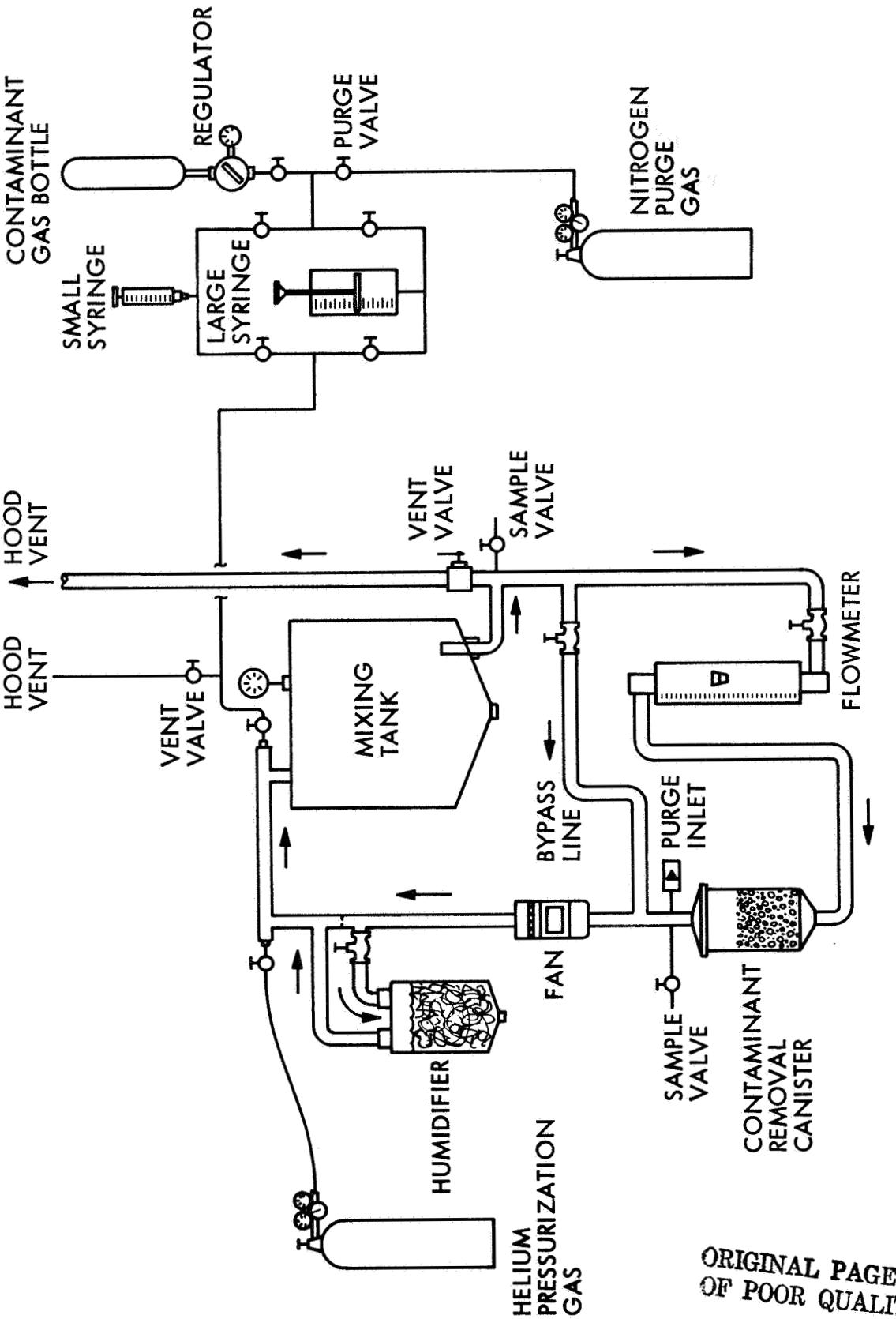

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Figure 1 Emergency Upset Contaminant Test Configuration

Table 11 presents a listing of the contaminants selected for test along with the contaminant time zero concentration, and the quantity of contaminant to be injected. The quantity of contaminant to be injected was based on a total system volume of 1.33 m^3 and the desired time zero concentration. Carbonyl bromide is not included in Table 11, because a source of the compound could not be found.

In selecting contaminant removal catalysts or sorbents for the test compounds, consideration was given to their chemical characteristics. The acid gases could best be removed by a base such as lithium hydroxide or base treated charcoal or Purafil. Halon 1301 could be removed by charcoal and carbon monoxide by a room temperature catalytic oxidizer. Based on this analysis and calculated sorbent capacities, the following quantities of sorbents or catalysts were used in the test.

Contaminant	Quantity of Removal Chemical
Carbon Monoxide	114 gm of Engelhard 2% Pt on 4x8 mesh Charcoal
F1301	1110 gms of Barnebey Cheney AC 6x10 mesh Charcoal
COF_2 HF Br_2 HCl HCN HBr	114 gms of BC-AC 6x10 mesh Charcoal Treated to 2 millimole KOH per gm of Charcoal

In conduct of the test, the chamber was first purged with room air and then closed out. The recirculation fan was run continuously with flow bypassing the contaminant removal canister, and a reference humidity measurement taken. Test chamber dew point was between 280 and 290°K for all test runs. The contaminant syringe was then loaded with the desired quantity of contaminant. The contaminant was injected and after a few minutes wait a time zero sample was taken. Flow through the removal canister was then set at 2.9 m^3/hr which was calculated to be the flow required to reduce the most difficult to remove contaminant to or near MAC in less than four hours. The four hours was selected as a reasonable length of time considering (1) the time the crew must wear a

Table 11 Contaminant Introduction Data

Contaminant	Desired Time Zero Tank Concentration (mg/m^3)	(ppm)	Quantity of Contaminant To Be Injected (mg)	(cc)
CO	513	445	680	590
HCl	30	20	40	27
HF	77	93	102	123
HBr	11	3.4	15	4.5
HCN	5.3	4.8	7	6.32 Pure gas 67.1 8% gas
COF_2	11	4	15	5.4
Br_2	18	2.7	24	*
F1301	10,500	1713	13,900	2270
Formaldehyde	33	27	44	*

*Liquid injection

Note: 1) All gases are 100% concentration except HCN which is 8% HCN in nitrogen.

2) Based on 1.33 m^3 system volume.

protective breather and (2) the size of the contaminant removal system. Samples of the contaminant removal device inlet and outlet were taken for carbon monoxide and F1301. Inlet samples only, were taken for the other contaminants, because a bubbler method of sample collection was used which required too much time to allow inlet and outlet samples to be taken. A gas chromatograph was used for CO and F1301 analysis and specific ion electrode for the others. A fresh load of sorbent was used for each contaminant introduced into the test system.

The results of the tests are summarized in Table 12 which shows that all contaminants were reduced to near or below MAC in less than four hours. Carbon monoxide has been previously shown to be readily oxidized on several noble metal catalysts and the 2% Pt on charcoal was the catalyst selected for Spacelab application. In order to insure that leakage or other factors were not a major contributor to the reduction in contaminant concentration a second run with carbon monoxide was made without any flow through the contaminant removal canister and with the bypass valve full open. Zero removal in the second run shows that all of the removal in run one can be attributed to the catalyst and none to other effects. Initial contaminant concentrations were reasonably close to desired values for these two tests. F1301 was also effectively removed to near MAC. The charcoal bed outlet concentrations show breakthrough and the final data point shows almost complete saturation at the 120 ppm level. Additional charcoal could be used to further reduce the cabin concentrations. The measured initial concentration for F1301 was also very close to the calculated value which shows that the injection system was working properly.

The remaining contaminants were reduced to below or near MAC relatively easily because they are so reactive. The contaminant removal device had to do a very small fraction of the job in most cases, because the initial concentration of the contaminants was only a fraction of the calculated value. These contaminants are so reactive that they combine with the moisture in the air and react with most any material with which they come in contact. Such was the case in the test system and such would also be the case in an actual spacecraft. The ratio

Table 12 Emergency Upset Model Test Data

Contaminant	Quantity of Contaminant Injected (cc)	Calculated Initial Concentration (ppm)	Test Time (min)	Measured Bed Inlet Concentration (ppm)	Measured Bed Outlet Concentration (ppm)
Carbon Monoxide	466	350	0	327	283
			35	51	ND
			60	20	ND
			90	5	ND
Carbon Monoxide	466	350	0	313	289
			20	348	295
			50	347	283
F1301	1793	1360	0	1324	1212
			53	1053	11
			120	116	140
			169	137	128
			236	121	113
Carbonyl Fluoride	6	4	0	0.13	-
			37	0.09	-
Carbonyl Fluoride	50	37	0	1.25	-
			26	0.36	-
			62	0.15	-
			95	0.10	-
Hydrogen Fluoride	180	93	0	0.25	-
			30	0.14	-
			111	0.10	-
Bromine	0.1*	2.7	0	0.31	-
			31	0.10	-
			85	ND (<0.03)	-

*Bromine/Ethanol Liquid Mixture Injection

Table 12 (continued)

Contaminant	Quantity of Contaminant Injected (cc)	Calculated Initial Concentration (ppm)	Test Time (min)	Measured Bed Inlet Concentration (ppm)	Measured Bed Outlet Concentration (ppm)
Hydrogen Chloride	30	20	0	261	-
			29	2.0	-
			72	1.8	-
Hydrogen Chloride	30	20	0	61	-
			30	1.1	-
			72	0.5	-
Hydrogen Cyanide	80	5.7	0	1.18	-
			31	0.44	-
			74	0.15	-
			129	0.02	-
			191	0.01	-
Hydrogen Bromide	10	3.4	0	0.23	-
			32	0.05	-
			87	0.02	

of initial measured contaminant concentration to calculated initial concentration varied according to an expected degree of stability or reactivity with one exception. Table 13 presents the order of reactivity and the contaminant introduction ratio.

Table 13

Contaminant Reactivity vs Introduction Ratio

Contaminant	Reactivity*	$\frac{\text{Measured Initial Conc.}}{\text{Calculated Initial Conc.}} \times 100$
HF	1	0.27
COF_2	1	3.2
HCl	2	305 to 1300
HBr	3	6.8
Br_2	4	11.5
HCN	5	20.7

*Arbitrary Number Assigned Depending on Degree of Reactivity (Not Quantitative)

Hydrogen chloride did not follow the expected rule. Initial measured concentration far exceeded the calculated value on the first run, so a second run was made, injecting the same quantity, but waiting five minutes longer before taking the time zero sample. Initial measured concentration was still much greater than calculated, but was lower. A yet unexplained problem with injection, sample taking or mixing in the tank must have produced the unexpected results. HCl concentrations were, however, very quickly reduced in both test runs.

PRELIMINARY DESIGN

The preliminary design was based on the contaminant load models established early in the program and on the emergency load model test program results. Separate steady state and emergency contaminant control systems have been evolved. The steady state model was used as input data to a computer program that sized elements of the system based on previously defined system analysis techniques. The emergency system was sized based on hand calculations, because the number of contaminants were fewer and the removal methods are easier to calculate.

Steady State System

In the development of a steady state system design, the first step was the preparation of a list of contaminants and the properties of each material required to carry out the analysis. A review of the list of contaminants showed none which required a base (such as lithium hydroxide) for control. It appeared that an activated carbon bed and a catalytic oxidizer would be sufficient. A post sorbent bed to remove possible toxic products formed in the catalytic oxidizer was also indicated. The data base was analyzed using the computer program ICHAR which was developed under NAS 1-11526. This program is described in reference 18. The computer analysis showed a required flow rate of slightly over 6.8 m^3/hr for a regenerable charcoal bed with trichloroethane being the design driver. There were no contaminants that required a greater flow, so a large fixed bed was not required. An analysis of contaminants not controlled by activated carbon showed that a flow of 2.9 m^3/hr was required for carbon monoxide removal, which established the flow rate through the catalytic oxidizer. Considering the sources of these design contaminants, a small safety factor was indicated for trichloroethane and a much larger one for carbon monoxide. Accordingly, a flow rate of 8.5 m^3/hr was selected for all components in the system.

With the flow rate through the regenerable bed set, the ICHAR program was run to define the quantity of activated carbon required. Several runs were made. The analysis showed a required bed size of 4.54 Kg for both the saturated and adsorption zones.

With a regenerable bed of this size and a catalytic oxidizer, two contaminants (ammonia and Freon 22) present potential problems. There is not sufficient activated carbon for removal of Freon 22 or for serving as a phosphoric acid substrate for removal of ammonia, therefore, breakthrough of the regenerable bed will occur. Poisoning of the oxidizer by these contaminants can probably be prevented by operating the oxidizer at an elevated temperature (550^{o}C). However, provisions must be made for control of the products of oxidation. LiOH should work well for the Freon 22 products, but no material with a large capacity for the NO_2 from ammonia oxidation, has been found. There are also those who feel that Freons should not be allowed to enter a high temperature catalytic oxidizer, because post sorbent bed performance becomes much more critical.

Contaminant Data Base

A list of 183 contaminants was prepared for input into the ICHAR computer program based on the steady state contaminant load model presented by Table 5. Many of the contaminants in the model have been identified in past tests, but were not quantifiable and were given zero generation rates. Of the 131 contaminants which have definable generation rates some fell into a general category of being non-structurally specific. Examples are:

C2 Styrene
C11 Alkanes
C12 Alkanes
C13 Alkanes
C14 Alkanes
Hydroxy Ketone

In addition several had no assigned spacecraft maximum allowable concentration (SMAC).

Table 14 and 15 present the contaminant data. Table 14 presents the SMAC in both ppm and mg/m^3. In some cases SMAC values were not available in which case, older data was searched to find SMAC values. Table 15 presents the contaminant properties necessary to carry out activated carbon adsorption calculations. They are molecular weight, density, solubility (0 = none, 1 = yes), and vapor pressure constants (A,B,C). The vapor pressure is calculated according to the following equations:

$$\log_{10} P = A - B/(C + t) \qquad \text{Note: } t \text{ in } {}^{o}C, \ P \text{ in mmHg}$$

if A = 0 then

$$\log_{10} P = C - \frac{(52.23)(B)}{T} \qquad \text{Note: } T \text{ in } {}^{o}K, \ P \text{ in mmHg}$$

The equations presented above and the values of A, B and C were obtained from the 10th edition of Lang "Handbook of Chemistry" and the 48th edition of CRC "Handbook of Chemistry and Physics". Much of the vapor pressure data was in tables of temperature vs pressure. In this case, the second form of the vapor pressure equation was derived in the temperature region of interest (277-322°K). For a few contaminants, complete data was not available, in which case, constants for similar materials were used. A zero in Table 14 for the constants A, B and C means, that data was not readily available and the generation rates were not given in the contaminant load model.

Charcoal Bed Analysis

The contaminant list was searched for all contaminants which could be reasonably removed by activated carbon and for which property data was available. This data was analyzed using the ICHAR computer program to determine the required bed flow rate and quantity of activated carbon required. A second run was then made using the selected flow of 8.5 m^3/hr and bed size (4536 gm). In the second run, contaminants for which breakthrough was indicated were allowed to rise to the SMAC level rather than to a level determined by 80% removal and 8.5 m^3/hr. The data from this run are included in Appendix A.

Table 14

Spacecraft Maximum Allowable Concentration

NAME	(PPM)	(MG/CU M)
ISO AMYL ALCOHOL	10.00	36.07
N AMYL ALCOHOL	10.00	36.07
ALLYL ALCOHOL	.20	.48
ISOBUTYL ALCOHOL	10.00	30.33
N BUTYL ALCOHOL	10.00	30.33
SEC BUTYL ALCOHOL	30.00	90.99
CAPRYL ALCOHOL	10.00	53.29
CYCLOHEXANOL	5.00	20.49
ETHYLENE GLYCOL	50.00	127.00
ETHYL ALCOHOL	100.00	188.52
METHYL ALCOHOL	40.00	52.44
HEXYL ALCOHOL	10.00	41.81
ISO PROPYL ALCOHOL	40.00	98.37
N PROPYL ALCOHOL	40.00	98.37
PHENOL	.50	1.93
ACETALDEHYDE	10.00	18.03
ACROLEIN	.05	.11
BUTYRALDEHYDE	50.00	147.54
FORMALDEHYDE	.10	.12
PROPIONALDEHYDE	50.00	118.83
BENZALDEHYDE	50.00	217.14
VALERALDEHYDE	50.00	176.22
BENZENE	1.00	3.20
ISO PROPYL BENZENE	5.00	24.59
N PROPYL BENZENE	10.00	49.19
ETHYL BENZENE	20.00	86.89
ETHYL METHYL BENZENE	5.00	24.55
TRIMETHYL BENZENE	3.00	14.76
DECAHYDRO NAPTHALENE	1.00	5.66
INDENE	1.00	4.75
MESITHYLENE	3.00	14.76
NAPHTHALENE	1.00	5.25
METHYL STYRENE	10.00	48.36
C2 STYRENE	.00	.00
STYRENE	20.00	85.24
XYLENE P	20.00	86.89
TOLUENE	20.00	75.41
ISO BUTYL ACETATE	30.00	142.60
BUTYL ACETATE	40.00	190.13
ETHOXY ETHYL ACETATE	10.00	54.08
METHYL ACETATE	40.00	121.25

METHYLBUTYRATE	7.00	29.25
METHYL METHACRYLATE	10.00	40.92
ETHYL ACETATE	50.00	180.27
ETHYL LACTATE	40.00	193.36
PROPYL ACETATE	40.00	167.17
ISO PROPYL ACETATE	50.00	208.96
BUTYL LACTATE	.50	2.99
DIOXANE	5.00	18.03
FURAN	.04	.11
METHYL FURAN	.04	.13
TETRAHYDRO FURAN	20.00	59.01
CARBON TETRACHLORIDE	.00	.00
CHLORO BENZENE	7.50	34.54
CHLORO BUTANE	50.00	189.40
CHLOROFORM	.00	.00
CHLOROETHANE	50.00	132.01
CHLORO PROPYLENE	7.50	23.49
CHLORO PROPANE	30.00	96.42
CHLORO ACETYLENE	.00	.00
DICHLORO BENZENE	5.00	30.08
DICHLORO ETHANE	10.00	40.49
DICHLORO ETHYLENE	1.00	3.97
ETHYLENE DICHLORIDE	.00	.00
ETHYL FLUORIDE	.00	.00
METHYL CHLORIDE	10.00	20.66
METHYL CHLOROFORM	.00	.00
DICHLORO METHANE	25.00	86.88
TETRACHLORO ETHYLENE	5.00	33.93
TRICHLORO ETHANE	1.00	5.46
TRICHLORO ETHYLENE	.00	.00
VINYLIDENE CHLORIDE	1.00	3.97
VINYL CHLORIDE	.10	.26
FREON 11	25.00	140.53
FREON 12	100.00	778.26
FREON 13	.00	.00
FREON 21	100.00	421.15
FREON 22	100.00	353.88
FREON 113	50.00	383.38
FREON 114	100.00	699.40
FREON 124	300.00	.00
FREON 112	25.00	208.52
TRIFLUORO CHLORO ETHYLENE	500.00	2382.98
CHLORO DIFLUORO ETHYLENE	.00	.00
DICHLORO DIFLUORO ETHYLEN	5.00	27.20
FLUORO CHLORO ETHYLENE	5.00	.00
DIFLUORO ETHYLENE	.00	.00
FLUORO PROPANE	.00	.00
FLUORO ETHANE	.00	.00
PENTAFLUORO ETHANE	.00	.00
TETRAFLUORO ETHYLENE	.00	.00
CHLORO TRIFLUORO ETHYLENE	.00	.00
HEXAFLUORO ETHANE	.00	.00
TRIFLUORO PROPENE	.00	.00
TRIFLUORO PROPANE	.00	.00

TRIFLUORO METHANE	5.00	.00
OCTAFLUORO BUTANE	.00	.00
OCTAFLUORO PROPANE	.00	.00
HEXAFLUORO PROPENE	.00	.00
VINYLIDENE FLUORIDE	.00	.00
TRIFLUORO ETHYLENE	.00	.00
BUTADIENE	100.00	221.34
ACETYLENE	175.00	186.47
N-BUTANE	75.00	178.37
ISO BUTANE	75.00	178.37
BUTENE-1	200.00	459.20
CYCLO HEXANE	60.00	206.63
CYCLO HEXENE	30.00	100.85
CYCLO PENTANE	.60	.00
CYCLO PROPANE	60.00	103.31
CYCLOPENTENE	30.00	83.61
DECANE	20.00	116.45
DIMETHYL BUTANE	30.00	105.79
DIMETHYL CYCLO HEXANE	25.00	114.80
DIMETHYL PENTANE	.00	.00
ETHANE	150.00	184.57
ETHYLENE	150.00	172.17
ETHYL ACETYLENE	80.00	177.07
HEPTANE	50.00	205.03
HEPTENE	40.00	160.72
HEXANE	200.00	705.30
LIMONENE	50.00	278.75
METHANE	2700.00	1767.74
ISOPRENE	200.00	557.49
HEXENE	50.00	172.19
METHYL CYCLOHEXANE	15.00	60.27
METHYL ACETYLENE	100.00	166.54
(2)METHYL PENTANE	500.00	1763.24
(3)METHYL PENTANE	500.00	1763.24
METHYL CYCLO PENTANE	25.00	86.10
METHYL CYCLO HEXENE	25.00	98.38
OCTANE	50.00	233.71
OCTENE	50.00	229.60
OCTYNE	.00	.00
NONANE	20.00	104.97
NONENE	50.00	258.29
ISO PENTANE	100.00	295.24
PENTENE-1	65.00	186.56
PROPANE	100.00	180.46
PROPADIENE	50.00	81.98
PROPYLENE	500.00	860.96
PENTENE-2	.00	.00
C11 ALKANES	.00	.00
C12 ALKANES	.00	.00
C13 ALKANES	.00	.00
C14 ALKANES	.00	.00
PENTANE	200.00	590.48
DODECANE	20.00	139.41
TRIMETHYL HEXANE	20.00	104.97

TRIMETHYL BUTANE	.00	.00
ACETONE	100.00	237.66
METHYL BUTYL KETONE	10.00	40.99
DIISOBUTYL KETONE	5.00	29.10
METHYL ETHYL KETONE	10.00	29.51
METHYL ISOBUTYL KETONE	10.00	40.99
METHYL ISOPROPYL KETONE	10.00	35.24
METHYL PROPYL KETONE	20.00	70.49
METHYL VINYL KETONE	1.00	2.87
OCTANONE	10.00	52.47
CYCLOHEXANONE	2.00	8.03
MESITYL OXIDE	2.50	10.04
HYDROXY KETONE	.00	.00
ETHYL MERCAPTAIN	.10	.00
METHYL MERCAPTAIN	.10	.00
PROPYL MERCAPTAN	.00	.00
ACETIC ACID	2.00	.00
BUTYRIC ACID	5.00	.00
CAPRYLIC ACID	25.00	.00
LACTIC ACID	.00	.00
VALERIC ACID	25.00	.00
AMMONIA	25.00	17.39
ACETOPHENONE	50.00	245.83
ACETONITRILE	4.00	6.72
BENZONITRILE	.00	.00
CARBON MONOXIDE	25.00	28.75
CYANIMIDE	25.00	.00
DIETHYL SULFIDE	.10	.00
DIMETHYL SULFIDE	1.00	2.54
DIETHYL DISULFIDE	.00	.00
DIMETHYL DISULFIDE	.00	.00
HYDROGEN	3000.00	.00
HYDROGEN SULFIDE	1.00	.00
METHOXY ACETIC ACID	.00	.00
NITROMETHANE	.00	.00

Table 15

Contaminant Properties

ORIGINAL PAGE IS
OF POOR QUALITY

NAME	MW	RHO	SOL	A	B	C
ISO AMYL AL	88.15	.819	.00	.00000	55.204	10.188
N AMYL ALCO	88.15	.813	.00	.00000	55.732	10.157
ALLYL ALCOH	58.08	.855	1.00	.00000	44.326	9.164
ISOBUTYL AL	74.12	.802	.00	.00000	48.374	9.571
N BUTYL ALC	74.12	.810	.00	.00000	49.878	9.587
SEC BUTYL A	74.12	.808	1.00	.00000	49.303	9.877
CAPRYL ALCO	130.23	.822	.00	.00000	53.984	9.220
CYCLOHEXANO	100.16	.962	.00	.00000	52.912	9.400
ETHYLENE GL	62.07	1.113	1.00	8.26210	2197.000	212.000
ETHYL ALCOH	46.07	.789	1.00	8.04494	1554.300	222.650
METHYL ALCO	32.04	.792	1.00	7.87863	1473.110	230.000
HEXYL ALCOH	102.18	.820	.00	.00000	47.512	9.011
ISO PROPYL	60.10	.785	1.00	6.66040	813.055	132.930
N PROPYL AL	60.10	.804	1.00	7.99733	1569.700	209.500
PHENOL	94.11	1.071	.00	7.13617	1518.100	175.000
ACETALDEHYD	44.05	.783	1.00	6.81089	992.000	230.000
ACROLEIN	56.06	.841	1.00	.00000	30.288	7.743
BUTYRALDEHY	72.11	.817	.00	.00000	33.860	7.959
FORMALDEHYD	30.03	.815	1.00	.00000	24.052	7.836
PROPIONALDE*	58.08	.807	1.00	.00000	30.288	7.743
BENZALDEHYD	106.13	1.046	.00	.00000	53.605	9.358
VALERALDEHY	86.13	.819	.00	.00000	.000	.000
BENZENE	78.11	.879	.00	6.90565	1211.033	220.790
ISO PROPYL	120.20	.862	.00	6.93666	1460.793	207.777
N PROPYL BE	120.20	.862	.00	6.95142	1491.297	207.140
ETHYL BENZE	106.17	.867	.00	6.95719	1424.255	213.206
ETHYL METHY	120.00	.870	.00	7.01582	1529.184	208.509
TRIMETHYL B	120.20	.876	.00	7.04383	1573.267	208.564
DECAHYDRO N	138.25	.884	.00	7.25013	1807.040	228.000
INDENE	116.16	.991	.00	.00000	43.630	7.874
MESITHYLENE	120.20	.865	.00	7.07436	1569.622	209.578
NAPHTHALENE	128.18	1.145	.00	6.84578	1606.529	187.227
METHYL STYR	118.18	.911	.00	7.27534	1695.400	220.000
C2 STYRENE	.00	.000	.00	.00000	.000	.000
STYRENE	104.15	.906	.00	6.92409	1420.000	206.000
XYLENE P	106.17	.861	.00	6.99052	1453.430	215.307
TOLUENE	92.14	.866	.00	6.95464	1344.800	219.482
ISO BUTYL A	116.16	.871	.00	.00000	38.960	8.120
BUTYL ACETA	116.16	.870	.00	.00000	38.950	8.110
ETHOXY ETHY*	132.16	.975	.00	.00000	38.960	8.120
METHYL ACET	74.08	.933	1.00	7.20211	1232.830	228.000

METHYLBUTYR	102.13	.889	.00	7.02835	1265.000	212.700
METHYL METH	100.00	.939	.00	.00000	40.063	8.597
ETHYL ACETA	88.11	.901	.00	7.09808	1238.710	217.000
ETHYL LACTA*	118.13	1.030	1.00	.00000	38.960	8.120
PROPYL ACET	102.13	.886	.00	.00000	40.176	8.550
ISO PROPYL	102.13	.874	.00	.00000	36.305	8.138
BUTYL LACTA*	146.19	.964	.00	7.09808	1238.710	217.000
DIOXANE	88.11	1.034	1.00	.00000	35.720	7.863
FURAN	68.08	.937	.00	6.97523	1060.851	227.740
METHYL FURA	82.00	.914	.00	.00000	.000	.000
TETRAHYDRO *	72.11	.888	1.00	7.20211	1232.830	228.000
CARBON TETR	153.82	1.594	.00	6.93390	1242.430	230.000
CHLORO BENZ	112.56	1.106	.00	7.10690	1500.000	224.000
CHLORO BUTA	92.57	.847	.00	6.75197	1125.800	212.000
CHLOROFORM	119.38	1.489	.00	6.90328	1163.030	227.400
CHLOROETHAN	64.52	.903	.00	6.80270	949.620	230.000
CHLORO PROP	76.53	.938	.00	.00000	25.340	7.150
CHLORO PROP	78.54	.859	.00	.00000	27.242	7.493
CHLORO ACET	60.48	.000	.00	.00000	.000	.000
DICHLORO BE	147.00	1.300	.00	6.88045	1496.200	201.000
DICHLORO ET	98.96	1.176	.00	7.18431	1358.460	232.200
DICHLORO ET	96.94	1.255	.00	.00000	30.760	7.890
ETHYLENE DI	96.94	1.250	.00	7.18431	1358.460	232.200
ETHYL FLUOR	48.06	.000	1.00	.00000	21.800	7.636
METHYL CHLO	50.49	.920	.00	.00000	21.270	7.348
METHYL CHLO	133.41	1.346	.00	.00000	32.450	7.778
DICHLORO ME	84.93	1.336	.00	.00000	30.024	7.880
TETRACHLORO	165.83	1.631	.00	.00000	39.357	8.168
TRICHLORO E	133.41	1.441	.00	6.85189	1262.570	205.170
TRICHLORO E	131.39	1.466	.00	7.02808	1315.040	230.000
VINYLIDENE	96.94	1.250	.00	.00000	27.690	7.628
VINYL CHLOR	62.50	.908	.00	6.49712	783.400	230.000
FREON 11	137.37	1.494	.00	.00000	26.217	7.496
FREON 12	190.19	1.486	.00	.00000	19.980	7.190
FREON 13	.00	.000	.00	.00000	.000	.000
FREON 21	102.92	1.426	.00	.00000	25.000	7.512
FREON 22	86.48	1.491	.00	.00000	19.804	7.364
FREON 113	187.38	1.576	.00	.00000	29.750	7.727
FREON 114	170.92	1.455	.00	.00000	23.940	7.405
FREON 124	.00	.000	.00	.00000	.000	.000
FREON 112	203.83	1.645	.00	.00000	36.650	8.143
TRIFLUORO C	116.47	.000	.00	.00000	21.243	7.426
CHLORO DIFL	.00	.000	.00	.00000	.000	.000
DICHLORO DI *	132.93	1.000	.00	.00000	28.284	7.911
FLUORO CHLO	.00	.000	.00	.00000	.000	.000
DIFLUORO ET	.00	.000	.00	.00000	.000	.000
FLUORO PROP	.00	.000	.00	.00000	.000	.000
FLUORO ETHA	.00	.000	.00	.00000	.000	.000
PENTAFLUORO	.00	.000	.00	.00000	.000	.000
TETRAFLUORO	.00	.000	.00	.00000	.000	.000
CHLORO TRIF	.00	.000	.00	.00000	.000	.000
HEXAFLUORO	.00	.000	.00	.00000	.000	.000
TRIFLUORO P	.00	.000	.00	.00000	.000	.000
TRIFLUORO P	.00	.000	.00	.00000	.000	.000

TRIFLUORO M	.00	.000	.00	.00000	.000	.000
OCTAFLUORO	.00	.000	.00	.00000	.000	.000
OCTAFLUORO	.00	.000	.00	.00000	.000	.000
HEXAFLUORO	.00	.000	.00	.00000	.000	.000
VINYLIDENE	.00	.000	.00	.00000	.000	.000
TRIFLUORO E	.00	.000	.00	.00000	.000	.000
BUTADIENE	54.09	.621	.00	6.85941	935.531	239.554
ACETYLENE	26.04	.000	.00	.00000	.000	.000
N-BUTANE	58.12	.579	.00	6.83029	945.900	240.000
ISO BUTANE	58.12	.557	.00	6.74808	882.800	240.000
BUTENE-1	56.11	.600	.00	6.84290	926.100	240.000
CYCLO HEXAN	84.16	.779	.00	6.84498	1203.526	222.863
CYCLO HEXEN	82.15	.810	.00	6.88617	1229.973	224.104
CYCLO PENTA	.00	.000	.00	.00000	.000	.000
CYCLO PROPA	42.08	.720	.00	.00000	21.570	7.584
CYCLOPENTEN	68.11	.774	.00	6.92066	1121.818	233.446
DECANE	142.29	.730	.00	7.31503	1705.600	212.590
DIMETHYL BU	86.18	.649	.00	.00000	28.565	7.506
DIMETHYL CY	112.22	.766	.00	6.84164	1369.525	216.040
DIMETHYL PE	100.21	.683	.00	.00000	32.960	7.765
ETHANE	30.07	.546	.00	6.80266	656.400	256.000
ETHYLENE	28.05	.566	.00	6.74756	585.000	255.000
ETHYL ACETY	54.09	.650	.00	.00000	.000	.000
HEPTANE	100.21	.684	.00	6.90240	1268.115	216.900
HEPTENE	98.19	.700	.00	6.90069	1257.505	219.179
HEXANE	86.18	.659	.00	6.87776	1171.366	224.366
LIMONENE	136.24	.843	.00	.00000	45.119	8.211
METHANE	16.00	.000	.00	6.61184	389.930	266.000
ISOPRENE	68.12	.681	.00	.00000	27.246	7.537
HEXENE	84.16	.673	.00	6.86572	1152.971	225.849
METHYL CYCL*	98.19	.769	.00	6.82689	1272.864	221.630
METHYL ACET	40.70	.660	.00	.00000	22.154	7.534
(2)METHYL P	86.18	.654	.00	6.83910	1135.410	226.572
(3)METHYL P	86.18	.664	.00	6.84887	1152.368	227.129
METHYL CYCL	84.16	.749	.00	6.86283	1186.059	226.042
METHYL CYCL	96.17	.800	.00	6.82689	1272.864	221.630
OCTANE *	114.23	.613	.00	6.93263	1353.486	212.764
OCTENE	112.22	.715	.00	6.93263	1353.486	212.764
OCTYNE	110.20	.743	.00	.00000	.000	.000
NONANE	128.26	.710	.00	7.25590	1567.000	225.000
NONENE	126.24	.754	.00	6.95387	1435.359	202.535
ISO PENTANE	72.15	.621	.00	6.78967	1020.012	233.097
PENTENE-1	70.14	.641	.00	6.84650	1044.895	233.516
PROPANE	44.10	.585	.00	6.82973	813.200	248.000
PROPADIENE	40.07	1.787	.00	5.64570	441.000	194.000
PROPYLENE	42.08	.609	.00	6.81960	785.000	247.000
PENTENE-2	.00	.000	.00	.00000	.000	.000
C11 ALKANES	.00	.000	.00	.00000	.000	.000
C12 ALKANES	.00	.000	.00	.00000	.000	.000
C13 ALKANES	.00	.000	.00	.00000	.000	.000
C14 ALKANES	.00	.000	.00	.00000	.000	.000
PENTANE	72.15	.626	.00	6.85221	1064.630	232.000
DODECANE	170.34	.750	.00	7.35518	1867.550	202.590
TRIMETHYL H	128.26	.703	.00	7.24570	1577.600	230.000

TRIMETHYL B	100.21	.690	.00	.00000	32.134	7.638
ACETONE	58.08	.791	1.00	7.02447	1161.000	224.000
METHYL BUTY	100.16	.816	.00	.00000	53.881	10.026
DIISOBUTYL	142.24	.806	.00	.00000	50.835	8.952
METHYL ETHY	72.11	.805	1.00	6.97421	1209.600	216.000
METHYL ISOB	100.16	.801	.00	.00000	53.528	10.200
METHYL ISOP	86.13	.803	.00	.00000	46.108	9.561
METHYL PROP	86.13	.812	.00	.00000	47.922	9.618
METHYL VINY	70.09	.864	.00	6.97421	1209.600	216.000
OCTANONE	128.22	.819	.00	.00000	50.835	8.952
CYCLOHEXANO	98.15	.947	1.00	.00000	43.903	8.357
MESITYL OXI	98.15	.858	.00	.00000	43.584	8.613
HYDROXY KET	.00	.000	.00	.00000	.000	.000
ETHYL MERCA	.00	.000	.00	.00000	.000	.000
METHYL MERC	.00	.000	.00	.00000	.000	.000
PROPYL MERC	.00	.000	.00	.00000	.000	.000
ACETIC ACID	.00	.000	.00	.00000	.000	.000
BUTYRIC ACI	.00	.000	.00	.00000	.000	.000
CAPRYLIC AC	.00	.000	.00	.00000	.000	.000
LACTIC ACID	.00	.000	.00	.00000	.000	.000
VALERIC ACI	.00	.000	.00	.00000	.000	.000
AMMONIA	17.00	.817	1.00	7.55466	1002.711	247.885
ACETOPHENON	120.15	1.028	.00	.00000	55.117	9.135
ACETONITRIL	41.05	.783	1.00	7.11988	1314.400	230.000
BENZONITRIL	103.12	1.001	.00	6.74631	1436.720	181.000
CARBON MONO	28.10	.000	.00	.00000	.000	.000
CYANIMIDE	.00	.000	.00	.00000	.000	.000
DIETHYL SUL	.00	.000	.00	.00000	.000	.000
DIMETHYL SU	62.13	.846	.00	6.93138	1081.587	229.746
DIETHYL DIS	.00	.000	.00	.00000	.000	.000
DIMETHYL DI	.00	.000	.00	.00000	.000	.000
HYDROGEN	.00	.000	.00	.00000	.000	.000
HYDROGEN SU	.00	.000	.00	.00000	.000	.000
METHOXY ACE	.00	.000	.00	.00000	.000	.000
NITROMETHAN	61.04	1.131	1.00	.00000	36.914	8.033

The charcoal data for BD carbon used in the analysis, was established during previous LMSC test programs. For the ICHAR run, those contaminants not removed by activated carbon were removed from the input data. The data has been put in a form compatible with the ICHAR program. Note that the index number assigned to each contaminant corresponds to its location in the master contaminant data base.

The unsorted and sorted output data tables are identical except that the sorted data is in the order of lowest to highest A value. The unsorted is in the order of data base position. The sorted output data table shows the expected cabin concentration (Ci) in mg/m^3 and required bed flow rate in CFM (Q). It is noted that the required Q is 999 CFM for several contaminants which are those with zero allowable levels. The problem of how to handle contaminants with zero allowable concentrations that have been found as off-gassing products from the equipment tests is yet to be resolved. The analysis showed that flow was 7.05 m^3/hr as established by trichloroethane.

The final table of the ICHAR output presents a summary of required carbon and expected time to breakthrough without regeneration for each contaminant (in days). Only 5 contaminants in the list will not be controlled by activated carbon. They are:

Nitromethane
Freon 22
Methyl alcohol
Propadiene
Ammonia

With a breakthrough of 0.94 days, nitromethane is almost totally controlled by charcoal and final control will be achieved with the catalytic oxidizer. Methyl alcohol is removed by both the catalytic oxidizer and condensing cabin heat exchanger, and propadiene will be removed in the catalytic oxidizer. This leaves only Freon 22 and ammonia as potential problem contaminants in addition to those with zero allowable concentrations. Ammonia will in the

most part be controlled by adsorption in the water of the cabin condensing heat exchanger, however, the equilibrium cabin level will be sufficiently high to result in the formation of significant quantities of NO_2 in the catalytic oxidizer. Data taken in previous contracts have shown that the best post sorbent material for NO_2 removal is Purafil or lithium hydroxide. Unfortunately, not enough data is available to make an accurate prediction of required bed size. Considering Purafil as 0.5% permanganate on alumina, excessive quantities would be required.

Freon 22 will be decomposed in the catalytic oxidizer if the temperature is sufficiently high. A lithium hydroxide post sorbent bed will probably remove the decomposition products. The charcoal bed breakthrough of Freon 22 and ammonia creates a requirement for high temperature operation of the catalytic oxidizer to prevent poisoning.

Catalytic Oxidizer Analysis

After completion of the activated charcoal bed analysis, the master data base was searched for those contaminants not included in the carbon analysis list. These contaminants, removed by the catalytic oxidizer, along with their generation rates and required flow rates are summarized by Table 16. A flow rate of 99 indicates a contaminant whose allowable level is not defined or is zero. Carbon monoxide requires the highest flow. Correcting the flow rate from Table 16, for the duty cycle of the regenerable bed, results in a required flow of 3.4 m^3/hr. Providing for a safety factor of 2.5 for carbon monoxide, which can come from a number of sources, matches the catalytic oxidizer flow to the regenerable bed flow.

System Description

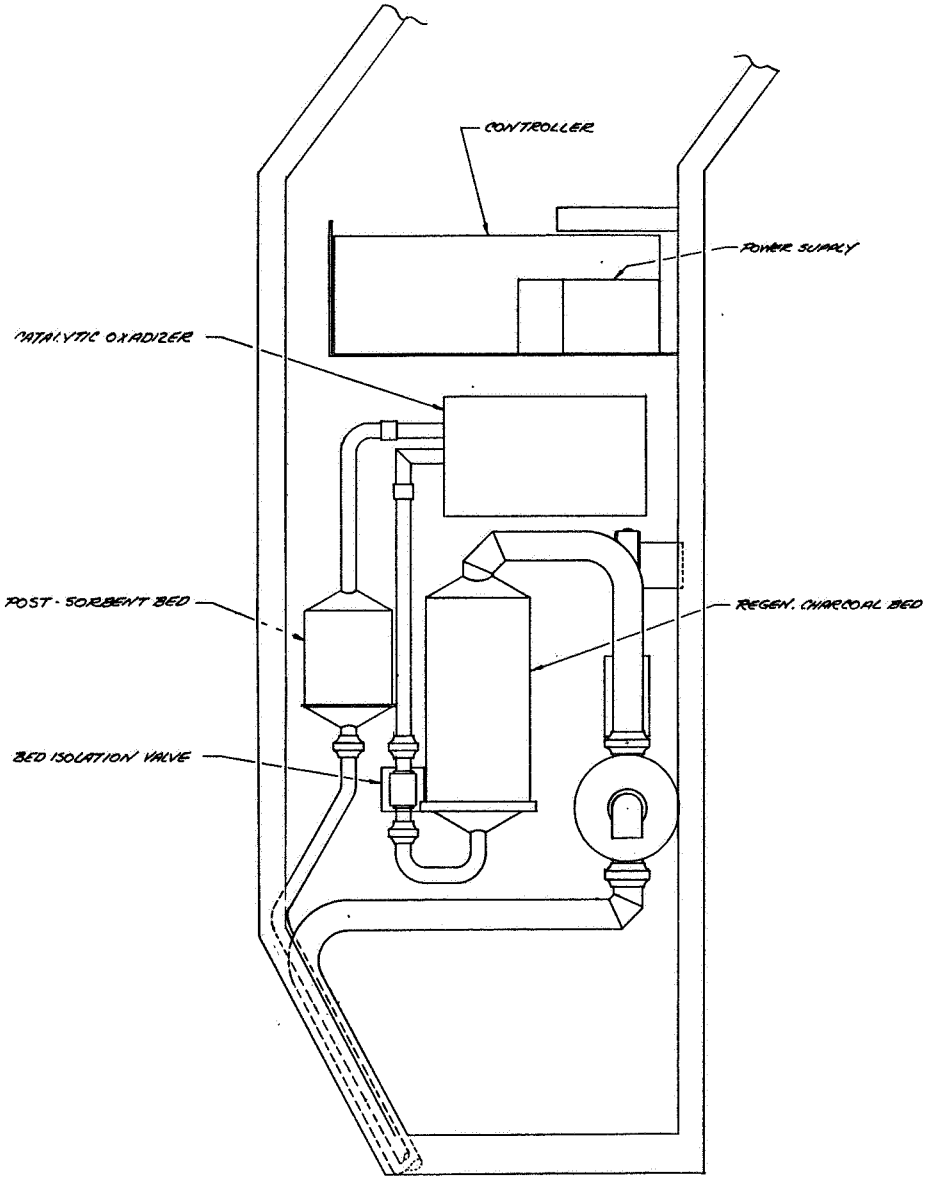
Figure 2 presents a layout drawing of the steady state trace contaminant control system packaged in a portion of a single Spacelab rack. The system consists of a centrifugal fan, regenerable charcoal bed, two bed isolation shut off valves, a vacuum vent valve, catalytic oxidizer, post sorbent bed, controller, control panel and miscellaneous ducting, brackets and wiring. In normal operation, the centrifugal fan draws air from the cabin and forces it

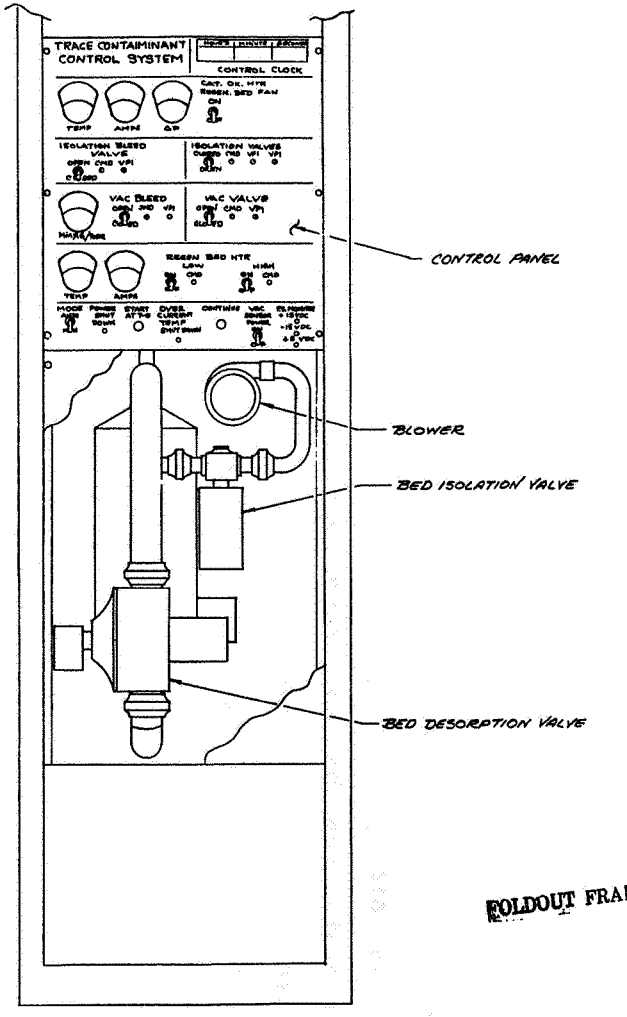
Table 16

Contaminants Not Included in Charcoal Bed Analysis

LOC	NAME	RATE	FLOW
19	FORMALDEHYDE	.00	.00
22	VALERALDEHYDE	.00	.00
29	DECAHYDRO NAPTHALENE	.00	.00
32	NAPHTHALENE	.00	.00
34	C2 STYRENE	96.00	99.00
51	METHYL FURAN	.00	.00
59	CHLORO PROPANE	.00	.00
60	CHLORO ACETYLENE	.00	.08
63	DICHLORO ETHYLENE	.00	.00
64	ETHYLENE DICHLORIDE	.00	.05
65	ETHYL FLUORIDE	.00	.10
73	VINYL CHLORIDE	.00	.00
76	FREON 13	.00	999.00
81	FREON 124	380.00	99.00
83	TRIFLUORO CHLORO ETHYLENE	920.00	.01
84	CHLORO DIFLUORO ETHYLENE	.08	99.00
86	FLUORO CHLORO ETHYLENE	17.60	99.00
87	DIFLUORO ETHYLENE	.00	99.00
88	FLUORO PROPANE	.00	99.00
89	FLUORO ETHANE	.00	99.00
90	PENTAFLUORO ETHANE	.00	99.00
91	TETRAFLUORO ETHYLENE	.00	99.00
92	CHLORO TRIFLUORO ETHYLENE	.00	99.00
93	HEXAFLUORO ETHANE	.00	99.00
94	TRIFLUORO PROPENE	.00	99.00
95	TRIFLUORO PROPANE	.00	99.00
96	TRIFLUORO METHANE	.00	99.00
97	OCTAFLUORO BUTANE	.00	99.00
98	OCTAFLUORO PROPANE	.00	99.00
99	HEXAFLUORO PROPENE	.00	99.00
100	VINYLIDENE FLUORIDE	.00	99.00
101	TRIFLUORO ETHYLENE	.00	99.00
103	ACETYLENE	13.20	.00
109	CYCLO PENTANE	.00	99.00
110	CYCLO PROPANE	.00	.00
115	DIMETHYL PENTANE	.00	.05
118	ETHYL ACETYLENE	.00	.00
123	METHANE	189.20	.00
128	(2)METHYL PENTANE	.00	.00
134	OCTYNE	.00	.04
142	PENTENE-2	.00	99.00
143	C11 ALKANES	8.80	99.00
144	C12 ALKANES	30.80	99.00
145	C13 ALKANES	2.80	99.00
146	C14 ALKANES.	8.80	99.00
150	TRIMETHYL BUTANE	.00	.05

156	METHYL ISOPROPYL KETONE	.00	.00
162	HYDROXY KETONE	132.00	99.00
163	ETHYL MERCAPTAIN	.00	99.00
164	METHYL MERCAPTAIN	.00	99.00
165	PROPYL MERCAPTAN	.00	99.00
166	ACETIC ACID	.00	99.00
167	BUTYRIC ACID	.00	99.00
168	CAPRYLIC ACID	.00	99.00
169	LACTIC ACID	.00	99.00
170	VALERIC ACID	.00	99.00
174	BENZONITRILE	.00	.05
175	CARBON MONOXIDE	2026.00	1.73
176	CYANIMIDE	.00	99.00
177	DIETHYL SULFIDE	.00	99.00
179	DIETHYL DISULFIDE	.00	99.00
180	DIMETHYL DISULFIDE	.00	99.00
181	HYDROGEN	156.00	99.00
182	HYDROGEN SULFIDE	.54	99.00
183	METHOXY ACETIC ACID	.00	99.00





FOLDOUT FRAME 1

FOLDOUT FRAME 2

Figure 2 Trace Contaminant Control System Arrangement

through the regenerable charcoal bed and the two bed isolation valves. The valves are open during the adsorption cycle to allow the removal of contaminants from the cabin atmosphere. The air leaving the regenerable bed passes through the catalytic oxidizer and post sorbent bed before returning to the cabin. During the desorption cycle of the regenerable bed, the fan is shutdown, the isolation valves are closed, the vacuum valve is opened and the regenerable bed heater is energized. The desorption cycle is initiated once every 24 hours and requires 200 minutes for completion of the cycle.

The centrifugal fan delivers a flow of 8.5 m^3/hr at a head rise of 5 kN/m^2 to the system. The fan is a Dynamic Air Engineering C050K unit operating at 22,500 rpm and 90 watts of power. The regenerable bed contains 4.54 Kg of 14 x 20 mesh Barnebey Cheney BD charcoal operating at a pressure drop of 0.7 kN/m^2 at a flow of 8.5 m^3/hr. The catalytic oxidizer contains 900 cc of ½% palladium on alumina catalyst, operating at 550°C, at a total pressure drop of 1.5 kN/m^2 and a total power consumption of 150 watts. The post sorbent bed contains 2 kg of 6 x 8 mesh lithium hydroxide operating at a pressure drop of .4 kN/m^2. The two regenerable bed isolation valves are one inch VACCO Industries V1D10237 solenoid operated shutoff valves with position indicators. The vacuum vent valve is a two inch ASCO HT 8215A80 VH-SW solenoid operated shutoff valve with position indicator.

Emergency System

The contaminants generated by the emergency upsets are presented by Table 10. The first step in the establishment of an emergency system was to derive the required flow rate through the system and postulate removal techniques. Table 17 presents this information for the contaminants generated by the emergency upsets. It can be seen that the system flowrate was established at 513 m^3/hr, by hydrogen fluoride removal, based on a time period of four hours to return contaminant concentrations to at or below SMAC.

In the experimental test program, a system flow rate of 2.9 m^3/hr was used and the system volume was 1.33 m^3. These values were both about 0.5% of the full sized system. The data presented in Table 12 shows control of all key con-

Table 17

Control of Emergency Upset Contaminants

Contaminants	Design Production Rate (gm)	Required Flow (m^3/hr)	Removal Technique
Carbon Dioxide	2270	0	-
Carbon Monoxide	154	215	Pt Treated Charcoal
Halon 1301	3150	317	Charcoal
Nitrous Oxide	3	0	-
Ammonia	3	0	-
Formaldehyde	10	250	Charcoal
Ethyl Alcohol	10	0	-
Isopropyl Alcohol	1.5	0	Base Treated Charcoal
Hydrogen Cyanide	1.6	125	" " "
Hydrogen Chloride	9.1	282	" " "
Hydrogen Fluoride	23	513	" " "
Hydrogen Bromide	3.4	438	" " "
Methane	8.8	0	-
Ethane	1.2	0	-
Propylene	12.1	0	-
Methyl Alcohol	0.8	0	-
Butanol	1.1	0	-
Acetaldehyde	0.12	0	-
Propionaldehyde	0.062	0	-
Acetone	0.32	0	-
Benzene	1.68	47	Charcoal
Toluene	0.7	0	-
Ethylene Benzene	0.32	0	-
Styrene	0.56	0	-
Vinyl Chloride	0.04	0	-
Carbonyl Fluoride	3.3	450	Base Treated Charcoal
Freon 14 (CF_4)	3.2	0	-
Tetrafluoroethylene	6.4	0	-
Carbonyl Bromide	3.0	364	Base Treated Charcoal
Bromine	5.4	422	Base Treated Charcoal
Nitrogen Oxide	0.014	0	-
Nitrogen Dioxide	0.021	0	-
Sulfur Dioxide	1.5	38	Base Treated Charcoal

taminants in the emergency model. It is clear that the emergency system requirements can be met with a fan, and a layered bed of activated carbon on which is deposited:

1) KOH for removal of acid gases, halogens, and carbonyl compounds
2) Phosphoric acid for control of ammonia
3) Platinum for oxidation of carbon monoxide.

Furthermore, the quantity of activated carbon required is set by the requirements for control of Freon 1301.

The removal of 3.15 Kg of Freon 1301 to a level of 100 ppm results in an A value of 20. The test data shows a capacity of about 0.8 of the Barnebey Chaney BD activated carbon curve. If a capacity of 4.5×10^{-3} cc/gm is assumed, the charcoal requirement is 361 Kg. This quantity of charcoal is excessive considering that the gas required to provide an entire atmospheric change is only about 400 Kg. If the allowable level of Freon 1301 was 1000 ppm instead of 100, the charcoal required would be reduced to 95 Kg There is some evidence that such an increase is justifiable.

REFERENCES

1. Lockheed Missiles and Space Company, Development of a Computer Program For Spacelab Contaminant Control Analysis, NASA MSFC Contract NAS 8-31551 January 15, 1977.
2. NHB 8060.1A, Flammability, Odor and Offgassing Requirements & Test Procedures for Materials in Environments that Support Combustion, NASA Office of Manned Space Flight, February 1974.
3. Beckman Instruments, Analysis of Multipurpose Equipment for Space Application, NASA-MSFC Contract NAS 8-29776, December 1973.
4. Analytical Research Lab., Collection and Measurement of Atmospheric Contaminants During Skylab AM/MDA Unmanned Altitude Chamber Test, NASA-JSC Contract NAS 9-11960, December 1972.
5. H. M. Liebich, W. Bertsch, A. Zlatkis, H. J. Schneider, Aviation, Space and Environ. Med., 46 (8) 1002, Volatile Organic Components in the Skylab 4 Spacecraft Atmosphere (1975).
6. Aerojet General, Analytical Chemical Lab., Report 3570, Trace Gas Analysis on Samples Taken from Apollo 101 Command Module Atmosphere, NASA KSC Contract NAS 10-5929, September 1968.
7. ERNO, Spacelab Mass Properties Status Report, RP-ER-0005K, Dec. 1975.
8. ERNO, Spacelab Mass Properties Status Report, RP-ER-0005L, January 1976.
9. E. A. Boettner, et. al., Combustion Products from the Incineration of Plastics", Grant EC-00386, University of Michigan Report 032050, February 1973.
10. Grumman Aerospace Co., Space Station Systems Analysis Study, NSS-SS-RP006, August 1976, Contract NAS 8-31993.
11. General Dynamics, Convair, Definition of Life Sciences Laboratories for Shuttle/Spacelab, Book 3, Preliminary Equipment Item Specification Catalogue.
12. Lockheed Missiles & Space Company, Conceptual Design for a Biological Specimen Holding Facility, LMSC-D056047, June 1976, Contract NAS 8-31491.
13. McDonnell Douglas Astronautics Co., Space Station Systems Analysis Study, MDC G6412, June 1976, Contract NAS 9-14958.
14. McDonnell Douglas Astronautics Co., Manned Orbital Systems Concepts Study, MDC G5919, September 1975, Contract NAS 8-31014.
15. Marshall Space Flight Center, Spacelab Design Reference Mission Analysis, Vol. IV, Mission C Space Processing Applications, April 1975.

16. Marshall Space Flight Center, Spacelab Design Reference Mission Analysis, Vol. V, Mission E, Life Sciences, Jan. 1975.

17. National Academy of Science - National Research Council Panel on Quality Air in Manned Spacecraft, June 1972.

18. Lockheed Missiles and Space Company, Design, Fabrication, and Test of a Trace Contaminant Control System, LMSC-D462467 Contract NAS 1-11526, November 28, 1975.

Appendix A

ICHAR PROGRAM INPUT & OUTPUT

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◆ ◆ ◆ ◆ ◆ CHARCOAL BED ANALYSIS PROGRAM ◆ ◆ ◆ ◆ ◆


TITLE
? REGENERABLE BED ANALYSIS WITH BT
WHAT IS THE TOTAL BED SIZE  GRAMS
? 4536
WHAT IS THE CHARCOAL DENSITY  LBS/FT3
? 30
WHAT IS THE LENGTH OF THE SHORT TERM MISSION PHASE  DAYS
? 1
WHAT IS THE LENGTH OF THE LONG TERM MISSION PHASE  DAYS
? 0



INPUT THE OPERATING CONDITIONS AS REQUESTED

DELTA A CRITICAL
? 16
PHOSPHORIC ACID TREATMENT (Y OR N)
? .8\8.\Y
WHAT IS THE BED REMOVAL EFFICIENCY DECIMAL
? .8
PROCESS FLOW (CFM)
? 5
TEMPERATURE (F)
? 100
IS THE BED REGENERABLE (Y OR N)
? Y
WHAT IS THE TOTAL CYCLE TIME ( HRS )
? 24
WHAT IS THE DESORPTION TIME ( HRS)
? 3



OUTPUT SUPPRESSION ( Y OR N )
CHARCOAL DATA
? N
CONTAMINANT DATA
? N
UNSORTED LIST
? Y
SORTED LIST
? N
SUMMARY
? N
OCHAR.: NEW FILE, OK? YES

END IN LINE 36601
```

ORIGINAL PAGE IS
OF POOR QUALITY

CHARCOAL DATA

CODE 1 = SOLUBLES
CODE 2 = INSOLUBLE NO ACID
CODE 3 = INSOLUBLE WITH ACID

A	CODE 1	CODE 2	CODE 3
000.00	.560+00	.560+00	.560+00
010.00	.180+00	.180+00	.180+00
030.00	.750-03	.275-03	.230-03
040.00	.480-04	.101-04	.880-05
050.00	.310-05	.440-06	.330-06
200.00	.100-09	.100-09	.100-09

PROGRAM INPUT DATA

INDEX NAME / RATE	MAC	RHO	VM	MW	PO	CODE
1 ISO AMYL ALCOHOL						
.920+01	.361+02	.819+00	.108+03	.882+02	.365+05	2
2 N AMYL ALCOHOL						
.140+02	.361+02	.813+00	.108+03	.882+02	.277+05	2
3 ALLYL ALCOHOL						
.188+02	.475+00	.855+00	.679+02	.581+02	.154+06	1
4 ISOBUTYL ALCOHOL						
.680+02	.303+02	.802+00	.924+02	.741+02	.104+06	2
5 N BUTYL ALCOHOL						
.372+03	.303+02	.810+00	.915+02	.741+02	.604+05	2
6 SEC BUTYL ALCOHOL						
.520+02	.910+02	.808+00	.917+02	.741+02	.147+06	1
7 CAPRYL ALCOHOL						
.480+01	.533+02	.822+00	.158+03	.130+03	.931+04	2
8 CYCLOHEXANOL						
.624+03	.205+02	.962+00	.104+03	.100+03	.164+05	2
9 ETHYLENE GLYCOL						
.480+01	.127+03	.111+01	.558+02	.621+02	.953+03	1
10 ETHYL ALCOHOL						
.320+03	.189+03	.789+00	.584+02	.461+02	.287+06	1
11 METHYL ALCOHOL						
.466+04	.524+02	.792+00	.405+02	.320+02	.398+06	1
12 HEXYL ALCOHOL						
.920+01	.418+02	.820+00	.125+03	.102+03	.553+05	2
13 ISO PROPYL ALCOHOL						
.137+04	.984+02	.785+00	.766+02	.601+02	.248+06	1
14 N PROPYL ALCOHOL						
.116+03	.984+02	.804+00	.748+02	.601+02	.140+06	1
15 PHENOL						
.640+02	.193+01	.107+01	.879+02	.941+02	.495+04	2
16 ACETALDEHYDE						
.280+02	.180+02	.783+00	.563+02	.441+02	.292+07	1
17 ACROLEIN						
.430+01	.115+00	.841+00	.667+02	.561+02	.129+07	1
18 BUTYRALDEHYDE						
.624+03	.148+03	.817+00	.883+02	.721+02	.684+06	2
20 PROPIONALDEHYDE						
.400+01	.119+03	.807+00	.720+02	.581+02	.134+07	1
21 BENZALDEHYDE						
.292+03	.217+03	.105+01	.101+03	.106+03	.121+05	2
23 BENZENE						

.112+03 .320+01 .879+00 .889+02 .781+02 .678+06 2
24 ISO PROPYL BENZENE
.240+01 .246+02 .862+00 .139+03 .120+03 .610+05 2
25 N PROPYL BENZENE
.116+03 .492+02 .862+00 .139+03 .120+03 .457+05 2
26 ETHYL BENZENE
.400+03 .869+02 .867+00 .122+03 .106+03 .106+06 2
27 ETHYL METHYL BENZENE
.760+01 .246+02 .870+00 .138+03 .120+03 .402+05 2
28 TRIMETHYL BENZENE
.420+03 .148+02 .876+00 .137+03 .120+03 .285+05 2
30 INDENE
.600+02 .475+01 .991+00 .117+03 .116+03 .206+05 2
31 MESITHYLENE
.224+02 .148+02 .865+00 .139+03 .120+03 .336+05 2
33 METHYL STYRENE
.600+02 .484+02 .911+00 .130+03 .118+03 .308+05 2
35 STYRENE
.112+02 .852+02 .906+00 .115+03 .104+03 .683+05 2
36 XYLENE P
.113+04 .869+02 .861+00 .123+03 .106+03 .980+05 2
37 TOLUENE
.542+04 .754+02 .866+00 .106+03 .921+02 .256+06 2
38 ISO BUTYL ACETATE
.392+03 .143+03 .871+00 .133+03 .116+03 .222+06 2
39 BUTYL ACETATE
.216+03 .190+03 .870+00 .134+03 .116+03 .217+06 2
40 ETHOXY ETHYL ACETATE
.204+03 .541+02 .975+00 .136+03 .132+03 .252+06 2
41 METHYL ACETATE
.520+02 .121+03 .933+00 .794+02 .741+02 .141+07 1
42 METHYLBUTYRATE
.800+00 .293+02 .889+00 .115+03 .102+03 .506+06 2
43 METHYL METHACRYLATE
.232+02 .409+02 .939+00 .106+03 .100+03 .373+06 2
44 ETHYL ACETATE
.556+03 .180+03 .901+00 .978+02 .881+02 .790+06 2
45 ETHYL LACTATE
.104+03 .193+03 .103+01 .115+03 .118+03 .225+06 1
46 PROPYL ACETATE
.600+02 .167+03 .886+00 .115+03 .102+03 .328+06 2
47 ISO PROPYL ACETATE
.988+03 .209+03 .874+00 .117+03 .102+03 .567+06 2
48 BUTYL LACTATE
.104+03 .299+01 .964+00 .152+03 .146+03 .131+07 2
49 DIOXANE
.520+01 .180+02 .103+01 .852+02 .881+02 .326+06 1
50 FURAN
.800+00 .111+00 .937+00 .727+02 .681+02 .338+07 2
52 TETRAHYDRO FURAN
.760+02 .590+02 .888+00 .812+02 .721+02 .137+07 1
53 CARBON TETRACHLORIDE
.360+02 .629-09 .159+01 .965+02 .154+03 .158+07 2
54 CHLORO BENZENE

.640+02 .345+02 .111+01 .102+03 .113+03 .140+06 2

55 CHLORO BUTANE
.136+03 .189+03 .847+00 .109+03 .926+02 .846+06 2

56 CHLOROFORM
.436+02 .489-09 .149+01 .802+02 .119+03 .204+07 2

57 CHLOROETHANE
.276+03 .132+03 .903+00 .715+02 .645+02 .604+07 2

58 CHLORO PROPYLENE
.172+02 .235+02 .938+00 .816+02 .765+02 .305+07 2

61 DICHLORO BENZENE
.304+02 .301+02 .130+01 .113+03 .147+03 .316+05 2

62 DICHLORO ETHANE
.880+02 .405+02 .118+01 .841+02 .990+02 .732+06 2

66 METHYL CHLORIDE
.800+00 .207+02 .920+00 .549+02 .505+02 .154+08 2

67 METHYL CHLOROFORM
.178+04 .546-09 .135+01 .991+02 .133+03 .144+07 2

68 DICHLORO METHANE
.478+04 .869+02 .134+01 .636+02 .849+02 .297+07 2

69 TETRACHLORO ETHYLENE
.560+02 .339+02 .163+01 .102+03 .166+03 .303+06 2

70 TRICHLORO ETHANE
.740+03 .546+01 .144+01 .926+02 .133+03 .314+06 2

71 TRICHLORO ETHYLENE
.120+03 .538-09 .147+01 .896+02 .131+03 .896+06 2

72 VINYLIDENE CHLORIDE
.880+01 .397+01 .125+01 .776+02 .969+02 .468+07 2

74 FREON 11
.292+03 .141+03 .149+01 .919+02 .137+03 .866+07 2

75 FREON 12
.176+02 .778+03 .149+01 .128+03 .190+03 .663+08 2

77 FREON 21
.290+01 .421+03 .143+01 .722+02 .103+03 .108+08 2

78 FREON 22
.474+04 .354+03 .149+01 .580+02 .865+02 .482+08 2

79 FREON 113
.414+04 .383+03 .158+01 .119+03 .187+03 .512+07 2

80 FREON 114
.920+02 .699+03 .146+01 .117+03 .171+03 .211+08 2

82 FREON 112
.520+02 .209+03 .165+01 .124+03 .204+03 .100+07 2

85 DICHLORO DIFLUORO ETHYLENE
.192+03 .272+02 .100+01 .133+03 .133+03 .978+07 2

102 BUTADIENE
.800+02 .221+03 .621+00 .871+02 .541+02 .859+07 2

104 N-BUTANE
.440+02 .178+03 .579+00 .100+03 .581+02 .802+07 2

105 ISO BUTANE
.484+02 .178+03 .557+00 .104+03 .581+02 .112+08 2

106 BUTENE-1
.264+02 .459+03 .600+00 .935+02 .561+02 .940+07 2

107 CYCLO HEXANE
.864+03 .207+03 .779+00 .108+03 .842+02 .739+06 2

108 CYCLO HEXENE

.176+02	.101+03	.810+00	.101+03	.822+02	.661+06	2
111 CYCLOPENTENE						
.660+02	.836+02	.774+00	.880+02	.681+02	.216+07	2
112 DECANE						
.120+01	.116+03	.730+00	.195+03	.142+03	.237+05	2
113 DIMETHYL BUTANE						
.572+02	.106+03	.649+00	.133+03	.862+02	.224+07	2
114 DIMETHYL CYCLO HEXANE						
.160+01	.115+03	.766+00	.147+03	.112+03	.163+06	2
116 ETHANE						
.836+02	.185+03	.546+00	.551+02	.301+02	.576+08	2
117 ETHYLENE						
.120+01	.172+03	.566+00	.496+02	.281+02	.815+08	2
119 HEPTANE						
.176+02	.205+03	.684+00	.147+03	.100+03	.437+06	2
120 HEPTENE						
.572+02	.161+03	.700+00	.140+03	.982+02	.519+06	2
121 HEXANE						
.132+03	.705+03	.659+00	.131+03	.862+02	.115+07	2
122 LIMONENE						
.840+02	.279+03	.843+00	.162+03	.136+03	.295+05	2
124 ISOPRENE						
.748+02	.557+03	.681+00	.100+03	.681+02	.317+07	2
125 HEXENE						
.880+01	.172+03	.673+00	.125+03	.842+02	.136+07	2
126 METHYL CYCLOHEXANE						
.520+01	.603+02	.769+00	.128+03	.982+02	.425+06	2
127 METHYL ACETYLENE						
.440+01	.167+03	.660+00	.617+02	.407+02	.135+08	2
129 (3)METHYL PENTANE						
.800-01	.176+04	.664+00	.130+03	.862+02	.141+07	2
130 METHYL CYCLO PENTANE						
.418+03	.861+02	.749+00	.112+03	.842+02	.102+07	2
131 METHYL CYCLO HEXENE						
.128+03	.984+02	.800+00	.120+03	.962+02	.417+06	2
132 OCTANE						
.352+02	.234+03	.613+00	.186+03	.114+03	.202+06	2
133 OCTENE						
.308+02	.230+03	.715+00	.157+03	.112+03	.198+06	2
135 NONANE						
.120+01	.105+03	.710+00	.181+03	.128+03	.131+06	2
136 NONENE						
.640+02	.258+03	.754+00	.167+03	.126+03	.631+05	2
137 ISO PENTANE						
.880+01	.295+03	.621+00	.116+03	.722+02	.396+07	2
138 PENTENE-1						
.176+02	.187+03	.641+00	.109+03	.701+02	.360+07	2
139 PROPANE						
.220+02	.180+03	.585+00	.754+02	.441+02	.220+08	2
140 PROPADIENE						
.189+03	.820+02	.179+01	.224+02	.401+02	.115+08	2
141 PROPYLENE						
.308+02	.861+03	.609+00	.691+02	.421+02	.252+08	2
147 PENTANE						

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.308+02    .590+03    .626+00    .115+03    .722+02    .302+07    2
 148  DODECANE
.280+01    .139+03    .750+00    .227+03    .170+03    .344+04    2
 149  TRIMETHYL HEXANE
.880+01    .105+03    .703+00    .182+03    .128+03    .151+06    2
 151  ACETONE
.189+04    .238+03    .791+00    .734+02    .581+02    .117+07    1
 152  METHYL BUTYL KETONE
.560+02    .410+02    .816+00    .123+03    .100+03    .476+05    2
 153  DIISOBUTYL KETONE
.360+03    .291+02    .806+00    .176+03    .142+03    .186+05    2
 154  METHYL ETHYL KETONE
.432+03    .295+02    .805+00    .896+02    .721+02    .606+06    1
 155  METHYL ISOBUTYL KETONE
.552+03    .410+02    .801+00    .125+03    .100+03    .815+05    2
 157  METHYL PROPYL KETONE
.116+03    .705+02    .812+00    .106+03    .861+02    .161+06    2
 158  METHYL VINYL KETONE
.200+01    .287+01    .864+00    .812+02    .701+02    .589+06    2
 159  OCTANONE
.180+02    .525+02    .819+00    .157+03    .128+03    .167+05    2
 160  CYCLOHEXANONE
.480+02    .803+01    .947+00    .104+03    .982+02    .476+05    1
 161  MESITYL OXIDE
.560+02    .100+02    .858+00    .114+03    .982+02    .973+05    2
 171  AMMONIA
.316+03    .174+02    .817+00    .208+02    .170+02    .977+07    1
 172  ACETOPHENONE
.640+02    .246+03    .103+01    .117+03    .120+03    .455+04    2
 173  ACETONITRILE
.420+02    .672+01    .783+00    .524+02    .411+02    .348+06    1
 178  DIMETHYL SULFIDE
.120+01    .254+01    .846+00    .734+02    .621+02    .250+07    2
 184  NITROMETHANE
.360+01    .250-09    .113+01    .540+02    .610+02    .210+06    1
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UNSORTED OUTPUT DATA

TITLE: REGENERABLE BED ANALYSIS WITH BT
CHARCOAL FILE: CHARD
CONTAMINENT DATA: CONTD2

INDEX	NAME	A	CI	MAC	RATE	REQ Q
1	ISO AMYL ALCOH	16.79	.564-01	.361+02	.920-02	.01
2	N AMYL ALCOHOL	15.80	.858-01	.361+02	.140-01	.01
3	ALLYL ALCOHOL	28.03	.115+00	.475+00	.188-01	1.21
4	ISOBUTYL ALCOH	18.16	.417+00	.303+02	.680-01	.07
5	N BUTYL ALCOHO	15.03	.228+01	.303+02	.372+00	.38
6	SEC BUTYL ALCO	19.20	.319+00	.910+02	.520-01	.02
7	CAPRYL ALCOHOL	10.79	.294-01	.533+02	.480-02	.00
8	CYCLOHEXANOL	10.85	.382+01	.205+02	.624+00	.93
9	ETHYLENE GLYCO	25.15	.294-01	.127+03	.480-02	.00
10	ETHYL ALCOHOL	27.50	.196+01	.189+03	.320+00	.05
11	METHYL ALCOHOL	29.82	.524+02	.524+02	.466+01	2.72
12	HEXYL ALCOHOL	14.95	.564-01	.418+02	.920-02	.01
13	ISO PROPYL ALC	18.15	.840+01	.984+02	.137+01	.43
14	N PROPYL ALCOH	22.02	.711+00	.984+02	.116+00	.04
15	PHENOL	14.51	.392+00	.193+01	.640-01	1.02
16	ACETALDEHYDE	28.79	.180+02	.180+02	.280-01	.05
17	ACROLEIN	35.64	.294-01	.115+00	.480-02	1.28
18	BUTYRALDEHYDE	18.50	.382+01	.148+03	.624+00	.13
20	PROPIONALDEHYD	33.42	.245-01	.119+03	.400-02	.00
21	BENZALDEHYDE	11.73	.179+01	.217+03	.292+00	.04
23	BENZENE	20.97	.686+00	.320+01	.112+00	1.07
24	ISO PROPYL BEN	14.75	.147-01	.246+02	.240-02	.00
25	N PROPYL BENZE	10.72	.711+00	.492+02	.116+00	.07
26	ETHYL BENZENE	11.77	.245+01	.869+02	.400+00	.14
27	ETHYL METHYL B	13.38	.466-01	.246+02	.760-02	.01
28	TRIMETHYL BENZ	9.16	.257+01	.148+02	.420+00	.87
30	INDENE	12.60	.368+00	.475+01	.600-01	.39
31	MESITHYLENE	12.06	.137+00	.148+02	.224-01	.05
33	METHYL STYRENE	11.80	.368+00	.484+02	.600-01	.04
35	STYRENE	16.22	.686-01	.852+02	.112-01	.00
36	XYLENE P	10.46	.693+01	.869+02	.113+01	.40
37	TOLUENE	11.36	.332+02	.754+02	.542+01	2.20
38	ISO BUTYL ACET	11.57	.240+01	.143+03	.392+00	.08
39	BUTYL ACETATE	12.14	.132+01	.190+03	.216+00	.03
40	ETHOXY ETHYL A	12.17	.125+01	.541+02	.204+00	.12
41	METHYL ACETATE	26.02	.319+00	.121+03	.520-01	.01
42	METHYLBUTYRATE	21.69	.490-02	.293+02	.800-03	.00
43	METHYL METHACR	18.74	.142+00	.409+02	.232-01	.02

44	ETHYL ACETATE	17.06	.341+01	.180+03	.556+00	.09
45	ETHYL LACTATE	15.04	.637+00	.193+03	.104+00	.02
46	PROPYL ACETATE	16.05	.368+00	.167+03	.600-01	.01
47	ISO PROPYL ACE	13.35	.544+01	.209+03	.888+00	.13
48	BUTYL LACTATE	12.94	.637+00	.299+01	.104+00	1.06
49	DIOXANE	25.58	.319-01	.180+02	.520-02	.01
50	FURAN	37.82	.490-02	.111+00	.800-03	.22
52	TETRAHYDRO FUR	24.77	.466+00	.590+02	.760-01	.04
53	CARBON TETRACH	22.08	.221+00	.629-09	.360-01	999.00
54	CHLORO BENZENE	16.96	.392+00	.345+02	.640-01	.06
55	CHLORO BUTANE	17.09	.833+00	.189+03	.136+00	.02
56	CHLOROFORM	26.69	.267+00	.489-09	.436-01	999.00
57	CHLOROETHANE	28.51	.169+01	.132+03	.276+00	.06
58	CHLORO PROPYLE	28.43	.105+00	.235+02	.172-01	.02
61	DICHLORO BENZE	14.38	.186+00	.301+02	.304-01	.03
62	DICHLORO ETHAN	22.66	.539+00	.405+02	.880-01	.07
66	METHYL CHLORID	33.26	.207+02	.207+02	.800-03	.00
67	METHYL CHLORDF	16.07	.109+02	.546-09	.178+01	999.00
68	DICHLORO METHA	24.48	.293+02	.869+02	.478+01	1.68
69	TETRACHLORO ET	18.18	.343+00	.339+02	.560-01	.05
70	TRICHLORO ETHA	16.26	.453+01	.546+01	.740+00	4.15
71	TRICHLORO ETHY	21.11	.735+00	.538-09	.120+00	999.00
72	VINYLIDENE CHL	31.82	.539-01	.397+01	.880-02	.07
74	FREON 11	22.60	.179+01	.141+03	.292+00	.06
75	FREON 12	21.35	.108+00	.778+03	.176-01	.00
77	FREON 21	37.90	.172-01	.421+03	.280-02	.00
78	FREON 22	27.52	.354+03	.354+03	.474+01	.41
79	FREON 113	13.87	.254+02	.383+03	.414+01	.33
80	FREON 114	20.04	.564+00	.699+03	.920-01	.00
82	FREON 112	16.30	.319+00	.209+03	.520-01	.01
85	DICHLORO DIFLU	16.18	.118+01	.272+02	.192+00	.22
102	BUTADIENE	25.86	.490+00	.221+03	.800-01	.01
104	N-BUTANE	23.15	.270+00	.178+03	.440-01	.01
105	ISO BUTANE	22.58	.296+00	.178+03	.484-01	.01
106	BUTENE-1	25.81	.162+00	.459+03	.264-01	.00
107	CYCLO HEXANE	14.81	.529+01	.207+03	.864+00	.13
108	CYCLO HEXENE	20.81	.108+00	.101+03	.176-01	.01
111	CYCLOPENTENE	23.77	.404+00	.836+02	.660-01	.02
112	DECANE	10.38	.735-02	.116+03	.120-02	.00
113	DIMETHYL BUTAN	15.93	.350+00	.106+03	.572-01	.02
114	DIMETHYL CYCLO	15.33	.980-02	.115+03	.160-02	.00
116	ETHANE	31.02	.185+03	.185+03	.836-01	.01
117	ETHYLENE	35.60	.172+03	.172+03	.120-02	.00
119	HEPTANE	14.02	.108+00	.205+03	.176-01	.00
120	HEPTENE	13.68	.350+00	.161+03	.572-01	.01
121	HEXANE	14.62	.811+00	.705+03	.132+00	.01
122	LIMONENE	9.15	.515+00	.279+03	.840-01	.01
124	ISOPRENE	21.26	.458+00	.557+03	.748-01	.00
125	HEXENE	18.40	.539-01	.172+03	.880-02	.00
126	METHYL CYCLOHE	17.35	.319-01	.603+02	.520-02	.00
127	METHYL ACETYLE	24.75	.167+03	.167+03	.440-02	.00
129	(3)METHYL PENT	22.66	.490-03	.176+04	.800-04	.00
130	METHYL CYCLO P	15.49	.256+01	.861+02	.418+00	.15
131	METHYL CYCLO H	14.81	.784+00	.984+02	.128+00	.04

132	OCTANE	9.96	.216+00	.234+03	.352-01	.00
133	OCTENE	11.93	.189+00	.230+03	.308-01	.00
135	NONANE	12.48	.735-02	.105+03	.120-02	.00
136	NONENE	9.67	.392+00	.258+03	.640-01	.01
137	ISO PENTANE	21.05	.539-01	.295+03	.880-02	.00
138	PENTENE-1	21.38	.108+00	.187+03	.176-01	.00
139	PROPANE	33.87	.135+00	.180+03	.220-01	.00
140	PROPADIENE	71.35	.820+02	.820+02	.189+00	.07
141	PROPYLENE	20.10	.861+03	.861+03	.308-01	.00
147	PENTANE	19.43	.189+00	.590+03	.308-01	.00
148	DODECANE	7.26	.172-01	.139+03	.280-02	.00
149	TRIMETHYL HEXA	10.99	.539-01	.105+03	.880-02	.00
151	ACETONE	21.20	.116+02	.238+03	.189+01	.24
152	METHYL BUTYL K	13.02	.343+00	.410+02	.560-01	.04
153	DIISOBUTYL KET	6.91	.221+01	.291+02	.360+00	.38
154	METHYL ETHYL K	18.60	.265+01	.295+02	.432+00	.45
155	METHYL ISOBUTY	10.89	.338+01	.410+02	.552+00	.41
157	METHYL PROPYL	15.70	.711+00	.705+02	.116+00	.05
158	METHYL VINYL K	29.43	.123-01	.287+01	.200-02	.02
159	OCTANONE	10.29	.110+00	.525+02	.180-01	.01
160	CYCLOHEXANONE	15.63	.294+00	.803+01	.480-01	.18
161	MESITYL OXIDE	14.82	.343+00	.100+02	.560-01	.17
171	AMMONIA	100.15	.194+01	.174+02	.316+00	.56
172	ACETOPHENONE	10.81	.392+00	.246+03	.640-01	.01
173	ACETONITRILE	36.35	.257+00	.672+01	.420-01	.19
178	DIMETHYL SULFI	36.11	.735-02	.254+01	.120-02	.01
184	NITROMETHANE	40.21	.221-01	.250-09	.360-02	999.00

SORTED OUTPUT DATA

TITLE: REGENERABLE BED ANALYSIS WITH BT
CHARCOAL FILE: CHARD
CONTAMINENT DATA: CONTD2

INDEX	NAME	A	CI	MAC	RATE	REQ Q
153	DIISOBUTYL KET	6.91	.221+01	.291+02	.360+00	.39
148	DODECANE	7.26	.172-01	.139+03	.280-02	.00
122	LIMONENE	9.15	.515+00	.279+03	.840-01	.01
28	TRIMETHYL BENZ	9.16	.257+01	.148+02	.420+00	.87
136	NONENE	9.67	.392+00	.258+03	.640-01	.01
132	OCTANE	9.96	.216+00	.234+03	.352-01	.00
159	OCTANONE	10.29	.110+00	.525+02	.180-01	.01
112	DECANE	10.38	.735-02	.116+03	.120-02	.00
36	XYLENE P	10.46	.693+01	.869+02	.113+01	.40
25	N PROPYL BENZE	10.72	.711+00	.492+02	.116+00	.07
7	CAPRYL ALCOHOL	10.79	.294-01	.533+02	.480-02	.00
172	ACETOPHENONE	10.81	.392+00	.246+03	.640-01	.01
8	CYCLOHEXANOL	10.85	.382+01	.205+02	.624+00	.93
155	METHYL ISOBUTY	10.89	.338+01	.410+02	.552+00	.41
149	TRIMETHYL HEXA	10.99	.539-01	.105+03	.880-02	.00
37	TOLUENE	11.36	.332+02	.754+02	.542+01	2.20
38	ISO BUTYL ACET	11.57	.240+01	.143+03	.392+00	.08
21	BENZALDEHYDE	11.73	.179+01	.217+03	.292+00	.04
26	ETHYL BENZENE	11.77	.245+01	.869+02	.400+00	.14
33	METHYL STYRENE	11.80	.368+00	.484+02	.600-01	.04
133	OCTENE	11.93	.189+00	.230+03	.308-01	.00
31	MESITHYLENE	12.06	.137+00	.148+02	.224-01	.05
39	BUTYL ACETATE	12.14	.132+01	.190+03	.216+00	.03
40	ETHOXY ETHYL A	12.17	.125+01	.541+02	.204+00	.12
135	NONANE	12.48	.735-02	.105+03	.120-02	.00
30	INDENE	12.60	.368+00	.475+01	.600-01	.39
48	BUTYL LACTATE	12.94	.637+00	.299+01	.104+00	1.06
152	METHYL BUTYL K	13.02	.343+00	.410+02	.560-01	.04
47	ISO PROPYL ACE	13.35	.544+01	.209+03	.888+00	.13
27	ETHYL METHYL B	13.38	.466-01	.246+02	.760-02	.01
120	HEPTENE	13.68	.350+00	.161+03	.572-01	.01
79	FREON 113	13.97	.254+02	.383+03	.414+01	.33
119	HEPTANE	14.02	.108+00	.205+03	.176-01	.00
61	DICHLORO BENZE	14.38	.186+00	.301+02	.304-01	.03
15	PHENOL	14.51	.392+00	.193+01	.640-01	1.02
121	HEXANE	14.62	.811+00	.705+03	.132+00	.01
24	ISO PROPYL BEN	14.75	.147-01	.246+02	.240-02	.00
107	CYCLO HEXANE	14.81	.529+01	.207+03	.864+00	.13

131	METHYL CYCLO H	14.81	.784+00	.984+02	.128+00	.04
161	MESITYL OXIDE	14.82	.343+00	.100+02	.560-01	.17
12	HEXYL ALCOHOL	14.95	.564-01	.418+02	.920-02	.01
5	N BUTYL ALCOHO	15.03	.228+01	.303+02	.372+00	.38
45	ETHYL LACTATE	15.04	.637+00	.193+03	.104+00	.02
114	DIMETHYL CYCLO	15.33	.980-02	.115+03	.160-02	.00
130	METHYL CYCLO P	15.49	.256+01	.861+02	.418+00	.15
160	CYCLOHEXANONE	15.63	.294+00	.803+01	.480-01	.18
157	METHYL PROPYL	15.70	.711+00	.705+02	.116+00	.05
2	N AMYL ALCOHOL	15.80	.858-01	.361+02	.140-01	.01
113	DIMETHYL BUTAN	15.93	.350+00	.106+03	.572-01	.02
46	PROPYL ACETATE	16.05	.368+00	.167+03	.600-01	.01
67	METHYL CHLOROF	16.07	.109+02	.546-09	.178+01	999.00
85	DICHLORO DIFLU	16.18	.118+01	.272+02	.192+00	.22
35	STYRENE	16.22	.686-01	.852+02	.112-01	.00
70	TRICHLORO ETHA	16.26	.453+01	.546+01	.740+00	4.15
82	FREON 112	16.30	.319+00	.209+03	.520-01	.01
1	ISO AMYL ALCOH	16.79	.564-01	.361+02	.920-02	.01
54	CHLORO BENZENE	16.96	.392+00	.345+02	.640-01	.06
44	ETHYL ACETATE	17.06	.341+01	.180+03	.556+00	.09
55	CHLORO BUTANE	17.09	.833+00	.189+03	.136+00	.02
126	METHYL CYCLOHE	17.35	.319-01	.603+02	.520-02	.00
13	ISO PROPYL ALC	18.15	.840+01	.984+02	.137+01	.43
4	ISOBUTYL ALCOH	18.16	.417+00	.303+02	.680-01	.07
69	TETRACHLORO ET	18.18	.343+00	.339+02	.560-01	.05
125	HEXENE	18.40	.539-01	.172+03	.880-02	.00
18	BUTYRALDEHYDE	18.50	.382+01	.148+03	.624+00	.13
154	METHYL ETHYL K	18.60	.265+01	.295+02	.432+00	.45
43	METHYL METHACR	18.74	.142+00	.409+02	.232-01	.02
6	SEC BUTYL ALCO	19.20	.319+00	.910+02	.520-01	.02
147	PENTANE	19.43	.189+00	.590+03	.308-01	.00
80	FREON 114	20.04	.564+00	.699+03	.920-01	.00
141	PROPYLENE	20.10	.861+03	.861+03	.308-01	.00
108	CYCLO HEXENE	20.81	.108+00	.101+03	.176-01	.01
23	BENZENE	20.97	.686+00	.320+01	.112+00	1.07
137	ISO PENTANE	21.05	.539-01	.295+03	.880-02	.00
71	TRICHLORO ETHY	21.11	.735+00	.538-09	.120+00	999.00
151	ACETONE	21.20	.116+02	.238+03	.189+01	.24
124	ISOPRENE	21.26	.458+00	.557+03	.748-01	.00
75	FREON 12	21.35	.108+00	.778+03	.176-01	.00
138	PENTENE-1	21.38	.108+00	.187+03	.176-01	.00
42	METHYLBUTYRATE	21.69	.490-02	.293+02	.800-03	.00
14	N PROPYL ALCOH	22.02	.711+00	.984+02	.116+00	.04
53	CARBON TETRACH	22.08	.221+00	.629-09	.360-01	999.00
105	ISO BUTANE	22.58	.296+00	.178+03	.484-01	.01
74	FREON 11	22.60	.179+01	.141+03	.292+00	.06
62	DICHLORO ETHAN	22.66	.539+00	.405+02	.880-01	.07
129	(3)METHYL PENT	22.66	.490-03	.176+04	.800-04	.00
104	N-BUTANE	23.15	.270+00	.178+03	.440-01	.01
111	CYCLOPENTENE	23.77	.404+00	.836+02	.660-01	.02
68	DICHLORO METHA	24.48	.293+02	.869+02	.478+01	1.68
127	METHYL ACETYLE	24.75	.167+03	.167+03	.440-02	.00
52	TETRAHYDRO FUR	24.77	.466+00	.590+02	.760-01	.04
9	ETHYLENE GLYCO	25.15	.294-01	.127+03	.480-02	.00

49	DIOXANE	25.58	.319-01	.180+02	.520-02	.01
106	BUTENE-1	25.81	.162+00	.459+03	.264-01	.00
102	BUTADIENE	25.86	.490+00	.221+03	.800-01	.01
41	METHYL ACETATE	26.02	.319+00	.121+03	.520-01	.01
56	CHLOROFORM	26.69	.267+00	.489-09	.436-01	999.00
10	ETHYL ALCOHOL	27.50	.196+01	.189+03	.320+00	.05
78	FREON 22	27.52	.354+03	.354+03	.474+01	.41
3	ALLYL ALCOHOL	28.03	.115+00	.475+00	.188-01	1.21
58	CHLORO PROPYLE	28.43	.105+00	.235+02	.172-01	.02
57	CHLOROETHANE	28.51	.169+01	.132+03	.276+00	.06
16	ACETALDEHYDE	28.79	.180+02	.180+02	.280-01	.05
158	METHYL VINYL K	29.43	.123-01	.287+01	.200-02	.02
11	METHYL ALCOHOL	29.82	.524+02	.524+02	.466+01	2.72
116	ETHANE	31.02	.185+03	.185+03	.836-01	.01
72	VINYLIDENE CHL	31.82	.539-01	.397+01	.880-02	.07
66	METHYL CHLORID	33.26	.207+02	.207+02	.800-03	.00
20	PROPIONALDEHYD	33.42	.245-01	.119+03	.400-02	.00
139	PROPANE	33.87	.135+00	.180+03	.220-01	.00
117	ETHYLENE	35.60	.172+03	.172+03	.120-02	.00
17	ACROLEIN	35.64	.294-01	.115+00	.480-02	1.28
178	DIMETHYL SULFI	36.11	.735-02	.254+01	.120-02	.01
173	ACETONITRILE	36.35	.257+00	.672+01	.420-01	.19
50	FURAN	37.82	.490-02	.111+00	.800-03	.22
77	FREON 21	37.90	.172-01	.421+03	.280-02	.00
184	NITROMETHANE	40.21	.221-01	.250-09	.360-02	999.00
140	PROPADIENE	71.35	.820+02	.820+02	.189+00	.07
171	AMMONIA	100.15	.194+01	.174+02	.316+00	.56

OUTPUT SUMMARY

TITLE: REGENERABLE BED ANALYSIS WITH BT
REGENERABLE BED 1 HRS CYCLE 0.0 HRS DESORPTION
TEMP=100F DACRIT= 16 BED EFFICIENCY = .800
ACID TREATED CHARCOAL

INDEX	NAME	MASS	SUM	TIME
112	DECANE	+.1323-01	+.1323-01	+.3051+06
148	DODECANE	+.2296-02	+.1553-01	+.2697+06
135	NONANE	+.1737-01	+.3289-01	+.1197+06
7	CAPRYL ALCOHOL	+.2290-01	+.5579-01	+.7200+05
149	TRIMETHYL HEXA	+.7396-01	+.1298+00	+.3089+05
114	DIMETHYL CYCLO	+.1446-01	+.1442+00	+.2634+05
24	ISO PROPYL BEN	+.3629-02	+.1478+00	+.2588+05
159	OCTANONE	+.2247-01	+.1703+00	+.2373+05
27	ETHYL METHYL B	+.8073-01	+.2510+00	+.1551+05
132	OCTANE	+.1414+00	+.3924+00	+.1034+05
31	MESITHYLENE	+.2831-01	+.4207+00	+.9403+04
136	NONENE	+.1278+00	+.5485+00	+.7422+04
122	LIMONENE	+.3622-01	+.5847+00	+.7004+04
172	ACETOPHENONE	+.1478-01	+.5995+00	+.6699+04
12	HEXYL ALCOHOL	+.5157-01	+.6511+00	+.5863+04
133	OCTENE	+.1143-01	+.6625+00	+.5981+04
33	METHYL STYRENE	+.2967+00	+.9592+00	+.4137+04
119	HEPTANE	+.2310-01	+.9823+00	+.3931+04
61	DICHLORO BENZE	+.6489-01	+.1047+01	+.3671+04
30	INDENE	+.1911+00	+.1238+01	+.3174+04
25	N PROPYL BENZE	+.8918-02	+.1247+01	+.3224+04
126	METHYL CYCLOHE	+.2209-02	+.1249+01	+.2956+04
35	STYRENE	+.5485-01	+.1304+01	+.2877+04
2	N AMYL ALCOHOL	+.1777+00	+.1482+01	+.2546+04
1	ISO AMYL ALCOH	+.8047-01	+.1563+01	+.2383+04
152	METHYL BUTYL K	+.1269+00	+.1689+01	+.2314+04
153	DIISOBUTYL KET	+.5891-01	+.1748+01	+.2404+04
129	(3)METHYL PENT	+.1122+00	+.1860+01	+.1843+04
42	METHYLBUTYRATE	+.3989+00	+.2259+01	+.1539+04
48	BUTYL LACTATE	+.1540+00	+.2413+01	+.1622+04
120	HEPTENE	+.8128-01	+.2495+01	+.1555+04
15	PHENOL	+.1158+00	+.2610+01	+.1470+04
160	CYCLOHEXANONE	+.9156-02	+.2620+01	+.1444+04
28	TRIMETHYL BENZ	+.4892-01	+.2669+01	+.1535+04
82	FREON 112	+.3185+00	+.2987+01	+.1255+04

161	MESITYL OXIDE	+.1290+00	+.3116+01	+.1227+04
40	ETHOXY ETHYL A	+.7941-01	+.3195+01	+.1236+04
125	HEXENE	+.9025-01	+.3286+01	+.1108+04
21	BENZALDEHYDE	+.2149+00	+.3501+01	+.1135+04
39	BUTYL ACETATE	+.1650+00	+.3666+01	+.1078+04
45	ETHYL LACTATE	+.1100+00	+.3776+01	+.1010+04
38	ISO BUTYL ACET	+.1261+01	+.5037+01	+.7900+03
46	PROPYL ACETATE	+.6299-02	+.5043+01	+.7457+03
8	CYCLOHEXANOL	+.3264+00	+.5370+01	+.7476+03
26	ETHYL BENZENE	+.1701+00	+.5540+01	+.7166+03
155	METHYL ISOBUTY	+.2365+00	+.5776+01	+.6946+03
113	DIMETHYL BUTAN	+.2990+00	+.6075+01	+.6200+03
43	METHYL METHACR	+.1108+00	+.6186+01	+.5855+03
54	CHLORO BENZENE	+.9339-01	+.6280+01	+.5914+03
69	TETRACHLORO ET	+.2352+00	+.6515+01	+.5604+03
131	METHYL CYCLO H	+.1707+00	+.6686+01	+.5720+03
121	HEXANE	+.9811+00	+.7667+01	+.4999+03
157	METHYL PROPYL	+.8835+00	+.8550+01	+.4420+03
36	XYLENE P	+.4351+00	+.8985+01	+.4488+03
75	FREON 12	+.1265+01	+.1025+02	+.3407+03
137	ISO PENTANE	+.1163+00	+.1037+02	+.3383+03
6	SEC BUTYL ALCO	+.2476+00	+.1061+02	+.3390+03
108	CYCLO HEXENE	+.2535+01	+.1315+02	+.2676+03
85	DICHLORO DIFLU	+.2155+00	+.1336+02	+.2809+03
4	ISOBUTYL ALCOH	+.7387+00	+.1410+02	+.2589+03
147	PENTANE	+.6202+00	+.1472+02	+.2436+03
9	ETHYLENE GLYCO	+.1500+01	+.1622+02	+.2040+03
55	CHLORO BUTANE	+.1171-01	+.1623+02	+.2284+03
5	N BUTYL ALCOHO	+.2700+01	+.1893+02	+.2014+03
141	PROPYLENE	+.1079+01	+.2001+02	+.1775+03
138	PENTENE-1	+.6215+00	+.2063+02	+.1692+03
47	ISO PROPYL ACE	+.1588+00	+.2079+02	+.1873+03
49	DIOXANE	+.2945+01	+.2374+02	+.1386+03
80	FREON 114	+.1807+00	+.2392+02	+.1486+03
53	CARBON TETRACH	+.2922+00	+.2421+02	+.1428+03
130	METHYL CYCLO P	+.3165+01	+.2738+02	+.1384+03
70	TRICHLORO ETHA	+.7057+01	+.3443+02	+.1089+03
127	METHYL ACETYLE	+.1124+01	+.3556+02	+.9362+02
107	CYCLO HEXANE	+.4613+01	+.4017+02	+.9520+02
71	TRICHLORO ETHY	+.9458+01	+.4963+02	+.7060+02
37	TOLUENE	+.6016+01	+.5564+02	+.7170+02
44	ETHYL ACETATE	+.1410+01	+.5705+02	+.6500+02
154	METHYL ETHYL K	+.1421+01	+.5847+02	+.6206+02
79	FREON 113	+.4257+01	+.6273+02	+.6168+02
14	N PROPYL ALCOH	+.8393+00	+.6357+02	+.5443+02
124	ISOPRENE	+.1952+01	+.6552+02	+.5337+02
23	BENZENE	+.3802+00	+.6590+02	+.5327+02
67	METHYL CHLOROF	+.7697+01	+.7360+02	+.5108+02
62	DICHLORO ETHAN	+.4484+01	+.7808+02	+.4392+02
105	ISO BUTANE	+.4511+01	+.8260+02	+.4157+02
104	N-BUTANE	+.6936+01	+.8953+02	+.3804+02
52	TETRAHYDRO FUR	+.4117+01	+.9365+02	+.3554+02
158	METHYL VINYL K	+.1362+01	+.9501+02	+.3267+02
18	BUTYRALDEHYDE	+.7210+01	+.1022+03	+.3555+02

41	METHYL ACETATE	+.1134+01	+.1034+03	+.3161+02
3	ALLYL ALCOHOL	+.5636+01	+.1090+03	+.2909+02
111	CYCLOPENTENE	+.5704+01	+.1147+03	+.2943+02
13	ISO PROPYL ALC	+.3902+01	+.1186+03	+.3080+02
74	FREON 11	+.1599+02	+.1346+03	+.2550+02
106	BUTENE-1	+.2459+01	+.1370+03	+.2392+02
56	CHLOROFORM	+.3374+01	+.1404+03	+.2304+02
16	ACETALDEHYDE	+.9463+01	+.1499+03	+.2091+02
66	METHYL CHLORID	+.3059+01	+.1529+03	+.1909+02
58	CHLORO PROPYLE	+.1703+02	+.1700+03	+.1854+02
20	PROPIONALDEHYD	+.1158+02	+.1815+03	+.1604+02
72	VINYLIDENE CHL	+.8238+02	+.2639+03	+.1132+02
102	BUTADIENE	+.5457+01	+.2694+03	+.1216+02
151	ACETONE	+.6630+02	+.3357+03	+.1043+02
17	ACROLEIN	+.4896+02	+.3846+03	+.7292+01
178	DIMETHYL SULFI	+.6335+02	+.4480+03	+.6211+01
117	ETHYLENE	+.4770+01	+.4528+03	+.6200+01
10	ETHYL ALCOHOL	+.2871+02	+.4815+03	+.6639+01
50	FURAN	+.1400+03	+.6214+03	+.4346+01
77	FREON 21	+.4103+03	+.1032+04	+.2614+01
57	CHL□ROETHANE	+.2042+03	+.1236+04	+.2547+01
139	PROPANE	+.3896+03	+.1626+04	+.1778+01
116	ETHANE	+.1193+03	+.1745+04	+.1735+01
173	ACETONITRILE	+.1368+03	+.1882+04	+.1473+01
68	DICHLORO METHA	+.7111+03	+.2593+04	+.1289+01
184	NITROMETHANE	+.1508+03	+.2744+04	+.9424+00
78	FREON 22	+.3905+04	+.6648+04	+.4807+00
11	METHYL ALCOHOL	+.2377+04	+.9025+04	+.3418+00
140	PROPADIENE	+.1017+07	+.1026+07	+.1054-02
171	AMMONIA	+.3961+07	+.4987+07	-.6297-04