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Working Fluid Selection for Space-Based Two-Phase Heat Transport Systems

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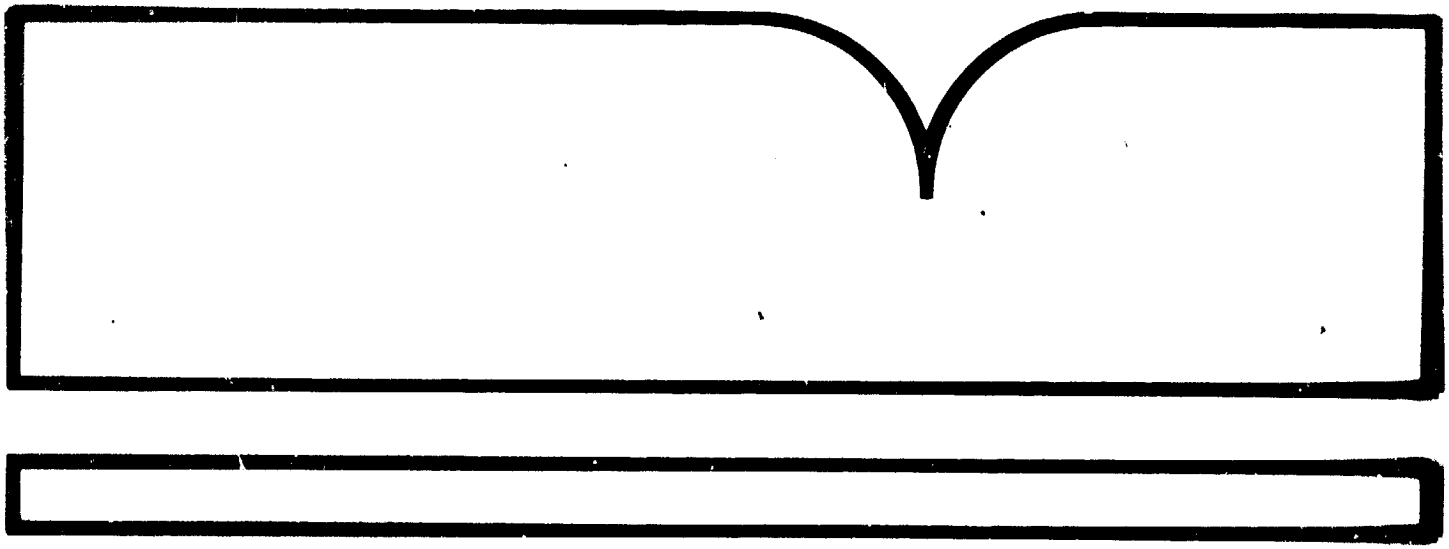

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Mark O. McLinden

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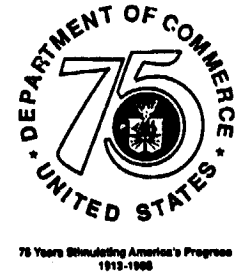

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U.S. DEPARTMENT OF COMMERCE, C. William Verity, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

ABSTRACT

The working fluid for externally-mounted, space-based two-phase heat transport systems is considered. A sequence of screening criteria involving freezing and critical point temperatures and latent heat of vaporization and vapor density are applied to a data base of 860 fluids. The thermal performance of the 52 fluids which pass this preliminary screening are then ranked according to their impact on the weight of a reference system. Upon considering other non-thermal criteria (flammability, toxicity and chemical stability) a final set of 10 preferred fluids is obtained. The effects of variations in system parameters is investigated for these 10 fluids by means of a factorial design.

INTRODUCTION

In order to remove the heat generated by electronics and other payloads on spacecraft some type of heat transport system is required. The heat generating equipment is typically attached to a 'cold plate'. In state-of-the art two-phase thermal control systems, these cold plates are cooled by the evaporation of a volatile working fluid contained in closed channels attached to the back of the cold plate. By using an evaporative process to remove heat, the entire cold plate can be maintained at a uniform temperature. The vaporized working fluid then flows to a condenser where the latent heat of vaporization is rejected either to the main spacecraft thermal loop or is radiated directly to space. The condensate is then pumped either mechanically or by capillary forces back to the cold plate to complete the loop.

The properties of the working fluid strongly influence the design and performance of the entire heat transport system. Yet, to date there has been no systematic and comprehensive evaluation of working fluids in these systems.

The working fluid in a two-phase heat transport system undergoes many of the same processes and at roughly the same temperature as the refrigerant in a vapor compression refrigeration system and will therefore possess many of the same desirable properties. Several sources (e.g. [1], [2]) present lists of desirable refrigerant properties; these are summarized in Table 1. No single fluid satisfies all of the criteria presented in Table 1, but through an evolutionary process extending over many decades a few classes of fluids dominate present applications. Ammonia has excellent thermal characteristics and is very inexpensive but operates at high

Table 1 - Desirable Properties of a Refrigerant

Chemical:

- Stable and inert

Health, Safety and Environmental

- Nontoxic
- Nonflammable
- Does not destroy stratospheric ozone

Thermal:

- Critical point and boiling point temperatures appropriate for the application
- Low vapor heat capacity
- Low viscosity
- High thermal conductivity

Materials compatibility:

- Soluble in lubricating oils
- Compatible with common materials

Miscellaneous

- Low freezing point
- High dielectric strength of vapor
- Easy leak detection
- Low cost

pressures and is toxic. The hydrocarbons are also inexpensive and have good thermal characteristics, are non-toxic but are flammable. The hazards associated with ammonia and hydrocarbons limit their use to industrial and large commercial systems. For smaller systems, the halogenated hydrocarbons are almost universally used because of their combination of very low toxicity and non-flammability. The tradeoffs, however, are a higher cost, lower heat of vaporization, and generally poorer transport properties.

The requirements of a working fluid in a heat transport system are somewhat different than those for a refrigeration system. In particular, since the heat transport system does not have a compressor, the properties that determine the behavior of a refrigerant in a compression process (e.g. entropy) will be of lesser importance and a high heat of vaporization of greater importance. For space-based systems the influence of fluid properties on total system weight is a prime concern. This includes not only the weight (density) of the fluid itself, but the required size and strength of the heat exchangers and piping, and a factor to account for the pump work necessary to circulate the fluid. For capillary-pumped systems a high surface tension is desirable.

As with terrestrial refrigeration systems, the safety-related characteristics of toxicity and flammability are of concern. The intended application will determine the relative importance of safety and thermal characteristics. The present study focuses on unmanned systems and thus a toxic and/or flammable fluid cannot be automatically eliminated. For manned spacecraft applications, the ranking criteria, and thus conclusions regarding the best fluid, may be entirely different.

For these reasons it is worthwhile to undertake a comprehensive evaluation of working fluids in heat transport systems rather than merely choosing a fluid based on refrigeration system criteria. The purpose of the present work is to establish criteria for the evaluation of potential working fluids for a specific class of space-based systems, apply these criteria to a large number of fluids to select the best fluid(s), and present the tradeoffs existing among these best fluids. This will then enable NASA designers to make a rational choice of working fluid for future systems. While focusing on space-based systems, the analysis presented here is applicable to ground-based systems as well.

The general approach will be to apply a series of screening criteria to the fluids contained in an extensive data base. As the number of fluids passing each successive set of criteria is reduced, the subsequent criteria will be increasingly sophisticated. The Physical Property Data Service (PPDS) data base of 860 industrially important fluids will be used. This proprietary data base has been compiled by the Institution of Chemical Engineers in the United Kingdom. NBS has purchased this data base in the form of an 'Electronic Data Module' which is connected to a host microcomputer. While no data base can contain all possible fluids, the PPDS data base contains representatives of every major class of fluid; as will be seen later, it is particularly complete for the types of fluids which are highly ranked in the analysis. (A more detailed description of this data base, including a listing of the 860 fluids, is given in Appendix I.)

Those fluids passing a set of preliminary criteria will then be evaluated in a reference heat transport system. The fluids will be ranked

according to a system weight which includes the fluid weight, the fluid-dependent portion of the component weights and an allowance for pumping power. At this point the ranking of the fluids will then be considered along with other, non-thermal, properties such as stability, toxicity, flammability and materials compatibility to arrive at a final set of preferred working fluids. Finally, the effects of changes in the parameters defining the reference heat transport system will be analyzed for the final set of fluids by means of a factorial design.

REFERENCE HEAT TRANSPORT SYSTEM

Proposed designs for next-generation spacecraft heat transport system are rather complex with numerous sensors, automatic valves, controllers, etc. Figure 1 depicts one proposed design for a Space Station attached payload active thermal control system. A very detailed design and analysis program has been developed for this system by Costello [3]. This program is currently limited to ammonia and R11 but could, in principle, be extended to other fluids.

But rather than analyze the effects of different fluids on a very specific system, the approach taken here is to reduce the heat transport system to its essential elements. The selection of the working fluid would be made early in the design process; details of the design would vary from fluid to fluid. Thus, consideration of a simplified, generic system is called for. Furthermore, the analysis is limited to those portions of the system which are fluid-dependent. For example, while the flow channels attached to a cold plate may vary in size or pressure rating according to the working fluid the actual cold plate itself will be independent of fluid. Similarly, a particular sensor or automatic valve will be required independent of the fluid. This sort of approach not only greatly simplifies the analysis but also generalizes the results. The system is specified in terms of a limited number of parameters which can easily be varied to examine different design parameters.

This study will consider two systems - mechanically-pumped and capillary. The reference pumped system is shown in Figure 2. The evaporator is taken to be 4 cold plates piped in parallel. Each cold plate has 5 parallel flow channels for a total of 20. Each channel is 0.76 m long and

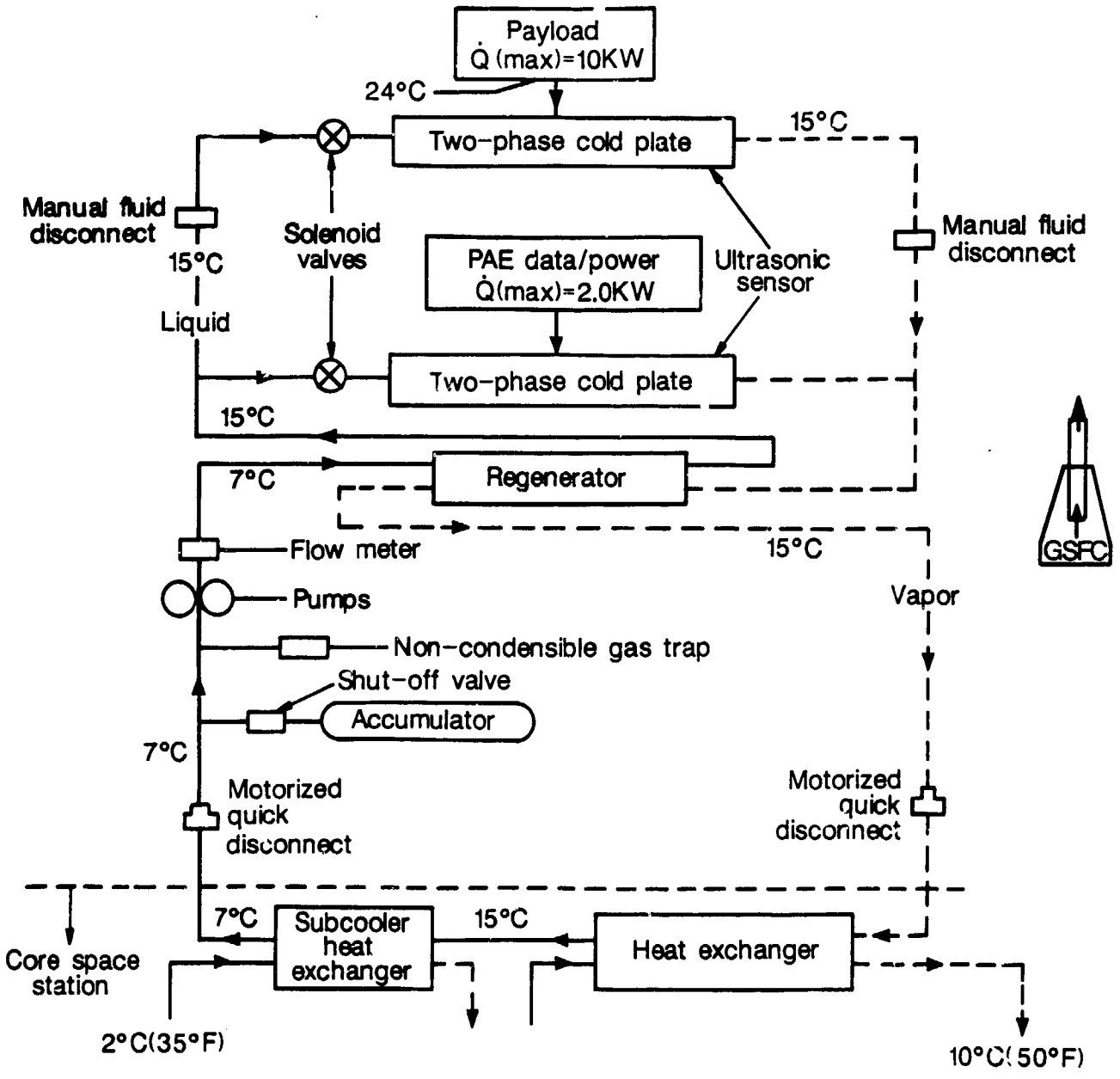

Figure 1 - Schematic of typical attached payload active thermal control system.

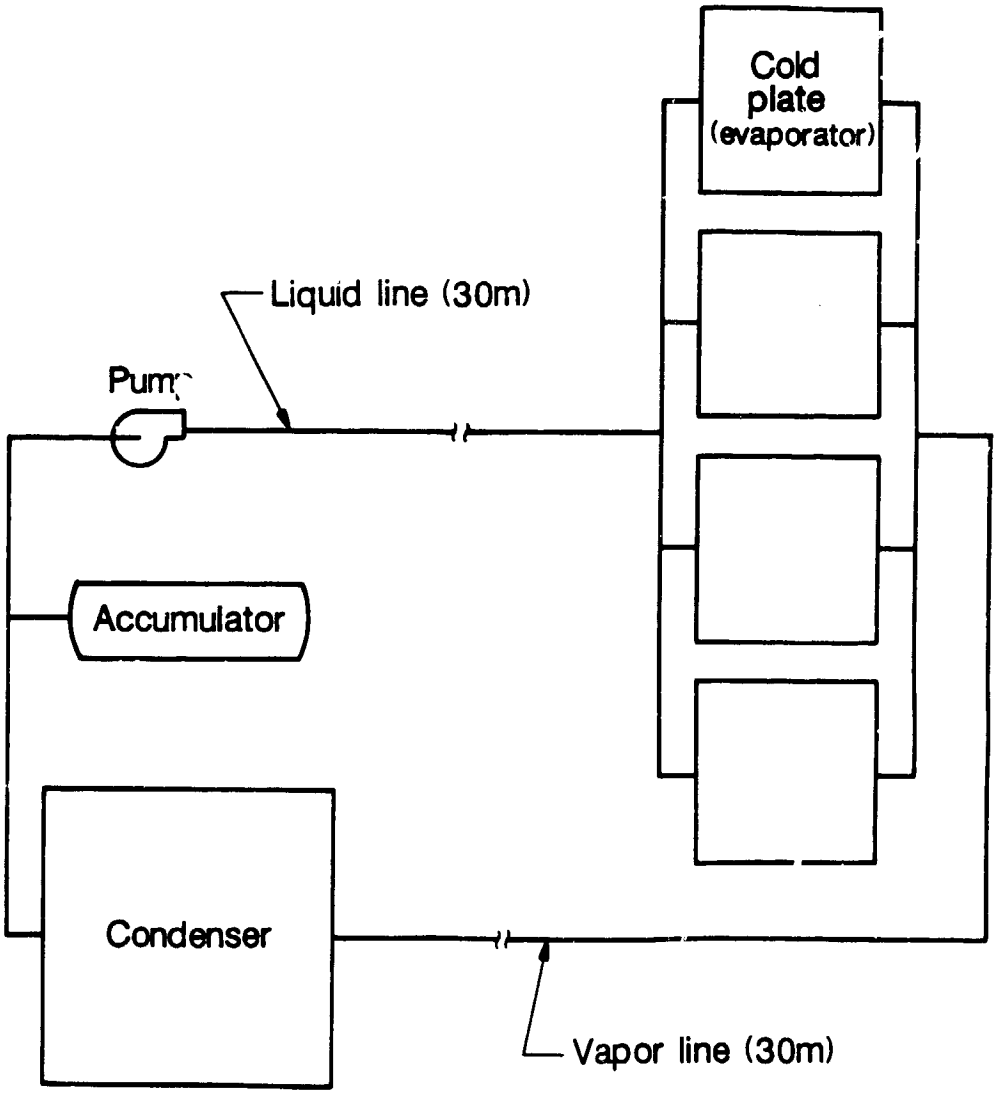

Figure 2 - Reference (base case) heat transport system, mechanically pumped.

consists of a 9.5 mm diameter liquid channel and a 25 mm vapor channel. The design heat load is 10 kW. The condenser consists of 8 parallel, 1.22 m long annuli with an inner and outer diameter of 20 and 25 mm respectively. Connecting the evaporators and condenser are liquid and vapor lines, each 30 m in length; the diameters and wall thickness of these lines will be optimized for each fluid subject to a maximum diameter of 38 mm and minimum wall thickness of 0.8 mm.

The accumulator is designed to store the entire fluid charge as liquid. Its volume is 1.2 times the total fluid volume of all the other components. This large accumulator volume represents a very conservative design approach which has significant weight implications. It is used here as representative of the current state-of-the-art. The circulating pump is specified in terms of an equivalent weight of 0.25 kilograms per watt of theoretical pump work. This factor includes the pump efficiency, the weight of the pump and an allowance for the weight of the power system necessary to supply the pump.

The nominal and maximum operating temperatures are 20°C and 45°C, respectively. The system would be expected to survive without damage from -40°C to 80°C. The upper temperature limit may impose a significant penalty on some fluids since the system must be designed for the fluid vapor pressure at 80°C.

For capillary systems (Figure 3) the circulating pump is replaced by a wick assembly which 'pumps' the fluid through capillary forces. An effective pore diameter of 10μm is assumed for the wick. The design heat

load is 2 kW for the single cold plate. The size of the condenser is also proportionally smaller compared to that in the 10 kW mechanically-pumped system. In all other aspects the capillary and pumped systems are identical.

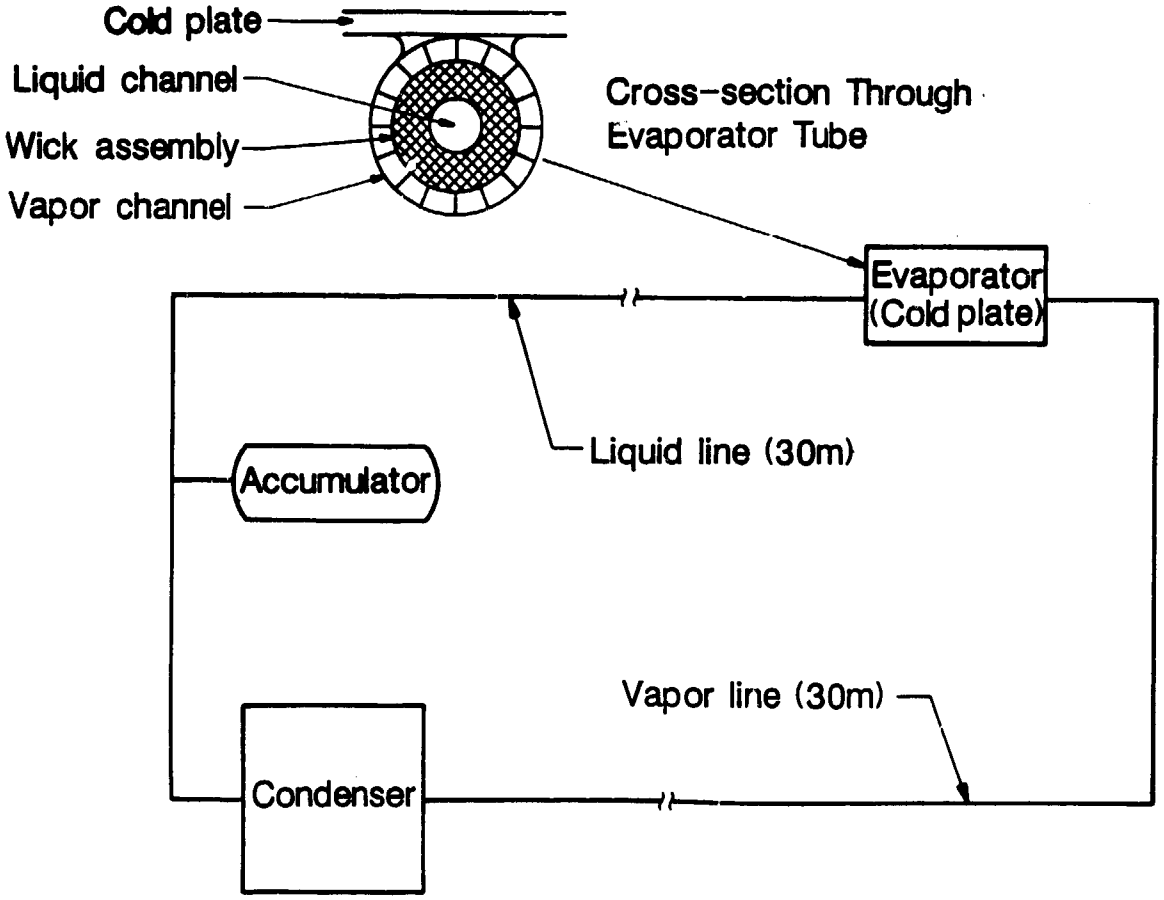

Figure 3 - Reference heat transport system - capillary.

FLUID EVALUATION PROCEDURE

A suitable working fluid must satisfy many requirements. Of primary concern is its long-term chemical stability. The relative importance of good thermal performance, low toxicity and non-flammability depend on the application. For systems which serve inhabited spaces, safety considerations would take precedence over thermal performance. For systems which would serve externally mounted equipment or experiments, a fluid of at least moderate toxicity and/or flammability might be chosen if it had superior thermal characteristics (as indicated by the present use of ammonia in some systems). Of secondary importance would be such criteria as materials compatibility, cost and availability. One would approach the problem of fluid evaluation according to relative importance of the various requirements and also according to the resources available.

In the present work, the focus is on thermal performance. This arises not only from the goals set forth at the outset of the project but also from the relative ease of evaluating thermal performance. The availability of a computerized data base for thermodynamic and transport (but not e.g. toxicological) properties makes it more efficient to evaluate the chemical stability, toxicity, flammability, materials compatibility, etc. of those fluids which pass the thermal criteria rather than vice-versa.

Preliminary Screening

The PPDS data base contains information on 860 materials, many of which are solids or super-critical fluids at normal temperatures. The first screening criteria, therefore, will select only those materials which have coexisting liquid and vapor phases in the temperature range of

interest, specifically a freezing temperature less than -40°C and a critical temperature greater than 50°C. The cutoff for critical temperature is 5°C above the maximum operating temperature.

An additional requirement is a vapor pressure of no more than 5000 kPa at the highest temperature the system is expected to survive (80°C). For fluids with critical temperatures between 50°C and 80°C this last criterion is for a critical pressure less than 5000 kPa. The vapor pressure criterion was selected on the basis that fluids operating at pressures substantially above those for ammonia (857 kPa at 20°C, 4129 kPa at 80°C) would not be acceptable.

Of the 860 fluids, 513 pass this first set of criteria. These 513 fluids were then screened according to their ability to remove heat by evaporation as measured by the product of the latent heat of vaporization and the saturated vapor density evaluated at 25°C. This parameter is a measure of the vapor volumetric flow necessary to remove a quantity of heat which in turn has a strong influence on required piping sizes, pressure drops, etc. A minimum value of 1.0 kJ/L, or about one order of magnitude lower than the value for ammonia, was selected. The application of this criterion reduces the list of fluids to 51. Eliminated were those fluids which would operate at very low vapor densities and would therefore require excessively large vapor ducts.

Upon examining the fluids which failed, only two - HBr and CH_2F_2 - were eliminated on the basis of excessive vapor pressure. HBr can reasonably be excluded because of its extreme toxicity and reactivity. Since the cut-off value for pressure was somewhat arbitrary, there would seem to be little reason to exclude only a single compound on the basis of vapor

pressure and thus CH_2F_2 was re-added to the list. Water failed the freezing point criteria but has the highest heat of vaporization of any fluid and was therefore also added. The vapor pressure data for $COCl_2$ (phosgene) in the data bank were seriously in error and would have required special treatment; in view of its extreme toxicity it was deleted from the list. These additions and deletions yield a list of 52 fluids, given in Table 2, which will be considered in greater detail.

Ranking By Incremental System Weight

For the ranking of thermal performance, a single figure-of-merit is desirable. For terrestrial thermal systems, total life cycle cost is an excellent index. Given the high cost of placing mass in orbit, system weight is the most appropriate index for space-based systems. The 52 fluids which passed the preliminary screening are evaluated in the reference heat transport systems with the resulting incremental system weight serving as a rating factor. This rating factor is a measure of the differences in system weight between fluids; it does not represent the total weight of the heat transport system. This weight is composed of four terms which will vary from fluid to fluid: the piping weight which is a function of its diameter and wall thickness; the fluid weight which is a function of the fluid density and total system volume; the accumulator weight which depends on system volume and operating pressure; and (for pumped systems) the equivalent weight associated with the pumping power.

Heat Transfer Considerations

The operation of the two-phase heat transport system involves the

Table 2 - Summary of Fluids Passing Preliminary Screening

PPDS No	Name and formula		Tmelt (K)	Tcrit (K)	VP@25 (kPa)	VP@80 (kPa)	Hfg/Vv (kJ/l)
HYDROCARBONS							
6	1,2-BUTADIENE	C4H6	137.	444.	168.	802.	1.62
7	BUTA-1,3-DIENE	C4H6	127.	425.	281.	1151.	2.55
8	BUTANE	C4H10	135.	425.	244.	1015.	2.20
9	BUT-1-ENE	C4H8	88.	420.	297.	1201.	2.57
10	2-BUTENE(CIS)	C4H8	134.	436.	214.	928.	2.03
11	2-BUTENE(TRANS)	C4H8	168.	429.	234.	996.	2.18
12	1-BUTYNE	C4H6	147.	464.	188.	842.	1.22
48	ISOBUTANE	C4H10	113.	408.	350.	1335.	2.98
49	2-METHYLPROPENE	C4H8	133.	418.	304.	1196.	2.68
57	PROPANE	C3H8	85.	370.	950.	3136.	6.95
58	PROPENE	C3H6	88.	365.	1155.	3719.	8.19
60	PROPYNE	C3H4	171.	402.	577.	2244.	4.95
66	ALLENE	C3H4	137.	394.	805.	2779.	5.36
170	VINYL ACETYLENE	C4H4	****	455.	202.	855.	1.97
313	3-METHYLBUT-1-ENE	C5H10	105.	453.	120.	566.	1.15
HALOCARBONS							
130	VINYL CHLORIDE	C2H3CL	119.	425.	389.	1485.	3.18
177	CHLOROETHANE(160)	C2H5CL	137.	460.	160.	751.	1.61
211	2-CHLOROPROPENE	C3H5CL	136.	478.	110.	551.	1.18
355	CHLOROMETHANE(40)	CH3CL	175.	416.	570.	2156.	4.88
369	CHLORODIFLUOROMETHANE	CHCLF2	127.	369.	1041.	3648.	7.97
431	DICHLORODIFLUOROMETHA	CCL2F2	115.	385.	651.	2291.	5.13
432	BROMOCHLORODIFLUOROME	CBRCLF2	113.	427.	275.	1128.	2.49
434	DICHLOROFLUOROMETHANE	CHCL2F	138.	452.	182.	853.	1.83
435	1,2-DICHLORO-1,1,2,2-	C2CL2F4	179.	419.	212.	929.	2.00
436	CHLOROPENTAFLUOROETHA	C2CLF5	174.	353.	916.	3150.	6.89
439	1-CHLORO-2,2,2-TRIFLU	C2H2CLF3	168.	429.	199.	947.	2.18
440	TRICHLOROFLUOROMETHAN	CCL3F	162.	471.	107.	527.	1.12
482	BROMOTRIFLUOROMETHANE	CBRF3	105.	340.	1614.	3965.	10.83
483	DIBROMODIFLUOROMETHAN	CBR2F2	132.	471.	110.	545.	1.20
485	DIFLUOROMETHANE(32)	CH2F2	137.	352.	1689.	5816.	11.92
486	BROMOMETHANE	CH3BR	180.	464.	218.	971.	2.14
487	1,1-DICHLORO-1,2,2,2-	C2CL2F4	216.	419.	218.	940.	2.10
490	1-CHLORO-1,1-DIFLUORO	C2H3CLF2	142.	410.	354.	1441.	3.22
492	1,1-DIFLUOROETHANE(15	C2H4F2	156.	387.	607.	2328.	5.12
649	VINYL BROMIDE	C2H3BR	135.	474.	141.	621.	1.39
C + H + O COMPOUNDS							
64	ACETALDEHYDE	C2H4O	150.	461.	118.	608.	1.29
111	METHYL ETHER	C2H6O	132.	400.	593.	2224.	5.00
143	FORMALDEHYDE	CH2O	181.	410.	533.	2318.	4.85
193	ETHYLENE OXIDE(EPOXYE	C2H4O	161.	469.	175.	872.	1.80
196	KETENE	C2H2O	139.	373.	1293.	3983.	9.73
NITROGEN COMPOUNDS							
70	AMMONIA	NH3	195.	405.	1003.	4141.	8.88
216	TRIMETHYLAMINE	C3H9N	156.	433.	219.	941.	2.06
422	ETHYLAMINE	C2H7N	192.	456.	141.	768.	1.63
423	DIMETHYLAMINE	C2H7N	181.	438.	205.	1016.	2.17
554	METHYLAMINE	CH5N	180.	430.	348.	1655.	3.55
SULFUR COMPOUNDS							
228	SULPHUR DIOXIDE	SO2	198.	431.	396.	1811.	3.88
373	METHANETHIOL	CH4S	150.	469.	202.	937.	2.01
375	CARBONYL SULPHIDE	COS	134.	375.	1245.	4000.	8.82
MISCELLANEOUS COMPOUNDS							
63	WATER	H2O	273.	647.	3.	47.	.06
154	CHLORINE	CL2	172.	417.	778.	2737.	6.24
380	HYDROGEN IODIDE	HI	222.	424.	788.	2668.	6.31
467	BORON TRICHLORIDE	BCL3	166.	452.	155.	702.	1.53

transfer of heat to and from the working fluid in the cold plate and condenser, respectively. This suggests that the varying heat transfer coefficients among the candidate fluids would have a significant impact on system design. Somewhat surprisingly, however, it will be seen that the application, reference system design, and fluid properties combine to yield very similar heat transfer performance among the 52 fluids considered in detail.

Evaporative heat transfer coefficients are most often correlated in terms of separate nucleate and convective contributions; an example is the correlation by Chen [4]:

$$h_{evap} = S\, h_{nb} + F\, h_{lo} \tag{1}$$

where the coefficients obtained from nucleate boiling, h_{nb}, and single phase convective, h_{lo}, correlations are multiplied by a suppression factor ($S \leq 1$) and two-phase multiplier ($F \geq 1$) respectively to obtain the two-phase coefficient. For conditions of low heat flux (such as the value of 8.4 kw/m^2 for the reference system) and/or high vapor quality, nucleate boiling is completely suppressed so that:

$$h_{evap} = F h_{lo} \tag{2}$$

The value of h_{lo} is given by a single-phase correlation such as Dittus-Boelter:

$$h_{lo} = 0.023 \frac{k_l}{D} \left[\frac{(1 - x)\, \dot{m})}{D\mu_l}\right]^{0.8} \left[\frac{C_{p,l}\mu_l}{k_l}\right]^{0.4} \tag{3}$$

where x is vapor quality and k_l and μ_l are the thermal conductivity and viscosity of the liquid. A widely-used correlation for the two-phase multiplier is that by Chen [4]:

$$F = 1.0 + 1.8 \left[\left(\frac{1-x}{x} \right)^{0.9} \left(\frac{\rho_v}{\rho_l} \right)^{0.5} \left(\frac{\mu_l}{\mu_v} \right)^{0.1} \right]^{-0.82} \quad (4)$$

The combination of equations (3) and (4) for a given mass flow rate, pipe diameter and quality and the assumption that the constant 1.0 in Equation (4) is small compared to the second term yields the dependence of evaporative heat transfer coefficient on fluid properties:

$$h_{evap} = f(k_l^{0.6},\ \mu_l^{-0.482},\ \mu_v^{0.082},\ C_{p,l}^{0.4},\ \rho_l^{0.41},\ \rho_v^{-0.41}) \quad (5)$$

To remove a given quantity of heat, the mass flow rate is inversely proportional to the heat of vaporization:

$$h_{evap} = f(h_{fg}^{-0.8},\ k_l^{0.6},\ \mu_l^{-0.482},\ \mu_v^{0.082},\ C_{p,l}^{0.4},\ \rho_l^{0.41},\ \rho_v^{-0.41}) \quad (6)$$

For condensation, the correlation of Shah [5] gives the average heat transfer coefficient for complete condensation of a wide variety of fluids:

$$h_{cond} = h_{lo}\ (0.55 + 2.09\ P_r^{-0.38}) \quad (7)$$

where P_r is the reduced pressure and h_{lo} is given by Equation (3). For a given mass flow rate and diameter:

$$h_{cond} = f(k_l^{0.6},\ \mu_l^{-0.4},\ C_{pl}^{0.4},\ P_r^{-0.38}) \quad (8)$$

Again, to remove a given quantity of heat:

$$h_{cond} = f(h_{fg}^{-0.8},\ k_l^{0.6},\ \mu_l^{-0.4},\ C_{pl}^{0.4},\ P_r^{-0.38}) \quad (9)$$

The properties groups given in Equations (5, 6, 8 and 9) are presented in Table 3 for the 52 fluids passing the preliminary screening. (The numerical values presented in Table 3 were evaluated at 20°C and have been

Table 3 - Comparison of two-phase heat transfer coefficients as given by Equations 5, 6, 8 and 9 for the cases of equal mass flow rate and equal heat load.

PPDS NO.	Formula	h_{fg} (kj/kg)	$\dot{m}$ = const		Q = const	
			h_{evap}	h_{cond}	h_{evap}	h_{cond}
HYDROCARBONS						
6	C_4H_6	433.5	.410	.422	.916	.944
7	C_4H_6	387.9	.340	.364	.831	.888
8	C_4H_{10}	359.5	.301	.329	.781	.855
9	C_4H_8	354.6	.299	.327	.784	.859
10	C_4H_8	398.8	.340	.363	.813	.866
11	C_4H_8	386.3	.320	.342	.783	.838
12	C_4H_6	441.1	.493	.440	1.087	.970
48	C_4H_{10}	331.7	.244	.276	.676	.765
49	C_4H_8	360.6	.279	.306	.722	.792
57	C_3H_8	344.9	.211	.249	.565	.669
58	C_3H_6	344.5	.220	.261	.590	.701
60	C_3H_4	481.5	.301	.330	.618	.677
66	C_3H_4	434.8	.289	.298	.643	.664
170	C_4H_4	443.3	.366	.401	.802	.881
313	C_5H_{10}	323.6	.340	.369	.960	1.041
HALOCARBONS						
130	C_2H_3Cl	300.5	.247	.260	.741	.778
177	C_2H_5Cl	372.1	.311	.326	.785	.823
211	C_3H_5Cl	326.4	.304	.333	.853	.934
355	CH_3Cl	386.0	.292	.314	.716	.771
369	$CHClF_2$	185.9	.126	.146	.553	.640
431	CCl_2F_2	141.2	.099	.115	.541	.629
432	$CBrClF_2$	127.1	.103	.114	.614	.681
434	$CHCl_2F$	232.6	.196	.212	.722	.779
435	$C_2Cl_2F_4$	128.3	.106	.121	.630	.714
436	C_2ClF_5	97.4	.073	.091	.541	.671
439	$C_2H_2ClF_3$	203.0	.147	.163	.604	.670
440	CCl_3F	183.5	.169	.186	.749	.828
482	$CBrF_3$	84.0	.061	.078	.510	.649
483	CBr_2F_2	125.1	.126	.139	.762	.842
485	CH_2F_2	272.2	.189	.211	.613	.684
486	CH_3Br	247.1	.192	.200	.673	.700
487	$C_2Cl_2F_4$	130.4	.094	.109	.549	.634
490	$C_2H_3ClF_2$	206.8	.132	.151	.534	.609
492	$C_2H_4F_2$	280.8	.203	.219	.643	.692
649	C_2H_3Br	220.6	.228	.224	.873	.860
C + H + O COMPOUNDS						
64	C_2H_4O	593.9	.608	.538	1.055	.934
111	C_2H_6O	409.2	.325	.355	.760	.831
143	CH_2O	695.0	.553	.513	.847	.786
193	C_2H_4O	561.4	.507	.518	.921	.941
196	C_2H_2O	383.6	.232	.249	.573	.614
NITROGEN COMPOUNDS						
70	NH_3	1184.5	1.000	1.000	1.000	1.000
216	C_3H_9N	372.9	.319	.347	.805	.874
422	C_2H_7N	622.2	.572	.596	.958	.998
423	C_2H_7N	561.1	.468	.482	.851	.877
554	CH_5N	772.9	.583	.595	.820	.837
SULFUR COMPOUNDS						
228	SO_2	359.7	.304	.324	.790	.840
373	CH_4S	496.4	.449	.474	.899	.950
375	COS	244.0	.196	.222	.693	.788
MISCELLANEOUS COMPOUNDS						
63	H_2O	2454.5	5.891	5.570	3.288	3.110
154	Cl_2	255.0	.146	.170	.498	.580
380	HI	141.3	.035	.043	.191	.238
467	BCl_3	199.6	.198	.205	.823	.853

Note: Heat transfer coefficients are relative to the values for ammonia.

normalized relative to ammonia.) The individual fluid properties of conductivity or viscosity vary by as much as an order of magnitude among the various fluids and likewise the two-phase heat transfer coefficients vary over a wide range when considered on the basis of equal mass flow rate.

When considered on the basis of removing a given quantity of heat, the differences in heat transfer among the various fluids is greatly reduced. Excluding those compounds in the "miscellaneous" category, for the equal heat case, the maximum variation among evaporative coefficients is 2.1:1 and only 1.7:1 among condensation coefficients compared to 16.3:1 and 12.8:1, respectively, for the equal mass flow rate case. Fluids, such as Halon 1301, which have low conductivities and heat capacities, (properties which lead to poor heat transfer coefficients) also tend to have low latent heats. In order to remove a given quantity of heat with such a fluid, the mass flow rate must be much higher than with a fluid with a high latent heat, such as ammonia. The higher mass flow rate implies increased velocities and Reynolds numbers and thus increased heat transfer coefficients. These increased coefficients come at the expense of higher pressure drops and thus increased pump work. An extreme example would be water which has very high heat transfer coefficients relative to ammonia because of the unrealistically high velocities arising from its very low vapor density.

Further reducing the practical differences between the fluids are the small temperature differences driving evaporation or condensation. As an example, the average condensing coefficient predicted by Equation (7) for ammonia in the reference case condenser design is 28,000 W/m^2 K; a heat load of 10 kW and a condensing area of 0.77m^2 implies a temperature

difference of 0.46 K. Even halving the heat transfer coefficient would require a temperature difference of less than 1.0 K to transfer the necessary heat. Thus, it seems reasonable to use the reference cold plate and condenser design for all the fluids.

Pumped System

For the reference heat transport system described in the previous section, the fluid mass flow rate, assuming complete evaporation in the cold plate, is:

$$\dot{m} = \frac{Q}{h_{fg}} \tag{10}$$

where Q is the heat load and h_{fg} is the latent heat of vaporization. The required strength of the piping and accumulator will depend on the operating pressure - the vapor pressure of the fluid at the maximum temperature of 80°C. The minimum wall thickness specified by the ASME pressure vessel code (as summarized by Perry [6]) is used:

$$\delta = \frac{PD_o}{2(SE+0.4\ P)} + C \tag{11}$$

where δ is wall thickness, P is pressure, D_o is the outside pipe diameter, E is a weld factor (taken here as 1.0 on the assumption of drawn tubing or fully-inspected welds) and the factor 0.4 is the stress reduction factor appropriate for non-ferrous materials. The corrosion allowance, C, is taken as zero. The allowable stress, S, is given in [6] for a wide variety of materials; it is 0.20 - 0.25 times the tensile strength and is 62,000 kPa (9,000 psi) for 6061-T6 aluminum and 200,000 kPa (29,000 psi)

for stainless steel. The wall thickness is subject to a minimum value of 0.8 mm to provide sufficient rigidity for handling, joining, etc.

The piping diameter has a large influence on system weight. Small diameters decrease the weight of not only the piping itself but also the required fluid charge and thus the weight of the accumulator. Offsetting these benefits are increased pressure drop and pumping power. The optimum diameters are determined by a Fibonacci search technique (described in Appendix B), applied separately to the liquid and vapor lines.

For a given fluid, the necessary fluid properties, fluid mass flow rate, etc. are evaluated at 20°C . The Reynolds number and resulting friction factor are computed for a given guess of liquid line diameter. For laminar flow:

$$f = 16\ Re^{-1} \tag{12}$$

For turbulent flow and hydraulically smooth tubes:

$$f = 0.046\ Re^{-0.2} \tag{13}$$

The theoretical pump work is given by:

$$W = \frac{32\ f\ L\ \dot{m}^3}{\pi^2\ \rho^2\ D_i^5} \tag{14}$$

where L is the pipe length (30m), ρ is the fluid density, and D_i is the inside pipe diameter. The equivalent weight due to pump work is then calculated by applying the factor of 0.25 kg/W.

The weight of the tubing M_t is simply:

$$M_t = \rho_t\ \pi\ \delta\ D_o L \tag{15}$$

where ρ_t is the density of the tube material.

The incremental volume of the accumulator is proportional to the pipe volume:

$$V_{ac} = \gamma\ 0.25\ \pi\ D_i^2 L \tag{16}$$

where γ is the proportionality factor between the volume of the accumulator and the remainder of the system (1.2 for the reference system). The mass of the fluid charge is then:

$$M_f = \rho V_{ac} \tag{17}$$

Assuming a cylindrical shape and ignoring for the moment the contribution of the ends, the weight of the accumulator itself is:

$$M_{ac} = \rho_{ac}\ \delta_{ac}\ \pi\ D_{ac}\ L_{ac} \tag{18}$$

where the wall thickness is given by Equation (2) to yield:

$$M_{ac} = \frac{\rho_{ac}\ P\ \pi\ D_{ac}^2\ L_{ac}}{2(S + 0.4\ P)} \tag{19}$$

But note that $\pi\ D_{ac}^2\ L_{ac}$ is just four times the volume so that:

$$M_{ac} = \frac{2\ \rho_{ac}\ P\ V_{ac}}{S + 0.4P} \tag{20}$$

Thus the weight of the accumulator is independent of the diameter/length ratio. The value given by Equation (20) is multiplied by 1.15 to allow for end fittings.

The above calculations yield values for the equivalent weight associated with the pump work, and piping, fluid and accumulator weights for the liquid line. These are summed and the process is repeated for different diameters until the minimum weight is found. (See Appendix B for a description of the optimization routine). The entire optimization process is then repeated for the vapor line. The diameter is constrained to a maximum of 38mm.

The pressure drop through the condenser (assuming complete phase change) is given by the Friedel model [7]:

$$\Delta P = \frac{0.0437\ L\ \dot{m}^{1.8}\ \mu_\ell^{0.2}}{\rho_\ell\ D^{4.8}} \left[1 + \frac{\rho_\ell}{\rho_g} \left[\frac{\mu_g}{\mu_\ell} \right]^{0.2} \right] \qquad (21)$$

where μ is viscosity and the ℓ and g subscripts refer to the liquid and vapor respectively. For the annular flow passage in the condenser the hydraulic diameter is used. Equation (12) applies to each of the parallel channels so that the total mass flow rate would be divided by eight. The pump work necessary to overcome this pressure gradient is given by:

$$W_p = \frac{\Delta P\ \dot{m}}{\rho} \qquad (22)$$

But since the average fluid density is changing as a function of quality, Equation (22) must be integrated over the quality range one to zero to yield for complete condensation:

$$W_p = \frac{0.1421\ \dot{m}^{2.8} L\ \mu_l^{0.2}}{\rho_l\ D^{4.8}\ (\rho_g - \rho_l)} \left\{ -2 + \ln\left[\frac{\rho_g}{\rho_l}\right] \left[1 + \frac{\rho_l}{\rho_g - \rho_l}\right] \right.$$

$$\left. + \frac{\rho_l}{\rho_g} \left[\frac{\mu_g}{\mu_l}\right]^{0.2} \frac{1}{(\rho_g - \rho_l)^2} \left[\frac{\rho_g^2 - \rho_l^2}{2} - 2\ \rho_l\ (\rho_g - \rho_l) + \rho_l^2\ \ln\left[\frac{\rho_g}{\rho_l}\right]\right]\right\} \tag{23}$$

The evaporator (cold plate) design is for parallel liquid and vapor channels. The pump work is evaluated by summing the individual single phase pressure drops and integrating over the length of the evaporator with vapor quality assumed to vary directly with length:

$$W_p = \int_{Z=0}^{Z=L} \left[\frac{(1-X)\ \dot{m}\ (\delta P/\delta Z)_l}{\rho_l} + \frac{X\ \dot{m}\ (\delta P/\delta Z)_v}{\rho_v}\right] dZ \tag{24}$$

where Z is distance and X is quality, so that $(1-X)\ \dot{m}$ represents the liquid mass flow rate. The pressure gradient, $\delta P/\delta Z$ is:

$$\frac{\delta P}{\delta Z} = \frac{32\ f\ \dot{m}^2}{\pi^2\ p\ D^5} \tag{25}$$

Carrying out the integration in Equation (24) yields:

$$W_p = 0.03739\ L\ \dot{m}^{2\ 8} \left[\frac{\mu_v^{0.2}}{\rho_l^2\ D_l^{4.8}} + \frac{\mu_v^{0.2}}{\rho_v^2\ D_v^{4.8}}\right] \tag{26}$$

where D_l and D_v are the diameters of the liquid and vapor channels, respectively.

The contributions of the pump work, fluid and accumulator weights in

the condenser and evaporator are added to those of the liquid and vapor lines to arrive at a total fluid-dependent system weight. This serves as the primary figure of merit for thermal performance.

Capillary System

For the capillary-pumped system, the circulating pump is replaced by a wick that induces flow through capillary forces. The maximum pressure differential that can be thus generated is:

$$\Delta P = \frac{2\sigma}{r} \qquad (27)$$

where σ is surface tension and r is the effective radius of the wick (5 μm for the reference case). The maximum pressure differential given by Equation (27) is multiplied by 0.9 to account for inefficiencies in the capillary pumping process.

The major difference between the analysis for the pumped and capillary systems is that, for the capillary system, the total ΔP is fixed by the fluid properties and the wick and cannot be arbitrarily varied by the input of pump work. The optimization problem will be to best allocate a fixed ΔP between the liquid and vapor lines. For a given fluid the pressure drops through the condenser and evaporator are evaluated as above. The remaining ΔP is allocated between the liquid and vapor lines and the diameters necessary to accommodate the flow rate at the specified ΔP are calculated. For laminar flow:

$$D = 2.526 \left[\frac{L \dot{m} \mu}{\rho \Delta P}\right]^{0.25} \qquad (28)$$

For turbulent flow:

$$D = 0.6660 \left[\frac{L \dot{m}^{1.8} \mu^{0.2}}{\rho \Delta P} \right]^{0.2083} \tag{29}$$

The system weight is then computed. The allocation of the ΔP is then varied by a Fibonocci search method to find the optimum value. The resulting system weight is then used for ranking each fluid.

FLUID SELECTION AND DISCUSSION

Pumped System

The 52 fluids which passed the preliminary screening were evaluated in terms of incremental system weight; the results are presented in Table 4. At this point one must consider the characteristics of chemical stability, toxicity, flammability, etc. to arrive at the 'best' fluid(s). If the thermally-top-ranked fluid (ammonia in this case) were also nontoxic and nonflammable there would be an unequivocable best choice, but unfortunately this is not the case.

The toxicity and flammability of the 52 fluids are classified in terms of the Threshold Limit Value (TLV) and lower explosive limit (LEL) and listed along with the maximum operating pressure in order of thermal ranking (incremental system weight) in Table 4. The Threshhold Limit Value is a measure of chronic toxicity; it is the concentration in air to which a worker may be exposed for 8 hours a day on a long-term basis. A higher value of TLV thus represents a less toxic compound; a value of 1000 ppm (parts per million) is generally the maximum value and is assigned only to compounds of very low toxicity. For some compounds, the status of toxicity testing is sufficient merely to classify as "toxic" rather than quantify with a numerical TLV. The indication of "simple asphyxiant" (S.A.) in Table 4 refers to a compound of such low toxicity that the major hazard to health would be asphyxiation through the displacement of oxygen. Flammability is quantified in terms of lower explosive limit; LEL is the concentration in air which will just ignite and sustain burning. A low value of LEL thus represents a more flammable compound. Sources for toxicity data include [8, 9, 10]; flammability data were taken from [9] as well as directly from

the PPDS data base.

Starting at the top of Table 4, ammonia has the highest thermal rating (i.e. lowest system weight) and is thus automatically a candidate for consideration. Ammonia is, however, moderately flammable and toxic and operates at high system pressures.

Table 4 Ranking of Fluids for Reference System
Based on Incremental System Weight

PPDS #	Formula	Inc. wt. (kg)	Pressure (kPa)	Flammability (LEL-v%)	Toxicity (TLV-ppm)	Name/comments	Consider Further
70	NH_3	27.5	4141.	15.0	25	ammonia	x
58	C_3H_6	32.5	3719.	2.0	S.A.	similar to propane	
57	C_3H_8	32.9	3136.	2.1	S.A.	propane	x
60	C_3H_4	34.9	2244.	-	1000	propyne- potentially unstable	
66	C_3H_4	35.2	2779.	-	-	similar to propane	
554	CH_3NH_2	35.5	1655.	5.0	10	methylamine	x
143	CH_2O	35.6	2318.	7.0	2		
196	C_2H_2O	36.5	3983.	-	0.5		
111	C_2H_6O	37.6	2224.	3.4	(toxic)		
485	CH_2F_2	43.1	5816.	-	-	R32-probably non toxic	x
355	CH_3Cl	45.2	2156.	10.7	50		
375	COS	45.3	4000.	12.0	(toxic)		
48	C_4H_{10}	46.1	1335.	1.8	1000	iso-butane	x
423	$(CH_3)_2NH$	47.0	1016.	2.8	10		
49	C_4H_8	48.0	1196.	1.7	S.A.	similar to iso-butane	
492	$C_2H_4F_2$	48.1	2328.	3.7	1000	R152a-mod. flammable	x
7	C_4H_6	48.5	1151.	1.4	1000	similar to iso-butane	
9	C_4H_8	49.4	1201.	1.6	S.A.	similar to iso-butane	
11	C_4H_8	52.3	996.	1.7	S.A.	similar to iso-butane	
422	$C_2H_5N_2$	52.9	768.	3.5	10		
8	C_4H_{10}	53.0	1015.	1.9	800	n-butane	
170	C_4H_4	53.8	855.	-	-	similar to iso-butane	
10	C_4H_8	54.0	928.	1.7	S.A.	similar to iso-butane	
369	$CHClF_2$	54.8	3648.	non	1000	R22-non toxic, non flammable	x
216	$(CH_3)_3N$	55.5	941.	2.0	(toxic)		
130	C_2H_3Cl	57.1	1485.	3.8	5		
373	CH_4S	58.2	937.	3.9	0.5		
154	Cl_2	59.1	2737.	non	1		
193	C_2H_4O	59.4	872.	3.7	10		
6	C_4H_6	60.5	802.	-	-		
228	SO_2	63.8	1811.	non	2		
64	C_2H_4O	64.3	608.	4.0	100		
12	C_4H_6	69.1	842.	-	-		
482	CF_3Br	71.0	3965.	non	1000	Halon-1301 fire fighting agent	x
431	CCl_2F_2	72.6	2291.	non	1000	R12-lower pres. than R22	x
490	$C_2H_3ClF_2$	72.8	1441.	6.2	1000		
436	C_2ClF_5	73.3	3150.	non	1000		
177	C_2H_5Cl	75.0	751.	3.8	1000		
313	C_5H_{10}	82.4	566.	1.5	-		
211	C_3H_5Cl	87.9	551.	4.5	(toxic)		
439	$C_2H_2ClF_3$	97.4	947.	-	-		
380	HI	100.0	2668.	-	(toxic)		
434	$CHCl_2F$	105.8	853.	non	10		
486	CH_3Br	107.1	971.	8.6	10		
467	BCl_3	114.7	702.	-	(toxic)		
649	C_2H_3Br	121.2	621.	5.6	1		
487	$C_2Cl_2F_4$	130.4	940.	non	-		
432	$CBrClF_2$	133.1	1128.	non	-		
435	$C_2Cl_2F_2$	133.1	929.	non	1000		
440	CCl_3F	143.7	527.	non	1000	R11-include for comparison	x
483	CBr_2F_2	197.4	545.	non	100		
63	H_2O	675.1	58.	non	non	water	

Notes: S.A. indicates a simple asphyxiant
- indicates no data

A fluid with a lower thermal rating would warrant consideration if it avoided the safety-related shortcomings of ammonia. Moving down the list, the next four fluids are hydrocarbons of low toxicity but which are highly flammable. These different tradeoffs relative to ammonia warrant inclusion in the final list. These four materials are all similar, three-carbon hydrocarbons and thus only one of the four need be considered further; propane is chosen because it is the most stable and readily available material among the four. Methylamine has a good thermal rating, is somewhat less flammable than propane, slightly more toxic than ammonia and, most significantly, operates at lower pressures than ammonia or propane. Continuing down the list, formaldehyde can be eliminated; it is toxic, flammable, and operates at moderately high pressures, i.e. it has no advantages over fluids with higher thermal ratings. Similarly, ketene can be eliminated - it is not only toxic, flammable and operates at high pressures but is also chemically unstable. Applying similar reasoning, difluoromethane (R32), iso-butane and 1,1-difluoroethane (R152a) are included in the final list.

Chlorodifluoromethane (R22) is the first nonflammable fluid; R22 is also of very low toxicity. These attributes come at the expense of high operating pressures and an incremental system weight nearly twice that for ammonia.

Flammable and/or toxic fluids with a thermal rating lower than R22 can be dismissed out of hand. There are several additional fluids, however, that warrant inclusion in the final list. Bromotrifluoromethane (Halon 1301) is a fire-fighting agent. The relatively poor thermal rating for Halon 1301 arises in large part from its very high liquid density;

this penalty might be offset if the heat-transport system could be integrated with the fire-fighting system. Dichlorodifluoromethane (R12) operates at lower pressures than R22. Chlorotrifluoromethane (R11) is ranked very low but since it is the currently used fluid in some systems it is included in the final list for comparison purposes.

Consideration of thermal, toxicity and flammability characteristics have reduced the original list of 860 candidates to a final 10: ammonia, propane, methyamine, R32, iso-butane, R152a, R22, Halon 1301, R12 and R11. They are all stable at normal temperatures. With the exception of R32 all of these materials are readily available at reasonable cost. For the most part, these fluids are in very widespread use with very good property data and a large store of materials compatibility data available. Ammonia and methyamine are the most demanding with regards to materials compatibility, but suitable materials exist even for these.

Variation in System Parameters

The selection process leading to the set of 10 preferred fluids was necessarily carried out for a system with a fixed set of parameters - the reference system described in a previous section. This raises the question of whether the ranking of fluids would be changed for a different set of system parameters. The effects of differing system parameters will be examined by means of a factorial design.

The statistical analysis method known as a factorial design is well suited to the investigation of a number of variables and the interactions among variables. The most common design, the one employed here, adjusts the variables (also called factors) between two levels in a specified

fashion. The results of the analysis are a main effect for each variable and interactions between variables. A main effect is the response of a dependent variable (e.g. incremental system weight) to a change from the low to high level of an independent variable (e.g. design heat load) taken over the average of all other factors. Interactions measure the result of two or more variables simultaneously changing from their low to high level. A thorough discussion of factorial designs may be found in [11].

The effects of changing nine key system parameters will be investigated by a factorial design for each of the 10 preferred fluids. The parameters of design heat load, transport (pipe) length, pump weight ratio, accumulator to system volume ratio, evaporator and condenser volume, minimum liquid and vapor tube wall thickness and maximum tube diameter will be varied from 30% below to 41% above the reference values (to yield a factor of 2.0 difference between the 'low' and 'high' levels for each variable). For the tube and accumulator material, the density and tensile strength for 6061-T6 aluminum will be taken as the low level and the properties for type 304 stainless steel will represent the high level. The final variable is the safety factor (over and above that allowed for in Equation (11)) for the pressure rating of the accumulator and piping; values of 1.0 and 2.0 are assumed for the low and high levels respectively.

The results of the factorial analysis are presented in Table 5. The first column gives the 'average' incremental system weight for each of the 10 fluids; this figure is the system weight evaluated with all of the variables at an average of the high and low values. These values are somewhat higher than the system weights for the reference case since for two of the variables (tube material and safety factor) the reference

system corresponds to the 'low' level rather than an average of the high and low levels.

The main effects presented in Table 5 are expressed as a fraction of the average incremental system weight. For example, the value of 0.251 for the effect of heat load for ammonia means that an increase in the heat load from 7 kW (the 'low' level) to 14 kW (the 'high' level) would increase the system weight 0.251 times the average (or 11.1 kg). One can use these results to examine the impact of different design parameters. (Interactions between variables were also computed but were generally much smaller than the main effects and are not presented here).

The main effects for the 10 fluids are all positive except for the factor of maximum tube diameter. For 9 of the 10 fluids this factor has a main effect that is very small or zero; for these fluids the optimum liquid and vapor line diameters are usually less than the maximum value so that varying this factor has little or no effect. For the low pressure R11, however, the effect is negative; larger diameter vapor lines result in a more efficient system.

Although, for the most part, the signs of the main effects presented in Table 5 are the same, the magnitude of the values vary considerably among the various fluids. For example, the weight for a system using ammonia is much less sensitive to pump efficiency than an R11 system. In general, the magnitude of the effects depends on the fluid vapor pressure. The high pressure fluids (e.g. ammonia and R32) and low pressure fluids (e.g. R11 and iso-butane) tend to have effects which are of opposite magnitudes. This, along with the observation that the high-ranked fluids tended to be those with high vapor pressures, suggests that a system with a different

Table 5 - Results of Factorial Design - Variation of System Parameters

Factors:		heat load (kW)	pipe length (m)	equiv. pump wt. (kg/W)	acc. vol. ratio -	material -	evap. & cond. vol. (L)	min. wall thick. (mm)	safety factor -	max.tube diameter (mm)
Levels:	low	7.07	21.2	0.177	0.85	Al	6.2/1.3	0.56	1.0	26.9
	high	14.14	42.4	0.354	1.70	S.S.	12.4/2.5	1.13	2.0	53.7

Average incremental system weight and main effects on system weight for the 10 preferred fluids:

Fluid	Average(kg)	Main effects (expressed as fraction of average)								
ammonia	44.2	.251	.364	.094	.438	.303	.148	.369	.252	.000
propane	52.96	.420	.468	.156	.352	.199	.160	.352	.195	.000
methyamine	50.96	.388	.483	.148	.370	.184	.172	.308	.107	.010
R32	68.31	.311	.374	.118	.444	.292	.095	.297	.258	.000
iso-butane	68.55	.623	.553	.265	.268	.113	.156	.262	.075	.007
R152a	68.54	.448	.477	.175	.379	.190	.129	.254	.112	.007
R22	78.29	.401	.434	.158	.416	.233	.103	.239	.145	.000
Halon 1301	99.81	.459	.442	.182	.407	.225	.083	.200	.126	.000
R12	98.43	.529	.495	.212	.372	.172	.094	.184	.077	.017
R11	234.77	.944	.602	.405	.230	.065	.077	.053	.003	-.125

set of parameter values might yield a substantially different ranking of fluids.

The parameters that would favor a low pressure fluid are low values of heat load, pipe length and pump weight ratio, and high values of accumulator volume ratio, condenser and evaporator volume, minimum tube wall thickness, maximum tube diameter, and tube safety factor, with stainless steel as the construction material. With this set of system parameters the full set of 52 fluids passing the preliminary screening were evaluated and ranked according to incremental system weight. The results are presented in Table 6; for comparison purposes, this table also summarizes the base case results. The previously highly-ranked (but also high pressure) ammonia and propane fell to about midway down the list. The top three fluids are methyamine, diethylamine and iso-butane, but considering the toxicity of the amines, the substantially less toxic, but only slightly more flammable iso-butane might be the best choice among the three. Applying criteria of toxicity and flammability as in the previous section, one might consider ammonia, R152a and R142b on the basis of reduced flammability compared to iso-butane. Sulfur dioxide is nonflammable but highly toxic. Again, R22 is the highest-ranked fluid which is both nontoxic and nonflammable, although R12 has a nearly identical thermal rating and would be preferred for its lower operating pressures. Perhaps the most surprising result is that for R11. Even though the parameters were selected to favor R11, it remains very near the bottom of the list, although the relative difference between it and the top ranked fluid has decreased. Even with a substantial change in system parameters, the list of preferred fluids is not substantially different. The relative thermal

ranking of some of the fluids within the list may have changed but the unquantifiable tradeoffs among thermal performance and safety considerations remain.

Among the set of 52 fluids, R11 has the lowest vapor pressure (apart from water) and was very near the cut off value for the product of latent heat and the vapor density. To check whether other fluids might perform well in the 'low pressure' system an expanded set of 204 fluids was considered. This set was comprised of those fluids having a latent heat times vapor density greater than 0.1 kJ/L (versus 1.0 kJ/L for the original set of 52 fluids). Twenty-seven fluids were ranked higher than the nontoxic, nonflammable R22; these are summarized in Table 7. all of these fluids are flammable. For the most part, they represent minor variations on fluids seen in the previous set of 52 fluids; for example, pentane and isopropylamine are added to the hydrocarbons and amines already examined. The one completely new compound is tetramethylsilane, $Si(CH_4)_4$. While this exercise does not alter the list of recommended fluids for the system considered in this study, it does point out the need to re-examine the choice of working fluids when system parameters or constraints change significantly.

Table 6 - Comparison of Thermal Rankings for Reference System with Those for System Favoring Low Pressure Fluids

Base Case			Low Pressure Case				
PPDS #	Formula	Inc. Wt. (kg)	PPDS #	Formula	Inc. Wt. (kg)	Name/comments	Consider Further
70	NH_3	27.5	554	CH_3NH_2	55.2	methyamine-toxic	
58	C_3H_6	32.5	423	$(CH_3)_2NH$	57.2		
57	C_3H_8	32.9	48	C_4H_{10}	57.5	iso-butane	x
60	C_3H_4	34.9	49	C_4H_8	58.0		
66	C_3H_4	35.2	7	C_4H_6	58.5		
554	CH_3NH_2	35.5	8	C_4H_{10}	58.5		
143	CH_2O	35.6	11	C_4H_8	58.6		
196	C_2H_2O	36.5	9	C_4H_8	58.7		
111	C_2H_6O	37.6	422	$C_2H_5NH_2$	59.0		
485	CH_2F_2	43.1	10	C_4H_8	59.2		
355	CH_3Cl	45.2	170	C_4H_4	59.8		
375	COS	45.3	60	C_3H_4	59.9		
48	C_4H_{10}	46.1	216	$(CH_3)_3N$	60.2		
423	$(CH_3)_2NH$	47.0	6	C_4H_6	61.9		
49	C_4H_8	48.0	111	C_2H_6O	62.2		
492	$C_2H_4F_2$	48.1	143	CH_2O	62.7		
7	C_4H_6	48.5	57	C_3H_8	63.9	propane	
9	C_4H_8	49.4	66	C_3H_4	64.1		
11	C_4H_6	52.3	64	C_2H_2O	65.3		
422	$C_2H_5N_2$	52.9	373	CH_3SH	66.2		
8	C_4H_{10}	53.0	193	C_2H_4O	66.5		
170	C_4H_4	53.8	12	C_4H_6	67.8		
10	C_4H_8	54.0	70	NH_3	68.0	ammonia-low flam.	x
369	$CHClF_2$	54.8	58	C_3H_6	68.3		
216	$(CH_3)_3N$	55.5	313	C_5H_{10}	69.6		
130	C_2H_3Cl	57.1	355	CH_3Cl	70.2		
370	CH_4S	58.2	130	C_2H_3Cl	70.9		
154	Cl_2	59.1	177	C_2H_5Cl	72.6		
193	C_2H_4O	59.4	492	$C_2H_4F_2$	73.2	R152a	x
6	C_4H_6	60.5	196	C_2H_2O	77.1		
228	SO_2	63.8	211	C_3H_5ClF	79.6		
64	C_2H_4O	64.3	490	$C_2H_3ClF_2$	81.7	R142b	
12	C_4H_6	69.1	228	SO_2	85.2		
482	CF_3Br	71.0	375	COS	86.0		
431	CCl_2F_2	72.6	154	Cl_2	90.9		
490	$C_2H_3ClF_2$	72.8	439	$C_2H_2ClF_3$	90.9		
436	C_2ClF_5	73.3	369	$CHClF_2$	92.7		
177	C_2H_5Cl	75.0	431	CCl_2F_2	92.8	R12 non-toxic, non-flam.	x
313	C_5H_{10}	82.4	434	$CHCl_2F$	96.3		
211	C_3H_5Cl	87.9	485	CH_2F_2	98.5		
439	$C_2H_2ClF_3$	97.4	436	C_2ClF_5	100.1		
380	HI	100.0	467	BCl_3	100.3		
434	$CHCl_2F$	105.8	486	CH_3Br	103.9		
486	CH_3Br	107.1	487	$C_2Cl_2F_4$	108.3		
467	BCl_3	114.7	649	C_2H_3Br	108.8		
649	C_2H_3Br	121.2	435	$C_2Cl_2F_4$	109.3		
487	$C_2Cl_2F_4$	130.4	482	$CBrF_3$	110.9	Halon 1301	x
432	$CBrClF_2$	133.1	432	$CBrClF_2$	118.0		
435	$C_2Cl_2F_4$	133.1	440	CCl_3F	120.4	R11	x
440	CCl_3F	143.7	380	HI	131.8		
483	CBr_2F2	197.4	63	H_2O	164.4		
63	H_2O	675.1	483	CBr_2F	166.2		

Table 7 - Summary of Fluids in Expanded Set With a Higher Thermal Rating Than R22 in 'Low Pressure' System

PPDS #	Formula	Inc. Wt. (kg)	Pressure (kPa)	Flammability (LEL - v%)	Toxicity (TLV-ppm)	Name
Selected fluids from set of 52:						
48	C_4H_{10}	57.5	1335	1.8	1000	iso-butane
57	C_3H_8	63.9	3136	2.1	S.A.	propane
70	NH_3	68.0	4141	15.0	25	ammonia
492	$C_2H_4F_2$	73.2	2328	3.7	1000	R152a
490	$C_2H_3C\ell F_2$	81.7	1441	6.2	1000	R142b
369	$CHC\ell F_2$	92.7	3648	non	1000	R22
431	$CC\ell_2F_2$	92.8	2291	non	1000	R12
Additional fluids considered:						
556	C_3H_9N	70.3	461	2.0	-	isopropylamine
42	C_5H_{12}	71.8	457	1.4	-	isopentane
311	C_5H_{10}	73.1	437	1.4	-	
109	C_5H_8	73.8	380	1.0	(toxic)	
312	C_5H_{10}	75.0	427	1.7	-	
578	$Si(CH_3)_4$	75.9	455	1.6	-	tetramethylsilane
56	C_5H_{12}	76.3	363	1.4	1000	pentane
121	C_5H_{10}	77.2	369	1.4	-	
120	C_5H_{10}	77.8	363	1.4	-	
97	$C_4H_{10}O$	77.9	402	1.9	400	diethylether
167	C_3H_6O	78.0	423	2.8	100	
110	C_5H_{10}	79.7	347	1.4	-	
517	C_4H_8O	80.7	391	1.7	-	
374	C_2H_6S	80.7	393	2.8	0.5	
555	C_3H_9N	81.6	290	2.0	(toxic)	n-propylamine
197	$C_2H_4O_2$	82.3	467	5.0	100	
514	$C_4H_{10}O$	83.1	352	2.0	-	
118	C_5H_8	83.3	305	1.5	-	
570	C_2H_6S	83.4	367	2.2	-	
117	C_5H_8	85.1	288	1.5	-	
17	C_5H_6	85.4	335	-	-	
194	C_4H_4O	85.5	450	2.3	(v. toxic)	
827	C_6H_{12}	86.6	310	-	-	
19	C_5H_8	86.7	292	1.8	(mod. toxic)	
384	$C_3H_7C\ell$	88.2	387	2.8	-	
123	C_3H_6O	88.8	276	2.3	(mod. toxic)	
445	$C_3H_8O_2$	90.7	331	3.1	1000	

Capillary System

A capillary-pumped system is also considered. The design of this system is basically the same as the reference system except that the lower design heat load of 2 kW (versus 10 kW) implies only one cold plate (versus four) and a smaller condenser. The transport length between the cold plate and condenser remains 30 m. The results for the set of 52 fluids is presented in Table 8.

As with the pumped system, ammonia receives the highest thermal rating (i.e. lowest system weight) for the capillary system. But again a fluid avoiding the hazards of ammonia would be desirable.

The choices for the capillary system are more limited - for 12 of the 52 fluids the pressure drop in the condenser and evaporator exceeded that which could be generated by capillary forces. (The allocation of ΔP between the liquid and vapor lines was optimized with 68% to 80% in the vapor line.)

Moving down from the top of the list, methylamine would warrant consideration for its lower operating pressures. Of the next 14 compounds, 9 are both more flammable than ammonia and highly toxic. The remaining five are hydrocarbons which are of low toxicity but, of course, highly flammable. Propane, although ranked lower than the unsaturated C_3H_4, C_3H_6 and C_4H_6 would be favored for its greater stability. Iso-butane is ranked lower than propane but would operate at substantially lower pressures. The fluorinated compounds R32 and R152a combine low toxicity with moderate flammability. Three nonflammable compounds appear feasible in the capillary system; the first two - sulfur dioxide and chlorine - are highly toxic. Only R22 is nonflammable and of low toxicity. R12 might be

considered for its lower operating pressure than R22. It, however, is on the verge of not operating - 88% of the 3.3 kPa pressure rise generated by capillary forces was consumed in the condenser and evaporator, leaving only 0.4 kPa to transport the liquid and vapor between the condenser and cold plate.

Table 8 - Ranking of Fluids for Capillary System

PPDS #	Formula	Inc. wt. (kg)	Pressure (kPa)	Flammability (LEL - v%)	Toxicity (TLV-ppm)	Name
70	NH_3	8.76	4141	15.0	25	ammonia
554	CH_5N	10.23	1655	5.0	10	methylamine
143	CH_2O	11.27	2318	7.0	2	
60	C_3H_4	12.68	2244	-	1000	propyne-unstable
196	C_2H_2O	12.77	3983	-	0.5	
422	C_2H_7N	12.80	768	3.5	10	
423	C_2H_7N	12.89	1016	2.8	10	
66	C_3H_4	13.28	2779	-	0.5	
193	C_2H_4O	13.70	872	3.7	10	
373	CH_4S	13.72	937	3.9	0.5	
111	C_2H_6O	13.82	2224	3.4	(toxic)	
170	C_4H_4	14.42	855	-	-	
64	C_2H_4O	14.75	608	4.0	100	
7	C_4H_6	14.78	1151	1.4	1000	
355	$CH_3C\ell$	15.00	2156	10.7	50	
57	C_3H_8	15.32	3136	2.1	S.A.	propane
58	C_3H_6	15.40	3719	2.0	S.A.	
10	C_4H_8	15.75	928	1.7	S.A.	
49	C_4H_8	15.99	1196	1.7	S.A.	
9	C_4H_6	16.08	1201	1.6	S.A.	
11	C_4H_8	16.13	996	1.7	S.A.	
6	C_4H_6	16.60	802	-	-	
216	C_3HqN	16.99	941	2.0	(toxic)	
48	C_4H_{10}	17.42	1335	1.8	1000	iso-butane
8	C_4H_{10}	17.44	1015	1.9	800	
228	SO_2	18.13	1811	non	2	
130	$C_2H_3C\ell$	18.47	1485	3.8	5	
177	$C_2H_5C\ell$	19.27	751	3.8	1000	
12	C_4H_6	19.59	842	-	-	
492	$C_2H_4F_2$	20.25	2328	3.7	1000	R152a
154	$C\ell_2$	21.00	2737	non	1	
375	COS	21.59	4000	12.0	(toxic)	
485	CH_2F_2	22.17	5816	-	-	R32
369	$CHC\ell F_2$	27.87	3648	non	1000	R22
486	$CH_3H_5C\ell$	30.45	971	8.6	10	
211	$C_3H_4C\ell$	32.98	551	4.5	(toxic)	
490	$C_2H_3C\ell F_2$	34.41	1441	6.2	1000	
434	$CHC\ell_2F$	37.76	853	non	10	
380	HI	40.11	2668	-	(toxic)	
431	$CC\ell_2F_2$	52.25	2291	non	1000	R12

The eight preferred fluids for the capillary system are all among the ten selected for the pumped system; the relative ranking among the eight is also nearly the same between the two systems. This is a most interesting result considering the differences between the systems. Although eight fluids are presented for the capillary system, in practice only the top two or three may really be feasible. R22 has an incremental system weight over 3 times that of ammonia (27.9 vs. 8.8kg) for the capillary system while for the pumped system the ratio is only 2:1 (54.8 vs. 27.5kg). The mechanical simplicity of the capillary system does not come without penalty.

OBSERVATIONS ON THE IDEAL FLUID

Upon examining the fluids which passed the various screening and ranking criteria set forth in this work, a number of general conclusions can be drawn relative to the characteristics of the ideal fluid for two-phase heat transport systems. The first, and most significant, is that all of the preferred fluids are simple, low molecular weight compounds. The most complex is iso-butane with 14 atoms; Halon 1301 with a molecular weight of 149 is the heaviest. Even considering the larger list of 52 fluids which passed the preliminary screening the largest molecule has only 17 atoms and the maximum molecular weight is 171 (for R114).

The major quality associated with a low molecular weight is a high latent heat of vaporization (on a per mass basis). This is reflected in Troutons Rule which is the empirical observation that for nearly all fluids the molar heat of vaporization is proportional to the boiling point temperature. Since only a relatively narrow range of boiling points will permit operation in the two-phase region, it follows that low molecular weights will yield high latent heats on a mass basis. A higher latent heat in turn requires a lower mass flow rate to remove a given quantity of heat. Pump work is further minimized by the general trend of simpler molecules having lower viscosities.

The second major observation is that the higher ranked fluids were those with higher vapor pressures. This applied not only to the group of fluids as a whole but also within classes of fluids; as examples, among the amines ammonia was ranked higher than methyamine and for the hydrocarbons, propane was ranked higher than iso-butane. High vapor pressures imply high vapor densities. This minimizes the pump work associated with moving

the vapor and permits the use of smaller diameter piping, which has further benefits in reducing the required fluid charge. Only with a substantial change to the parameters of the base case system did the high pressure fluids fall in the rankings; but even then, the very low pressure fluids such as R11 remained near the bottom.

These considerations limit the possibilities for the ideal fluid--only a few elements form stable, volatile compounds. In particular, nearly all of the 52 fluids passing the preliminary screening were composed entirely of eight elements: carbon, hydrogen, nitrogen, oxygen, sulfur and the halogens fluorine, chlorine, and bromine. (The only exceptions were the highly reactive and toxic boron trichloride and hydrogen iodide). It is no coincidence that these same elements constitute the vast bulk of the non-metallic materials in industrial use today.

The chemistry among the simple compounds of these eight elements is generally well known. While the data base employed here is not exhaustive it certainly has many representatives of all of the major classes of compounds--hydrocarbons, amines, ethers, alcohols, halocarbons, etc. It is possible that similar promising compounds exist, but it seems unlikely that a completely new class of compounds would be discovered for this application. (As an example, 1,1,1,2-tetrafluoroethane, R134a, has been receiving intense scrutiny as a refrigerant to replace the environmentally harmful R12. Although a new fluid not yet in commercial production, R134a is chemically and thermally similar to the compound it might eventually replace). Only if the rules of the evaluation were to change drastically would substantially different conclusions be reached. For example, if safety concerns (including toxicity, flammability and operation at very

low pressures) were to take total precedence over thermal performance a different set of preferred fluids might emerge.

Only pure fluids were considered in this study; mixtures of fluids may offer some advantages. Fluid mixtures which form azeotropes would behave essentially like a pure fluid. Although the thermal performance of an azeotrope is not likely to be superior to a pure fluid, there are opportunities to manipulate other properties. For example, a mixture of a highly-ranked but flammable fluid such as propane with a nonflammable fluid with a lower thermal ranking might yield an azeotropic mixture with reduced flammability and a moderately good thermal rating. The more general class of nonazeotropic mixtures offer additional possibilities to manipulate propeties. In constrast to pure fluids a nonazeotropic mixture does not boil or condense at a constant temperture but rather over a range of tempertures. While this effect may be a liability if a highly uniform temperature is desired across the entire cold plate, it has also been utilized to better control a two-phase heat transport system [12].

CONCLUSIONS

The effect of different working fluids on the thermal performance (measured in terms of system weight) of a two-phase heat transport system has been considered. This study has examined the externally-mounted payload thermal control system where thermal performance is paramount. Applying a sequence of screening and ranking criteria to a data base of 860 fluids has resulted in the selection of 10 recommended fluids. Among these 10 fluids, tradeoffs exist among thermal performance and safety consideration such as flammability and toxicity as summarized in Table 9.

This study has identified the best fluids within the various categories of safety-related properties (e.g. toxic but flammable versus nontoxic and nonflammable, etc.). The selection between a fluid such as ammonia with excellent thermal characteristics but safety-related shortcomings versus a less hazardous but also thermally-inferior fluid such as R12 represents a question of design philosophy that can only be made by NASA.

An examination of the molecular characteristics of the highly-ranked fluids reveals that all are simple molecules of low molecular weight with moderate to high vapor pressures at the operating temperature. The data base used here covers very well the few classes of chemically-stable compounds that possess these qualities. Thus while minor variations on the compounds identified here may prove to be better, it is unlikely that a completely different class of compounds with better characteristics would exist.

Table 9 - Summary of Tradeoffs Among the Preferred Heat Transport Fluids

Formula	Name	Incremental Weight(kg) pumped (10 kW)	Incremental Weight(kg) capillary (2 kW)	Pressure @ 80°C (kPa)	Flammability	Toxicity
NH_3	ammonia	27.5	8.8	4141.	moderate	high
C_3H_8	propane	32.9	15.3	3136.	high	low
CH_3NH_2	methyamine	35.5	10.2	1655.	mod. high	high
CH_2F_2	R32	43.1	22.2	5816.	moderate	low?
C_4H_{10}	iso-butane	46.1	17.4	1335.	high	low
$C_2H_4F_2$	R152a	48.1	20.3	2328.	moderate	low
$CHClF_2$	R22	54.8	27.9	3648.	non	low
$CBrF_2$	Halon 1301	71.0	xxx	3965.	non	low
CCl_2F_2	R12	72.6	52.3	2291.	non	low
CCl_3F	R11	143.7	xxx	527.	non	low

Notes: xxx indicates not feasible for capillary system.

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APPENDIX A - PPDS DATA BASE

The PPDS data base is a proprietary data base produced by the Physical Property Data Service of the Institution of Chemical Engineers in association with the National Engineering Laboratory (both in the United Kingdom). It is a comprehensive collection of data on 860 pure fluids; it can also calculate mixtures of up to 20 components. The data base contains two types of information: constant (temperature-independent) properties such as critical pressure and dipole moment and temperature-dependent properties such as viscosity and vapor pressure. These properties are listed in Table A-1. Each fluid is referenced by a code number. Table A-2 contains a listing of the available fluids.

NBS has acquired the PPDS data base in the form of an 'Electronic Data Module.' This device is based on a Motorola MC68000 microprocessor and stores the fluid data in 2 MBytes of EPROM memory. It communicates with a host microcomputer over an interface (in this case a Hewlett-Packard series 9000 model 217 communicating over an IEEE-488 parallel interface).

The FORTRAN application program on the host computer accesses the data module by calling an interface subroutine with the desired fluid, property, etc. input to the subroutine in terms of code numbers. The interface routine then interprets this input and transmits a coded character string over the IEEE interface to the data module. The data module receives this transmission, interprets it, and returns the requested data to the host computer as another character string. The interface subroutine receives this return string, interprets it, and finally supplies the requested data to the application (main) program. The first part of the

interface routine, containing a description of inputs and outputs is given in Table A-3; the remaining details of the interface routine are machine-dependent and not relevant to this report.

Table A-1 Fluid Properties Available on the PPDS Data Base

Constant (temperature - independent) properties.

Code Number	Description and units
1	Molecular weight
2	Critical temperature (K)
3	Critical pressure (Pa)
4	Critical volume (ℓ/mol)
5	Melting point (K)
6	Boiling point (K)
7	Parachor (dyne • cm)
8	Vapor heat or formation (kJ/mol)
9	Liquid heat of formation (kJ/mol)
10	Flash point (K)
11	Lower flammability limit (vol %)
12	Upper flammability limit (vol %)
13	Autoignition temperature (K)
14	Solubility parameter (cal/cm^3)
15	Acentric factor
16	Vapor entropy at 298.15 K (J/mol K)
17	Acentric factor of the homomorph
18	Dipole moment (Debye)
19	Compound name and formula

Temperature - dependent properties

Code Number	Description and units
1	Vapor heat capacity (kJ/kg K)
2	Vapor viscosity (cps)
3	Vapor thermal conductivity (W/m K)
4	Vapor enthalpy (kJ/mol)
5	Liquid heat capacity (kJ/kg K)
6	Liquid thermal conductivity (W/mol K)
7	Liquid density (kg/m^3)
8	Liquid coefficient of cubical expansion (K^{-1})
9	Liquid enthalpy (kJ/mol)
10	Enthalpy of vaporization (kJ/mol)
11	Surface tension (N/m)
12	Saturated vapor pressure (Pa)
13	Liquid viscosity (cps)
14	Vapor density (kg/m^3)
15	Total heat of formation (kJ/mol)
16	Vapor entropy (J/mol K)
17	Liquid entropy (J/mol K)
18	Entropy of vaporization (J/mol K)
19	Vapor Gibbs free energy (kJ/mol)
20	Liquid Gibbs free energy (kJ/mol)

Table A-2 Fluids Contained in the PPDS Data Base
(organized by PPDS code number for each of six fluids classes)

HYDROCARBONS

2	C2H2	ACETYLENE
5	C6H6	BENZENE
6	C4H6	1,2-BUTADIENE
7	C4H6	BUTA-1,3-DIENE
8	C4H10	BUTANE
9	C4H8	BUT-1-ENE
10	C4H8	2-BUTENE(CIS)
11	C4H8	2-BUTENE(TRANS)
12	C4H6	1-BUTYNE
14	C6H8	1,3-CYCLOHEXADIENE
15	C6H12	CYCLOHEXANE
16	C6H10	CYCLOHEXENE
17	C5H6	1,3-CYCLOPENTADIENE
18	C5H10	CYCLOPENTANE
19	C5H8	CYCLOPENTENE
20	C10H22	DECANE
24	C8H16	1,1-DIMETHYLCYCLOHEXANE
25	C7H14	1,1-DIMETHYLCYCLOPENTANE
26	C8H18	2,4-DIMETHYLHEXANE
28	C12H26	DODECANE
30	C2H6	ETHANE
31	C8H12	1,5-ETHYLCYCLOHEXADIENE
32	C8H16	ETHYLCYCLOHEXANE
33	C7H14	ETHYLCYLOPENTANE
34	C2H4	ETHYLENE
35	C7H16	HEPTANE
36	C7H14	HEPT-1-ENE
37	C6H14	HEXANE
41	CH4	METHANE
42	C5H12	ISOPENTANE
43	C6H12	METHYLCYCLOPENTANE
44	C7H14	4-METHYL-1-HEXENE
45	C10H22	3-METHYLNONANE
46	C6H14	ISOHEXANE
47	C6H14	3-METHYLPENTANE
48	C4H10	ISOBUTANE
49	C4H8	2-METHYLPROPENE
52	C9H20	NONANE
53	C8H18	OCTANE
56	C5H12	PENTANE
57	C3H8	PROPANE
58	C3H6	PROPENE
60	C3H4	PROPYNE
61	C7H8	TOLUENE
62	C11H24	UNDECANE
66	C3H4	ALLENE
68	C9H10	ALPHA-METHYLSTYRENE
80	C9H12	ISOPROPYLBENZENE(CUMENE)
89	C12H24	DODEC-1-ENE
94	C8H10	ETHYLBENZENE
98	C8H16	2-ETHYL-1-HEXENE
101	C6H10	2,4-HEXADIENE
103	C6H12	HEX-1-ENE
109	C5H8	2-METHYLBUTA-1,3-DIENE (ISOPRENE
110	C5H10	2-METHYL-2-BUTENE
114	C6H12	4-METHYLPENT-1-ENE
115	C6H12	CIS-4-METHYLPENT-2-ENE
116	C6H12	TRANS-4-METHYLPENT-2-ENE
117	C5H8	1,3-PENTADIENE(CIS)
118	C5H8	1,3-PENTADIENE(TRANS)
120	C5H10	2-PENTENE(CIS)
121	C5H10	2-PENTENE(TRANS)
126	C8H8	STYRENE
131	C8H10	M-XYLENE
132	C8H10	O-XYLENE

133	C8H10	P-XYLENE
148	C7H12	2-METHYL-2,4-HEXADIENE
170	C4H4	VINYL ACETYLENE
223	C8H18	2,2,4-TRIMETHYLPENTANE
224	C8H18	2-METHYLHEPTANE
241	C5H12	2,2-DIMETHYLPROPANE
242	C6H14	2,2-DIMETHYLBUTANE
243	C6H14	2,3-DIMETHYLBUTANE
244	C7H16	2,2,3-TRIMETHYLBUTANE
245	C8H18	3-METHYLHEPTANE
246	C8H18	4-METHYLHEPTANE
247	C8H18	3-ETHYLHEXANE
248	C8H18	2,2-DIMETHYLHEXANE
249	C8H18	2,3-DIMETHYLHEXANE
250	C8H18	2,5-DIMETHYLHEXANE
251	C8H18	3,3-DIMETHYLHEXANE
252	C8H18	3,4-DIMETHYLHEXANE
253	C8H18	2-METHYL-3-ETHYLPENTANE
254	C8H18	3-METHYL-3-ETHYLPENTANE
255	C8H18	2,2,3-TRIMETHYLPENTANE
256	C8H18	2,3,3-TRIMETHYLPENTANE
257	C8H18	2,3,4-TRIMETHYLPENTANE
258	C7H16	2-METHYLHEXANE
259	C7H16	3-METHYLHEXANE
260	C7H16	3-ETHYLPENTANE
261	C7H16	2,2-DIMETHYLPENTANE
262	C7H16	2,3-DIMETHYLPENTANE
263	C7H16	2,4-DIMETHYLPENTANE
264	C7H16	3,3-DIMETHYLPENTANE
265	C9H20	2-METHYLOCTANE
266	C9H20	3-METHYLOCTANE
267	C9H20	2,2-DIMETHYLHEPTANE
268	C9H20	2,6-DIMETHYLHEPTANE
269	C9H20	2,2,4-TRIMETHYLHEXANE
270	C9H20	2,2,5-TRIMETHYLHEXANE
271	C9H20	4-METHYLOCTANE
272	C9H20	3-ETHYLHEPTANE
273	C9H20	2,3,3-TRIMETHYLHEXANE
274	C9H20	2,3,5-TRIMETHYLHEXANE
275	C9H20	2,4,4-TRIMETHYLHEXANE
276	C9H20	3,3,4-TRIMETHYLHEXANE
277	C9H20	3,3-DIETHYLPENTANE
278	C9H20	2,2-DIMETHYL-3-ETHYLPENTANE
279	C9H20	2,2,3,3-TETRAMETHYLPENTANE
280	C9H20	2,2,3,4-TETRAMETHYLPENTANE
281	C9H20	2,2,4,4-TETRAMETHYLPENTANE
282	C9H20	2,3,3,4-TETRAMETHYLPENTANE
283	C9H12	PROPYLBENZENE
284	C7H14	1,CIS-2-DIMETHYLCYCLOPENTANE
285	C7H14	1,TRANS-2-DIMETHYLCYCLOPENTANE
286	C7H14	1,CIS-3-DIMETHYLCYCLOPENTANE
287	C7H14	1,TRANS-3-DIMETHYLCYCLOPENTANE
288	C7H14	METHYLCYCLOHEXANE
289	C8H16	CIS-1,2-DIMETHYLCYCLOHEXANE
290	C8H16	TRANS-1,2-DIMETHYLCYCLOHEXANE
291	C8H16	1,CIS-3-DIMETHYLCYCLOHEXANE
292	C8H16	1,TRANS-3-DIMETHYLCYCLOHEXANE
293	C8H16	1,CIS-4-DIMETHYLCYCLOHEXANE
294	C8H16	1,TRANS-4-DIMETHYLCYCLOHEXANE
295	C9H12	1-METHYL-2-ETHYLBENZENE
296	C9H12	1-METHYL-3-ETHYLBENZENE
297	C9H12	1-METHYL-4-ETHYLBENZENE
298	C9H12	1,2,3-TRIMETHYLBENZENE
299	C9H12	1,2,4-TRIMETHYLBENZENE(PSEUDOCUM
300	C9H12	1,3,5-TRIMETHYLBENZENE(MESITYLEN
301	C10H14	BUTYLBENZENE
302	C11H16	PENTYLBENZENE
303	C13H28	TRIDECANE
304	C14H30	TETRADECANE

305	C15H32	N-PENTADECANE
306	C16H34	HEXADECANE
307	C17H36	HEPTADECANE
308	C18H38	OCTADECANE
309	C19H40	N-NONADECANE
310	C20H42	N-EICOSANE
311	C5H10	PENT-1-ENE
312	C5H10	2-METHYLBUT-1-ENE
313	C5H10	3-METHYLBUT-1-ENE
314	C8H18	2,2,3,3-TETRAMETHYLBUTANE
315	C9H20	2,4-DIMETHYL-3-ETHYLPENTANE
316	C8H16	PROPYLCYCLOPENTANE
317	C8H16	ISOPROPYLCYCLOPENTANE
318	C8H16	1-METHYL-1-ETHYLCYCLOPENTANE
319	C8H16	1-METHYL-CIS-2-ETHYLCYCLOPENTAN
320	C8H16	1-METHYL-TR-2-ETHYLCYCLOPENTANE
321	C8H16	1-METHYL-CIS-3-ETHYLCYCLOPENTAN
322	C8H16	1-METHYL-TR-3-ETHYLCYCLOPENTANE
323	C8H16	1,C-2,C-3-TRIMETHYLCYCLOPENTANE
324	C8H16	1,C-2,T-3-TRIMETHYLCYCLOPENTANE
325	C8H16	1,1,2-TRIMETHYLCYCLOPENTANE
326	C8H16	1,1,3-TRIMETHYLCYCLOPENTANE
327	C8H16	1,T-2,C-3-TRIMETHYLCYCLOPENTANE
328	C8H16	1,C-2,C-4-TRIMETHYLCYCLOPENTANE
329	C8H16	1,C-2,T-4-TRIME HYLCYCLOPENTANE
330	C8H16	1,T-2,C-4-TRIMETHYLCYCLOPENTANE
331	C7H14	CYCLOHEPTANE
332	C8H16	CYCLOOCTANE
333	C9H18	CYCLONONANE
334	C10H14	ISOBUTYLBENZENE
335	C10H14	SECBUTYLBENZENE
336	C10H14	TERTBUTYLBENZENE
337	C10H14	1-METHYL-2-ISOPROPYLBENZENE
338	C10H14	1-METHYL-3-ISOPROPYLBENZENE
339	C10H14	1-METHYL-4-ISOPROPYLBENZENE
340	C10H14	1,2,4,5-TETRAMETHYLBENZENE
341	C10H8	NAPHTHALENE
342	C11H10	1-METHYLNAPHTHALENE
343	C11H10	2-METHYLNAPHTHALENE
344	C12H12	1-ETHYLNAPHTHALENE
345	C12H12	2-ETHYLNAPHTHALENE
346	C13H14	1-PROPYLNAPHTHALENE
347	C13H14	2-PROPYLNAPHTHALENE
348	C14H16	1-BUTYLNAPHTHALENE
349	C14H16	2-BUTYLNAPHTHALENE
350	C16H20	1-HEXYLNAPHTHALENE
351	C16H20	2-HEXYLNAPHTHALENE
352	C19H24	1-NONYLNAPHTHALENE
353	C19H26	2-NONYLNAPHTHALENE
354	C9H18	BUTYLCYCLOPENTANE
357	C8H12	VINYLCYCLOHEXENE
367	C12H26	2,2,4,6,6-PENTAMETHYLHEPTANE
376	C10H14	1,4-DIETHYLBENZENE
475	C9H18	1,TRANS-3,5-TRIMETHYLCYCLOHEXANE
476	C8H16	OCT-1-ENE
477	C6H10	HEXA-1,5-DIENE
478	C18H14	O-TERPHENYL
479	C18H14	M-TERPHENYL
480	C18H14	P-TERPHENYL
481	C13H12	DIPHENYLMETHANE
591	C6H12	2,3-DIMETHYLBUT-2-ENE
628	C21H44	N-HENEICOSANE
629	C22H46	N-DOCOSANE
630	C23H48	N-TRICOSANE
631	C24H50	N-TETRACOSANE
632	C6H12	2-METHYLPENT-1-ENE
633	C6H12	3-METHYLPENT-1-ENE
634	C6H12	2-ETHYLBUT-1-ENE
635	C7H14	HEPT-2-ENE

636	C8H16	OCT-2-ENE
637	C9H18	NON-1-ENE
638	C10H20	DEC-1-ENE
639	C11H22	UNDEC-1-ENE
640	C13H26	TRIDEC-1-ENE
641	C14H28	TETRADEC-1-ENE
642	C10H14	1-METHYL-2-PROPYLBENZENE
643	C10H14	1-METHYL-3-PROPYLBENZENE
644	C10H14	1-METHYL-4-PROPYLBENZENE
702	C15H16	4-ISOPROPYLDIPHENYL
704	C10H20	CYCLODECANE
705	C7H12	CYCLOHEPTENE
706	C8H14	CYCLOOCTENE
707	C8H16	METHYLCYCLOHEPTANE
792	C10H18	CIS-DECALIN
793	C10H18	TRANS-DECALIN
794	C12H10	BIPHENYL
795	C14H10	PHENANTHRENE
796	C14H10	ANTHRACENE
797	C9H10	INDANE
814	C10H12	1,2,3,4-TETRAHYDRONAPHTHALENE
815	C16H10	PYRENE
825	C6H12	TRANSHEX-2-ENE
826	C6H12	2,3-DIMETHYLBUT-1-ENE
827	C6H12	3,3-DIMETHYLBUT-1-ENE
828	C10H14	1,3-DIETHYLBENZENE
830	C12H10	ACENAPHTHENE
859	C10H16	ALPHA-PINENE
860	C10H16	BETA-PINENE

HALOCARBONS

22	C3H6CL2	1,2-DICHLOROPROPANE
78	CCL4	CARBON TETRACHLORIDE(10)
83	C2H4CL2	1,2-DICHLOROETHANE
128	C2HCL3	TRICHLOROETHYLENE
130	C2H3CL	VINYL CHLORIDE
153	CHCL3	CHLOROFORM(20)
177	C2H5CL	CHLOROETHANE(160)
178	C2CL4	PERCHLOROETHYLENE
182	C2H2CL2	VINYLIDENE CHLORIDE
183	C2H2CL2	1,2-DICHLOROETHYLENE(CIS)
184	C2H2CL2	1,2-DICHLOROETHYLENE(TRANS)
185	C4H5CL	1-CHLORO-1,3-BUTADIENE
186	C4H5CL	2-CHLORO-1,3-BUTADIENE
187	C4H6CL2	1,4-DICHLOROBUTENE-2(TRANS)
211	C3H5CL	2-CHLOROPROPENE
212	C4H6CL2	3,4-DICHLOROBUTENE-1
220	C2H4CL2	1,1-DICHLOROETHANE(150A)
231	C4H8CL2	2,3-DICHLOROBUTANE
232	C4H8CL2	1,2-DICHLOROBUTANE
233	C4H7CL	3-CHLOROBUTENE-1
234	C4H7CL	1-CHLOROBUTENE-2(CIS)
235	C5H11CL	2-CHLORO-2-METHYLBUTANE
236	C5H10CL2	2,3-DICHLOROPENTANE
237	C5H10CL2	2,3-DICHLORO-2-METHYLBUTANE
238	C5H9CL3	1,2,3-TRICHLORO-2-METHYLBUTANE
239	C5H9CL	3-CHLORO-2-METHYLBUTENE-1
240	C5H9CL	2-CHLORO-3-METHYLBUTENE-2
355	CH3CL	CHLOROMETHANE(40)
366	CH2CL2	DICHLOROMETHANE(30)
368	C2H3CL3	1,1,1-TRICHLOROETHANE(140A)
369	CHCLF2	CHLORODIFLUOROMETHANE(22)
370	C4H4CL2	2,3-DICHLOROBUTADIENE-1,3
371	C4H6CL2	1,3-DICHLOROBUTENE-2(TRANS)
372	C4H5CL3	2,3,4-TRICHLOROBUTENE-1
377	C4H9CL	2-CHLOROBUTANE
379	CH3I	IODOMETHANE
382	C3H5CL	ALLYL CHLORIDE
383	C3H7CL	1-CHLOROPROPANE

384	C3H7CL	2-CHLOROPROPANE
385	C3H5CL3	1-2-3 TRICHLOROPROPANE
387	C2H3CL3	1,1,2-TRICHLOROETHANE
388	C2H2CL4	1-1-1-2-TETRACHLOROETHANE
389	C2H2CL4	1,1,2,2-TETRACHLOROETHANE
390	C2HCL5	PENTACHLOROETHANE(120)
391	C2CL6	HEXACHLOROETHANE
392	C4CL6	HEXACHLOROBUTADIENE
393	C6CL6	HEXACHLOROBENZENE
406	C3H4CL2	1-3-DICHLOROPROPENE
412	C2HBRCLF3	BROMOCHLORO2,2,2-TRIFLUOROETHANE
431	CCL2F2	DICHLORODIFLUOROMETHANE(12)
432	CBRCLF2	BROMOCHLORODIFLUOROMETHANE(12B1)
433	CCLF3	CHLOROTRIFLUOROMETHANE(13)
434	CHCL2F	DICHLOROFLUOROMETHANE(21)
435	C2CL2F4	1,2-DICHLORO-1,1,2,2-TETRAFLUORO
436	C2CLF5	CHLOROPENTAFLUOROETHANE(115)
437	C2F6	HEXAFLUOROETHANE
438	C2HCL2F3	11-DICHLORO-222-TRIFLUOROETHANE
439	C2H2CLF3	1-CHLORO-2,2,2-TRIFLUOROETHANE
440	CCL3F	TRICHLOROFLUOROMETHANE(11)
441	CHF3	FLUOROFORM(23)
442	C2CL4F2	1,1,2,2-TETRACHLORO-1,2-DIFLUORO
443	C2CL3F3	1,2,2-TRICHLORO-1,1,2-TRIFLUORDE
482	CBRF3	BROMOTRIFLUOROMETHANE(13B1)
483	CBR2F2	DIBROMODIFLUOROMETHANE(12B2)
484	CF4	CARBON TETRAFLUORIDE(14)
485	CH2F2	DIFLUOROMETHANE(32)
486	CH3BR	BROMOMETHANE
487	C2CL2F4	1,1-DICHLORO-1,2,2,2-TETRAFLUORO
488	C2BR2F4	1,2-DIBROMOTETRAFLUOROETHANE(114
489	C2BR2CLF3	1,2-DIBROMO-1-CHLORO-1,2,2-TRIFL
490	C2H3CLF2	1-CHLORO-1,1-DIFLUOROETHANE(142B
491	C2H4BR2	1,2-DIBROMOETHANE
492	C2H4F2	1,1-DIFLUOROETHANE(152A)
493	C2H5BR	BROMOETHANE
494	C2H5I	IODOETHANE
495	C5F12	PERFLUOROPENTANE
496	C6F14	PERFLUOROHEXANE
497	C6F14	PERFLUORO-2-METHYLPENTANE
498	C7F16	PERFLUOROHEPTANE
499	C8F18	PERFLUOROOCTANE
500	C9F20	PERFLUORONONANE
501	C10F22	PERFLUORODECANE
502	C4F8	PERFLUOROCYCLOBUTANE(C318)
503	C7F14	PERFLUOROMETHYLCYCLOHEXANE
504	C6F6	PERFLUOROBENZENE
505	C6H4CL2	1,2-DICHLOROBENZENE
506	C6H5BR	BROMOBENZENE
507	C6H5CL	CHLOROBENZENE
508	C6H5F	FLUOROBENZENE
509	C6H5I	IODOBENZENE
510	C10F18	PERFLUORODECALIN
592	CHBR3	BROMOFORM
593	CH2BRCL	BROMOCHLOROMETHANE
594	CH2BR2	DIBROMOMETHANE
595	C3H7BR	1-BROMOPROPANE
596	C3H7BR	2-BROMOPROPANE
597	C3H7I	1-IODOPROPANE
598	C3H7I	2-IODOPROPANE
599	C4H9BR	1-BROMOBUTANE
600	C4H9BR	2-BROMOBUTANE
601	C4H9CL	1-CHLOROBUTANE
602	C4H9I	1-IODOBUTANE
603	C4H9I	2-IODOBUTANE
604	C5H11CL	1-CHLOROPENTANE
605	C6H13BR	1-BROMOHEXANE
606	C7H7CL	BENZYL CHLORIDE
607	C7H7CL	O-CHLOROTOLUENE

608	C7H7CL	M-CHLOROTOLUENE
609	C7H7CL	P-CHLOROTOLUENE
610	C7H7F	P-FLUOROTOLUENE
645	CBRCL3	BROMOTRICHLOROMETHANE
646	C2H4F2	1,2-DIFLUOROETHANE
647	C2H3BR3	1,1,2-TRIBROMOETHANE
648	C2H2BR4	1,1,2,2-TETRABROMOETHANE
649	C2H3BR	VINYL BROMIDE
715	C7H7BR	O-BROMOTOLUENE
716	C7H7BR	M-BROMOTOLUENE
717	C7H7BR	P-BROMOTOLUENE
726	C5H10CL2	1,5-DICHLOROPENTANE
727	C6H13CL	1-CHLOROHEXANE
732	C6H4F2	1,3-DIFLUOROBENZENE
733	C6H4F2	1,4-DIFLUOROBENZENE
734	C7H7F	O-FLUOROTOLUENE
735	C7H7F	M-FLUOROTOLUENE
736	C6H4CL2	1,3-DICHLOROBENZENE
737	C6H4CL2	1,4-DICHLOROBENZENE
738	C6H3CL3	1,2,3-TRICHLOROBENZENE
739	C6H3CL3	1,2,4-TRICHLOROBENZENE
740	C6H3CL3	1,3,5-TRICHLOROBENZENE
741	C10H7CL	1-CHLORONAPHTHALENE
742	C6H4BR2	1,2-DIBROMOBENZENE
743	C6H4BR2	1,4-DIBROMOBENZENE
744	C10H7BR	1-BROMONAPHTHALENE
823	C6HF5	PENTAFLUOROBENZENE
824	C7F8	PERFLUOROTOLUENE
834	C6H4F2	1,2-DIFLUOROBENZENE
835	C6H3F3	1,3,5-TRIFLUOROBENZENE
836	C10H7F	1-FLUORONAPHTHALENE

C + H + O COMPOUNDS

1	C3H6O	ACETONE
23	C28H4604	DIDECYL PHTHALATE
27	C10H10O4	DIMETHYL PHTHALATE
29	C12H2402	LAURIC ACID
39	C3H8O	PROPAN-2-OL
40	C6H14O	DI-ISOPROPYL ETHER
54	C8H18O	OCTAN-1-OL
59	C3H8O	PROPAN-1-OL
64	C2H4O	ACETALDEHYDE
65	C3H4O	ACROLEIN
67	C3H6O	PROP-2-ENE-1-OL
71	C4H8O	METHYL ETHYL KETONE
72	C8H18O	DI-N-BUTYL ETHER
73	C4H8O	BUTYRALDEHYDE
74	C6H12O2	CAPROIC ACID
76	C6H10O2	CAPROLACTONE
79	C4H6O	CROTONALDEHYDE
81	C6H10O	CYCLOHEXANONE
82	C16H2204	DIBUTYL PHTHALATE
84	C6H14O2	1,1-DIETHOXYETHANE
87	C12H14O4	DIETHYL PHTHALATE
88	C24H3804	DI-ISOOCTYL PHTHALATE
90	C4H10O2	ETHYLENE GLYCOL MONOETHYL ETHER
91	C6H12O3	2-ETHOXYETHYL ACETATE
92	C5H8O	3-ETHYL ACROLEIN
93	C2H6O	ETHANOL
96	C2H6O2	ETHYLENE GLYCOL
97	C4H10O	DIETHYL ETHER
99	C6H10O4	ETHYLIDENE DIACETATE
104	C6H14O	HEXAN-1-OL
106	C6H12O2	ISOBUTYL ACETATE
107	C4H8O	ISOBUTYRALDEHYDE
111	C2H6O	METHYL ETHER
112	C5H8O	METHYL ISOPROPENYL KETONE
113	C6H12O	METHYL ISOBUTYL KETONE
119	C5H10O	METHYL N-PROPYL KETONE

122	C6H6O	PHENOL
123	C3H6O	PROPIONALDEHYDE
125	C5H10O2	N-PROPYL ACETATE
134	C2H4O2	ACETIC ACID
135	C3H4O2	ACRYLIC ACID
136	C7H12O2	BUTYL ACRYLATE
137	C4H10O	BUTAN-1-OL
139	C10H22O	DECAN-1-OL
140	C5H8O2	ETHYL ACRYLATE
142	C8H18O	2-ETHYLHEXANOL
143	CH2O	FORMALDEHYDE
144	C7H16O	HEPTAN-1-OL
145	C5H10O2	ISOPROPYL ACETATE
146	CH4O	METHANOL
147	C4H6O2	METHYL ACRYLATE
149	C9H20O	NONAN-1-OL
151	CH2O2	FORMIC ACID
152	C3H6O2	PROPIONIC ACID
158	C4H8O2	ETHYL ACETATE
159	C10H20O2	2-ETHYLHEXYL ACETATE
160	C4H6O2	VINYL ACETATE
162	C3H8O2	PROPYLENE GLYCOL
164	C8H4O3	PHTHALIC ANHYDRIDE
167	C3H6O	PROPYLENE OXIDE(1,2-EPOXYPROPANE
168	C6H12O2	N-BUTYL ACETATE
171	C4H10O	2-METHYLPROPAN-1-OL(ISOBUTANOL)
172	C4H10O	BUTAN-2-OL(SECBUTANOL)
173	C4H10O	2-METHYLPROPAN-2-OL(TERTBUTANOL)
174	C3H6O2	METHYL ACETATE
175	C7H14O3	ETHYL 3-ETHOXY PROPIONATE
176	C5H10O3	METHYL 3-METHOXY PROPIONATE
188	C6H14O2	HEXYLENE GLYCOL
189	C6H14O	4-METHYL-2-PENTANOL
190	C5H12O	PENTAN-2-OL
191	C4H6O3	ACETIC ANHYDRIDE
192	C4H2O3	MALEIC ANHYDRIDE
193	C2H4O	ETHYLENE OXIDE(EPOXYETHANE)
194	C4H4O	FURAN
195	C9H12O2	CUMENE HYDROPEROXIDE
196	C2H2O	KETENE
197	C2H4O2	METHYL FORMATE
198	C3H6O2	ETHYL FORMATE
199	C5H10O2	ETHYL PROPIONATE
200	C4H8O2	N-BUTYRIC ACID
201	C4H8O2	ISOBUTYRIC ACID
203	C8H8O	ACETOPHENONE (METHYL PHENYL KETO
204	C9H14O	ISOPHORONE
205	C6H12O3	PARALDEHYDE(2,4,6-TRIMETHYL-S-TR
206	C5H8O	ETHYLIDENE ACETONE
207	C6H10O	MESITYL OXIDE
208	C5H12O2	DIETHOXYMETHANE
210	C4H6O	METHACROLEIN
213	C6H12O2	DIACETONE ALCOHOL
214	C4H4O2	DIKETENE
215	C5H10O2	TETRAHYDROFURFURYL ALCOHOL
218	C7H14O2	METHOXYHEXANONE
219	C6H10O3	ETHYL ACETOACETATE
221	C6H12O	CYCLOHEXANOL
222	C9H12O	2-PHENYL-2-PROPANOL
225	C15H16O	P-CUMYL PHENOL
227	C4H8O	TETRAHYDROFURAN
229	C3H8O2	ETHYLENE GLYCOL MONOMETHYL ETHER
230	C5H10O3	2-METHOXYETHYL ACETATE
358	C5H8O4	GLUTARIC ACID
359	C5H8O3	LEVULINIC ACID
363	C5H4O2	FURFURAL
364	C6H14O2	ETHYLENE GLYCOL MONO-N-BUTYL ETH
394	C5H12O	PENTAN-1-OL
395	C5H8O2	METHYL METHACRYLATE

397	C5H12O	ETHYL PROPYL ETHER
399	C4H10O3	DIETHYLENE GLYCOL
402	C2H2O2	GLYOXAL
403	C5H8O2	ISOPROPENYL ACETATE
404	C5H8O2	ACETYL ACETONE
408	C7H8O	O-CRESOL
409	C7H8O	M-CRESOL
410	C7H8O	P-CRESOL
416	C6H10O4	ADIPIC ACID
417	C7H6O2	BENZOIC ACID
418	C7H8O	BENZYL ALCOHOL
427	C3H8O3	GLYCERINE
445	C3H8O2	DIMETHOXYMETHANE
511	C5H12O	3-METHYLBUTAN-1-OL
512	C5H12O	2-METHYLBUTAN-2-OL
513	C8H18O	OCTAN-2-OL
514	C4H10O	METHYL PROPYL ETHER
515	C5H12O	METHYL TERTBUTYL ETHER
516	C6H14O	DIPROPYL ETHER
517	C4H8O	ETHYL VINYL ETHER
518	C5H10O	ETHYL ALLYL ETHER
519	C5H10O	DIETHYL KETONE
520	C5H10O	METHYL ISOPROPYL KETONE
521	C6H12O	METHYL N-BUTYL KETONE
522	C6H12O	ETHYL N-PROPYL KETONE
523	C7H14O	METHYL N-PENTYL KETONE
524	C9H18O	DI-N-BUTYL KETONE
525	C5H10O2	N-VALERIC ACID
526	C5H10O2	ISOVALERIC ACID
527	C4H8O2	PROPYL FORMATE
528	C5H10O2	ISOBUTYL FORMATE
529	C6H12O2	N-PENTYL FORMATE
530	C6H12O2	ISOPENTYL FORMATE
531	C7H14O2	ISOPENTYL ACETATE
532	C4H8O2	METHYL PROPIONATE
533	C6H12O2	N-PROPYL PROPIONATE
534	C7H14O2	ISOBUTYL PROPIONATE
535	C5H10O2	METHYL BUTYRATE
536	C5H10O2	METHYL ISOBUTYRATE
537	C6H12O2	ETHYL BUTYRATE
538	C6H12O2	ETHYL ISOBUTYRATE
539	C7H14O2	N-PROPYL BUTYRATE
540	C7H14O2	N-PROPYL ISOBUTYRATE
541	C8H16O2	ISOBUTYL BUTYRATE
542	C6H12O2	METHYL VALERATE
543	C7H14O2	ETHYL VALERATE
544	C10H20O2	ETHYL OCTANOATE (CAPRYLATE)
545	C11H22O2	ETHYL NONANOATE (PELARGONATE)
546	C13H26O2	METHYL LAURATE
547	C8H14O4	DIETHYL SUCCINATE
548	C8H8O3	METHYL SALICYLATE
549	C10H14O	THYMOL (P-CYMEN-3-OL)
550	C10H20O	MENTHOL
551	C7H8O	ANISOLE(METHYL PHENYL ETHER)
552	C8H10O	PHENETOLE(ETHYL PHENYL ETHER)
553	C7H6O	BENZALDEHYDE
567	C5H10O	TETRAHYDROPYRAN
568	C4H8O2	1,4-DIOXAN
611	C6H14O4	TRIETHYLENE GLYCOL
612	C8H16O2	CAPRYLIC ACID
613	C7H14O2	N-PENTYL ACETATE
614	C8H16O2	N-HEXYL ACETATE
615	C9H18O2	N-HEPTYL ACETATE
616	C10H20O2	N-OCTYL ACETATE
617	C12H24O2	N-DECYL ACETATE
618	C7H14O2	N-BUTYL PROPIONATE
619	C8H16O2	N-PENTYL PROPIONATE
620	C9H18O2	N-PENTYL N-BUTYRATE
621	C8H16O2	N-PROPYL-N-VALERATE

622	C9H18O2	ISOBUTYL VALERATE
623	C7H14O2	METHYL-N-CAPROATE
624	C22H44O2	BUTYL STEARATE
626	C5H12O	2-METHYLBUTAN-1-OL
650	C11H24O	UNDECAN-1-OL
651	C12H26O	DODECAN-1-OL
652	C16H34O	HEXADECAN-1-OL
653	C18H38O	OCTADECAN-1-OL
654	C5H10O	VALERALDEHYDE
655	C7H14O	HEPTANAL
656	C8H16O	OCTANAL
657	C6H12O	METHYL SECBUTYL KETONE
658	C6H12O	ETHYL ISOPROPYL KETONE
659	C6H12O	METHYL TERTBUTYL KETONE
660	C7H14O	ETHYL BUTYL KETONE
661	C7H14O	DIPROPYL KETONE
662	C7H14O	PROPYL ISOPROPYL KETONE
663	C7H14O	DI-ISOPROPYL KETONE
664	C8H16O	METHYL N-HEXYL KETONE
665	C9H18O	METHYL N-HEPTYL KETONE
666	C9H18O	DI-ISOBUTYL KETONE
667	C6H10O	ISOMESITYL OXIDE
668	C7H14O2	N-HEPTANOIC ACID
669	C9H18O2	N-NONANOIC ACID
670	C10H20O2	N-DECANOIC ACID
671	C11H22O2	N-UNDECANOIC ACID
672	C13H26O2	N-TRIDECANOIC ACID
673	C14H28O2	MYRISTIC ACID
674	C15H30O2	N-PENTADECANOIC ACID
675	C16H32O2	PALMITIC ACID
676	C17H34O2	MARGARIC ACID
677	C18H36O2	STEARIC ACID
678	C22H44O2	BEHENIC ACID
688	C16H22O4	DI-ISOBUTYL PHTHALATE
689	C24H38O4	DI(2-ETHYLHEXYL) PHTHALATE
690	C8H8O2	METHYL BENZOATE
691	C9H10O2	ETHYL BENZOATE
692	C8H18O2	ETHYLENE GLYCOL MONO-N-HEXYL ETH
693	C4H10O2	ETHYLENE GLYCOL DIMETHYL ETHER
694	C6H14O2	ETHYLENE GLYCOL DIETHYL ETHER
695	C10H22O2	ETHYLENE GLYCOL DI-N-BUTYL ETHER
696	C5H12O3	DIETHYLENE GLYCOL MONOMETHYL ETH
697	C6H14O3	DIETHYLENE GLYCOL MONOETHYL ETHE
698	C8H18O3	DIETHYLENE GLYCOL MONO-N-BUTYL E
699	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER
700	C8H18O3	DIETHYLENE GLYCOL DIETHYL ETHER
701	C12H26O3	DIETHYLENE GLYCOL DI-N-BUTYL ETH
708	C5H10O	CYCLOPENTANOL
709	C7H14O	CYCLOHEPTANOL
710	C8H16O	CYCLOOCTANOL
711	C5H8O	CYCLOPENTANONE
712	C7H12O	CYCLOHEPTANONE
713	C8H14O	CYCLOOCTANONE
718	C6H14O	ETHYL N-BUTYL ETHER
719	C8H18O	DI-ISOBUTYL ETHER
720	C8H18O	DI-TERTBUTYL ETHER
721	C10H22O	DI-N-PENTYL ETHER
722	C10H22O	DI-ISOPENTYL ETHER
730	C3H4O2	VINYL FORMATE
745	C5H10O2	N-BUTYL FORMATE
746	C7H14O2	N-HEXYL FORMATE
747	C8H16O2	N-HEPTYL FORMATE
748	C9H18O2	N-OCTYL FORMATE
749	C9H18O2	N-HEXYL PROPIONATE
750	C10H20O2	N-HEPTYL PROPIONATE
751	C11H22O2	N-OCTYL PROPIONATE
752	C8H16O2	N-BUTYL BUTYRATE
753	C10H20O2	N-HEXYL BUTYRATE
754	C11H22O2	N-HEPTYL BUTYRATE

755	C12H24O2	N-OCTYL BUTYRATE
756	C9H18O2	N-BUTYL VALERATE
757	C10H20O2	N-PENTYL VALERATE
758	C11H22O2	N-HEXYL VALERATE
759	C12H24O2	N-HEPTYL VALERATE
760	C13H26O2	N-OCTYL VALERATE
798	C8H10O	2,5-XYLENOL
799	C8H10O	3,4-XYLENOL
800	C8H10O	3,5-XYLENOL
801	C12H10O	DIPHENYL ETHER
829	C10H20O	DECANAL
837	C6H10O3	PROPIONIC ANHYDRIDE
838	C8H14O3	BUTYRIC ANHYDRIDE
847	C6H10O4	DIETHYL OXALATE
856	C6H6O2	CATECHOL
857	C7H8O2	GUAIACOL
858	C10H8O	1-NAPHTHOL

NITROGEN COMPOUNDS

50	C5H9NO	1-METHYL-2-PYRROLIDONE
51	N2	NITROGEN
69	C6H15N3	AMINO-ETHYL PIPERAZINE
70	NH3	AMMONIA
75	C6H11NO	CAPROLACTAM
85	C4H10N2	DIETHYLENEDIAMINE
86	C4H13N3	DIETHYLENETRIAMINE
95	C2H8N2	ETHYLENE DIAMINE
100	CH3NO	FORMAMIDE
102	C6H16N2	1,6-HEXANEDIAMINE
108	C10H22N2	ISOPHORONEDIAMINE
124	C3H5N	PROPIONITRILE
127	C8H23N3	TETRAETHYLENEPENTAMINE
129	C6H18N4	TRIETHYLENETETRAMINE
138	C12H21NO2	11-CYANOUNDECANOIC ACID
150	C13H21NO2	1,1-PEROXYDICYCLOHEXYLAMINE
156	C4H7NO	ACETONE CYANOHYDRIN
157	C12H25NO2	12-AMINODODECANOIC ACID
161	C4H5NO	ACROLEIN CYANOHYDRIN
165	C5H5N	PYRIDINE
166	C6H7N	4-METHYLPYRIDINE(GAMMA-PICOLINE)
169	C3H5NO	LACTONITRILE
179	HCN	HYDROGEN CYANIDE
180	C2H3N	ACETONITRILE (ETHANENITRILE)
181	C3H3N	ACRYLONITRILE
202	C7H9N	BENZYLAMINE
209	C3H7NO	DIMETHYL FORMAMIDE
216	C3H9N	TRIMETHYLAMINE
217	C6H15N	TRIETHYLAMINE
226	C5H5N	1-CYANOBUTADIENE
356	C4H12N2O	AMINO-ETHYL ETHANOLAMINE
360	C3H3NO	OXAZOLE
361	C4H5N	CROTONITRILE(TRANS)
378	C3H7NO	2-NITROPROPANE
398	C2H7NO	ETHANOLAMINE
411	C4H11N	DIETHYLAMINE
413	NO	NITRIC OXIDE
414	NO2	NITROGEN DIOXIDE
415	C6H7N	ANILINE
419	C10H15N	N,N-DIETHYLANILINE
421	C6H5NO2	NITROBENZENE
422	C2H7N	ETHYLAMINE
423	C2H7N	DIMETHYLAMINE
424	C6H13N	CYCLOHEXYLAMINE
425	C6H8N2	ADIPONITRILE
426	C5H11N	PIPERIDINE
428	C3CL3N3	CYANURIC CHLORIDE
429	C6H8N2	PHENYLHYDRAZINE
430	C9H6N2O2	TOLUENE-2,4-DIISOCYANATE
459	N2H4	HYDRAZINE

461	N2O4	DINITROGEN TETROXIDE
554	CH5N	METHYLAMINE
555	C3H9N	N-PROPYLAMINE
556	C3H9N	ISOPROPYLAMINE
557	C4H11N	N-BUTYLAMINE
558	C6H15N	DI-N-PROPYLAMINE
559	C4H7N	BUTYRONITRILE
560	C6H11N	CAPRONITRILE (HEXANONITRILE)
561	C7H9N	N-METHYLANILINE
562	C8H11N	N,N-DIMETHYLANILINE
563	C8H11N	N-ETHYLANILINE
564	C9H13N	N,N-DIMETHYL-O-TOLUIDINE
565	C7H5N	BENZONITRILE
566	C8H7N	P-TOLUNITRILE
569	C4H9N	PYRROLIDINE
577	CH3NO2	NITROMETHANE
625	C4H11N	ISOBUTYLAMINE
627	C12H27N	TRI-N-BUTYLAMINE
679	C5H13N	N-PENTYLAMINE
680	C6H15N	N-HEXYLAMINE
681	C6H15N	DI-ISOPROPYLAMINE
682	C7H17N	N-HEPTYLAMINE
683	C8H19N	N-OCTYLAMINE
684	C8H19N	DI-N-BUTYLAMINE
685	C8H19N	DI-ISOBUTYLAMINE
686	C9H21N	TRIPROPYLAMINE
687	C3H7N	ALLYLAMINE
703	C5H4CLN	2-CHLOROPYRIDINE
714	C5H11N	CYCLOPENTYLAMINE
723	C7H7NO2	2-NITROTOLUENE
724	C7H7NO2	3-NITROTOLUENE
725	C7H7NO2	4-NITROTOLUENE
728	C9H13N	N,N-DIMETHYL-P-TOLUIDINE
731	C4H9NO	MORPHOLINE
761	C10H9N	1-NAPHTHYLAMINE
762	C10H9N	2-NAPHTHYLAMINE
763	C13H13N	N-METHYLDIPHENYLAMINE
764	C14H15N	DIBENZYLAMINE
765	C8H7N	PHENYLACETONITRILE
766	C8H7N	O-TOLUNITRILE
767	C8H7N	M-TOLUNITRILE
768	C12H10N2	AZOBENZENE
769	C7H9NO	O-ANISIDINE
770	C8H11NO	O-PHENETIDINE
771	C8H9NO	ACETANILIDE
772	C8H9NO2	2-NITROETHYLBENZENE
773	C6H4N2O4	1,3-DINITROBENZENE
774	C6H3N3O6	1,3,5-TRINITROBENZENE
775	C6H6CLN	2-CHLOROANILINE
776	C6H6CLN	3-CHLOROANILINE
777	C6H6CLN	4-CHLOROANILINE
802	C7H9N	O-TOLUIDINE
803	C7H9N	M-TOLUIDINE
804	C7H9N	P-TOLUIDINE
805	C4H5N	PYRROLE
806	C6H7N	2-METHYLPYRIDINE(ALPHA--PICOLINE)
807	C6H7N	3-METHYLPYRIDINE(BETA-PICOLINE)
808	C7H9N	2,4-DIMETHYLPYRIDINE(2,4-LUTIDIN
809	C7H9N	2,6-DIMETHYLPYRIDINE(2,6-LUTIDIN
810	C9H7N	QUINOLINE
811	C9H7N	ISOQUINOLINE
816	C10H9N	QUINALDINE (2-METHYLQUINOLINE)
817	C10H9N	LEPIDINE (4-METHYLQUINOLINE)
818	C10H9N	6-METHYLQUINOLINE
819	C10H9N	8-METHYLQUINOLINE
820	C8H11N	2,6-DIMETHYLANILINE
821	C8H11N	4-ETHYLANILINE
822	C12H11N	DIPHENYLAMINE
831	C7H9N	2-ETHYLPYRIDINE

832	C7H9N	4-ETHYLPYRIDINE
833	C8H11N	2,4,6-COLLIDINE
842	C4H11NO2	DIETHANOLAMINE
843	C6H15NO3	TRIETHANOLAMINE
844	C2H5NO2	NITROETHANE
845	C3H7NO2	1-NITROPROPANE
846	C4H9NO2	1-NITROBUTANE
854	C6H5NO3	2-NITROPHENOL
855	C6H5NO3	4-NITROPHENOL

SULFUR COMPOUNDS

163	H2S	HYDROGEN SULPHIDE
228	SO2	SULPHUR DIOXIDE
365	CS2	CARBON DISULPHIDE
373	CH4S	METHANETHIOL
374	C2H6S	ETHYL MERCAPTAN (ETHANETHIOL)
375	COS	CARBONYL SULPHIDE
452	CS	CAESIUM
454	S	SULPHUR
462	SO3	SULPHUR TRIOXIDE
464	SF6	SULPHUR HEXAFLUORIDE
470	SNCL4	STANNIC CHLORIDE
570	C2H6S	DIMETHYLSULPHIDE
571	C3H8S	ETHYLMETHYLSULPHIDE
572	C4H10S	DIETHYLSULPHIDE
573	C10H22S	DI-ISOPENTYLSULPHIDE
574	C4H10S2	DIETHYLDISULPHIDE
575	C4H10O3S	DIETHYL SULPHITE
778	C3H8S	PROPANE-1-THIOL
779	C3H8S	PROPANE-2-THIOL
780	C4H10S	BUTANE-1-THIOL
781	C4H10S	2-METHYLPROPANE-1-THIOL
782	C4H10S	2-METHYLPROPANE-2-THIOL
783	C5H12S	PENTANE-1-THIOL
784	C5H12S	PENTANE-2-THIOL
785	C5H12S	2-METHYLBUTANE-2-THIOL
786	C6H14S	HEXANE-1-THIOL
787	C6H14S	HEXANE-2-THIOL
788	C7H16S	HEPTANE-1-THIOL
789	C8H18S	OCTANE-1-THIOL
790	C2H6OS	DIMETHYLSULPHOXIDE
791	C4H8O2S	SULPHOLANE
812	C4H4S	THIOPHENE
813	C4H8S	TETRAHYDROTHIOPHENE
848	C6H6S	BENZENETHIOL
849	C5H6S	2-METHYLTHIOPHENE
850	C5H6S	3-METHYLTHIOPHENE

MISCELLANEOUS COMPOUNDS

3		AIR
4		ALPHANOL
13	CO	CARBON MONOXIDE
21	C6H12OCL2	DICHLORO-DIISOPROPYL ETHER
38	H2	HYDROGEN (NORMAL)
55	O2	OXYGEN
63	H2O	WATER
77	CO2	CARBON DIOXIDE
105	H2O2	HYDROGEN PEROXIDE
141	T0H20O2	2-ETHYLHEXYL ACRYLATE
154	CL2	CHLORINE
155	HCL	HYDROGEN CHLORIDE
362	AR	ARGON
380	HI	HYDROGEN IODIDE
381	C2HOCL3	CHLORAL
386	C3H5OCL	EPICHLOROHYDRIN
396	HF	HYDROGEN FLUORIDE
400	KR	KRYPTON
401	XE	XENON
405	C3H6OCL2	2-3-DICHLOROPROPANOL

407	C6H12OCL2	DI-(3-CHLOROPROPYL)ETHER
420	C7H5OCL	BENZOYL CHLORIDE
444	COCL2	PHOSGENE
446	H2	HYDROGEN (PARA)
447	HD	HYDROGEN DEUTERIDE
448	D2	DEUTERIUM (NORMAL)
449	4HE	HELIUM-4
450	NE	NEON
451	RB	RUBIDIUM
453	O3	OZONE
455	F2	FLUORINE
456	BR2	BROMINE
457	I2	IODINE
458	HG	MERCURY
460	D2O	HEAVY WATER
463	OF2	OXYGEN FLUORIDE
465	NBF5	NIOBIUM PENTAFLUORIDE
466	UF6	URANIUM HEXAFLUORIDE
467	BCL3	BORON TRICHLORIDE
468	ALCL3	ALUMINIUM TRICHLORIDE
469	SICL4	SILICON TETRACHLORIDE
471	TICL4	TITANIUM TETRACHLORIDE
472	HBR	HYDROGEN BROMIDE
473	ALBR3	ALUMINIUM TRIBROMIDE
474	CD4	DEUTEROMETHANE
576	C2HF3O2	TRIFLUOROACETIC ACID
578	C4H12SI	TETRAMETHYLSILANE
579	C8H20SI	TETRAETHYLSILANE
580	C6H18OSI2	HEXAMETHYLDISILOXANE
581	C8H24O2SI3	OCTAMETHYLTRISILOXANE
582	C10H30O3SI4	DECAMETHYLTETRASILOXANE
583	C12H36O4SI5	DODECAMETHYLPENTASILOXANE
584	C14H42O5SI6	TETRADECAMETHYLHEXASILOXANE
585	C16H48O6SI7	HEXADECAMETHYLHEPTASILOXANE
586	C18H54O7SI8	OCTADECAMETHYLOCTASILOXANE
587	C8H24O4SI4	OCTAMETHYLCYCLOTETRASILOXANE
588	C10H30O5SI5	DECAMETHYLCYCLOPENTASILOXANE
589	K	POTASSIUM
590	NA	SODIUM
729	C2H3CLO	ACETYL CHLORIDE
839	C6H5CLO	2-CHLOROPHENOL
840	C6H5CLO	3-CHLOROPHENOL
841	C6H5CLO	4-CHLOROPHENOL
851	C3H2CLF5O	ISOFLURANE
852	C3H2CLF5O	ENFLURANE
853	C2H3CLO2	CHLOROACETIC ACID

Table A-3 Interface Routine to Access PPDS Data Module
(partial listing)

```
      SUBROUTINE PPDS (NC,ICODE,XFRAC,ITY,IPROP,T,P,IPH,NE,IE,VP,CP,HP)
C
C   THIS SUBROUTINE ACCESSES THE PPDS DATA BASE AS CONTAINED IN THE
C   ELECTRONIC DATA MODULE.
C
C   INPUTS:
C      NC - NUMBER OF COMPONENTS IN THE STREAM (NC = 1—20)
C      ICODE - ARRAY OF INTEGERS SPECIFYING THE PPDS CODE NUMBER
C         FOR EACH PURE COMPONENT IN THE STREAM
C      XFRAC - COMPOSITION (MOLE FRACTION) OF THE STREAM; REAL
C         ARRAY OF DIMENSION 20
C      ITY - CODE FOR TYPE OF PROPERTY REQUESTED:
C         ITY = -1 — TEMPERATURE DEPENDENT PROPERTY WITH PHASE UNKNOWN
C         ITY = 0 — CONSTANT (TEMPERATURE-INDEPENDENT PROPERTY)
C         ITY = 1 — TEMPERATURE-DEPENDENT PROPERTY WITH PHASE SPECIFIED
C         ITY = 2 — TEMPERATURE-DEPENDENT PROPERTY ALONG SATURATION LINE
C      IPROP - CODE FOR SPECIFIC PROPERTY (SEE TABLE A1 OR PPDS MANUAL)
C         FOR EXAMPLE: IPROP = 1 — MOLECULAR WEIGHT IF ITY = 0
C                                  VAPOR HEAT CAPACITY IF ITY = 1 OR 2
C      T - TEMPERATURE (K) (IGNORED FOR ITY = 0)
C      P - PRESSURE (PA) (IGNORED FOR ITY = 0 OR 2)
C
C   OUTPUTS:
C      IPH - PHASE INDICATOR
C         IPH = 1 — LIQUID PHASE
C         IPH = 2 — VAPOR PHASE
C         IPH = 3 — PROPERTY INDEPENDENT OF PHASE
C      NE - NUMBER OF ERRORS
C      IE - CHARACTER VARIABLE ARRAY (CHARACTER*1 IE(20)) RETURNING CODE
C         FOR EACH OF THE NE ERRORS
C      VP - VALUE OF THE REQUESTED VARIABLE PROPERTY FOR THE MIXTURE
C      CP - ARRAY OF THE REQUESTED CONSTANT PROPERTY (ONE ARRAY ELEMENT
C         FOR EACH COMPONENT OF THE MIXTURE)
C      HP - ARRAY OF CHARACTER VARIABLES RETURNING THE NAME AND FORMULA
C         FOR EACH COMPONENT OF THE MIXTURE (CHARACTER*44 HP(20))
```

APPENDIX B - OPTIMIZATION TECHNIQUE

For the determination of the optimum pipe diameter for the pumped system and the optimum allocation of pressure drop for the capillary system, a Fibonnaci search technique is used. This technique is only applicable for a function, f, having a single extremum within the known interval, $[X_0, X_1]$. The function f is evaluated at two values of X - X_{38} and X_{62} - where $X_0 < X_{38} < X_{62} < X_1$. If $f(X_{38})$ is greater than $f(X_{62})$ then the maximum in f must lie in the interval $X_0 < X < X_{62}$. If, on the other hand, $f(X_{38})$ is less than $f(X_{62})$ the maximum must lie within $X_{38} < X < X_1$. The size of the interval containing the solution is thus reduced, with X_{38} becoming the new X_0 or X_{62} becoming the new X_1.

The power of the Fibonnaci technique lies in the selection of the values of X at which to evaluate f(X); these points lie at approximately 38% and 62% of the distance between X_0 and X_1:

$$X_{38} = X_0 + (1 - G)(X_1 - X_0) \qquad [B-1]$$

$$X_{62} = X_0 + G\,(X_1 - X_0) \qquad [B-2]$$

The constant G is the so-called golden ratio and is equal to 0.61803. (This optimization technique is also known as the golden search method.) This constant has the property:

$$G^2 = (1 - G) \qquad [B-3]$$

This means that when the original interval $[X_0, X_1]$ is reduced to $[X_0, X_{62}]$ the old X_{38} becomes the new X_{62} and thus $f(X_{62})$ does not need to be recalculated. Likewise, when the original interval is reduced to $[X_{38}, X_1]$ the old X_{62} is equal to the new X_{38} as defined by Eqn. B-2. This ability to 'reuse' previous function evaluations speeds convengence and allows the Fibonnaci search to locate the extremum within an interval

of size $(X_1 - X_0)G^{N-1}$ where $(X_1 - X_0)$ is the original interval containing the extremum and N is the number of function evaluations.

The Fibonnaci search is implemented as a subroutine, called GOLD, which returns the location and value of the extremum (either a minimum or maximum) given a starting interval and an external function GEVAL which returns a value of f(X) for a given guess of X. As an example, for the optimization of pipe diameter, GEVAL would return the system weight for a given value of pipe diameter. The use of subroutine GOLD is described in comment statements in the program listing, given as Table B-1.

Table B-1 Subroutine to Implement Fibonnaci Search Optimization Technique

```
      SUBROUTINE GOLD (X0I,X1I,NC,LMAX,GEVAL,XOPT,YOPT)
C
C   SUBROUTINE WHICH CARRIES OUT A FIBONNACI (GOLDEN) SEARCH
C   TECHNIQUE TO LOCATE AN EXTREMUM (MAXIMUM OR MINIMUM) IN A
C   FUNCTION WITHIN A SPECIFIED INTERVAL.
C
C   INPUTS:
C      X0I - LOWER BOUND OF INTERVAL CONTAINING EXTREMUM
C      X1I - UPPER BOUND OF INTERVAL CONTAINING EXTREMUM
C      NC - NUMBER OF FUNCTION EVALUATIONS; THE EXTREMUM IS
C        LOCATED WITHIN AN INTERVAL OF (X1I-X0I)*(0.618)**NCC
C      LMAX - LOGICAL FLAG; IF LMAX:
C        .TRUE. - LOCATE MAXIMUM VALUE
C        .FALSE. - LOCATE MINIMUM VALUE
C
C   EXTERNAL FUNCTION:
C      GEVAL - RETURNS VALUE OF FUNCTION TO BE OPTIMIZED GIVEN
C        VALUE OF INDEPENDENT VARIABLE X
C
C   OUTPUTS:
C      XOPT - LOCATION OF EXTREMUM
C      YOPT - VALUE OF FUNCTION AT EXTREMUM
C
      EXTERNAL GEVAL
      LOGICAL LMAX
      DATA GR/0.61803398875/
      X0=X0I
      X1=X1I
      IF (LMAX) THEN
        XMAX=1.0
      ELSE
        XMAX=-1.0
      END IF
      X62=X0+GR*(X1-X0)
      Y62=XMAX*GEVAL(X62)
      DO 200 IG=1,NC
      X38=X0+(1.0-GR)*(X1-X0)
      Y38=XMAX*GEVAL(X38)
      IF (Y62.LT.Y38) THEN
        X1=X62
        X62=X38
        Y62=Y38
      ELSE
        X0=X1
        X1=X38
      END IF
  200 CONTINUE
      XOPT=0.5*(X0+X1)
      YOPT=XMAX*MAX(Y38,Y62)
      RETURN
      END
```

APPENDIX C - SELECTED REFERENCES FOR FLUID PROPERTIES

Listed below are references for the thermodynamic and transport properties of the ten 'preferred' fluids identified in this study. Most of the references selected include comprehensive evaluations of experimental data from many laboratories and include convenient tabulations and/or mathematical fits to the data.

General references:

ASHRAE Handbook of fundamentals, American Society of Heating, Refrigerating and Air Conditioning Engineers, Atlanta, GA, 1985. (This is a convenient reference to all of the preferred fluids except methylamine and R32. The thermodynamic formulations have been recently updated and are generally good; the transport properties, however, are out of date and in some cases seriously in error. A project to update the transport properties should be complete by 1990.)

ASHRAE Thermodynamic Properties of Refrigerants, American Society of Heating, Refrigerating and Air Conditioning Engineers, Atlanta, GA, 1988. (Contains more extensive tabulations of formulations in the ASHRAE Handbook of Fundamentals.)

Encyclopedia des Gaz (Gas Encyclopedia, English translation by N. Marshall) Elsevier, Amsterdam, the Netherlands, 1976. (A good source of materials compatibility data on all ten preferred fluids; thermodynamic and transport data are not always up to date.)

W. Braker and A.L. Mossman, Matheson Gas Data Book, Matheson, Division of Searle Medical Products USA, Inc., Lyndhurst, NJ, 1980. (A good source of materials compatibility data and safe handling recommendations; also contains information on availability of ultra-pure materials.)

T.E. Daubert and R.P. Danner 'Data Compilation - Tables of Properties of Pure Compounds,' Design Institute for Physical Property Data (DIPPR), American Institute of Chemical Engineers, New York, NY, 1985. (Gives convenient empirical fits to saturation properties for several hundred compounds.)

References for specific fluids:

ammonia (thermodynamic properties):

L. Haar and J.S. Gallagher, Thermodynamic Properties of Ammonia, J. Phys. Chem. Ref. Data 7 635-792 (1978).

ammonia (transport properties):
Daubert and Danner (see reference above).

propane and iso-butane (thermodynamic and transport):
B.A. Younglove and J.F. Ely 'Thermophysical Properties of Fluids, II. Methane, Ethane, Propane, Isobutane and Normal Butane,' J. Phys. Chem. Ref. Data 16 577-798 (1987).

methylamine (thermodynamic and transport):
Daubert and Danner (see reference above).

R32 (thermodynamic):
P.F. Malbrunot, P.A. Meunier, G.M. Scatena, W.H. Mears, K.P. Murphy and J.V. Sinka 'Pressure-Volume-Temperature Behavior of Difluoromethane,' Journal of Chemical and Engineering Data 13 16-21 (1968).

R32 (transport):
T.W. Phillips and K.P. Murphy, 'Liquid Viscosity of Halocarbons,' Journal of Chemical and Engineering Data 15 304-307 (1970).

W. Tauscher, 'Measurement of the Thermal Conductivity of Liquid Refrigerant by an Unsteady-State Hot Wire Method,' ASHRAE Journal, 11(1) 97-104 (1969).

R152a (thermodynamic):
ASHRAE Handbook of Fundamentals (see reference above).

R152a (transport):
'Thermophysical Properties of Refrigerants,' 2nd ed. American Society of Heating, Refrigerating and Air Conditioning Engineers, Atlanta, GA, 1976. (As noted above, the current edition of this reference is not always the most reliable but it will be updated by 1990.)

R22 (thermodynamic and transport):
'Therma' Properties of Refrigerant - R22, Chlorodifluoromethane Japanese Association of Refrigeration, 1975. (The thermodynamic, but not transport, formulations in this work have been adopted by ASHRAE.)

Halon 1301 (thermodynamic and transport):
ASHRAE Handbook of Fundamentals (see reference above).

R12 (thermodynamic and transport):
'Thermophysical Properties of Refrigerants - R12, Dichlorodifluoromethanes, Japanese Association of Refrigeration, 1981. (The thermodynamic, but not transport, formulations in this work have been adopted by ASHRAE.)

R11 (thermodynamic):
ASHRAE Thermodynamic Properties of Refrigerants (see reference above).

R11 (thermodynamic and transport):
V.V. Altunin, V.Z. Geller, E.A. Kremenevskaya, I.I. Perelshtein and E.K. Petrov, 'Thermophysical Properties of Freons, Methane Series, Part 2,' Hemisphere Publishing Corporation, Washington, DC, 1987. (translation of 'Teplofizicheskiye Svoystva Freonov, Vol. 2' Monograph Series of the National Standard Reference Data Service of the USSR, 1985).
Note: heat transfer coefficients are relative to the values for ammonia.

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☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

The working fluid for externally-mounted space-based two-phase heat transport systems is considered. A sequence of screening criteria involving freezing and critical point temperatures and latent heat of vaporization and vapor density are applied to a data base of 860 fluids. The thermal performance of the 52 fluids which pass this preliminary screening are then ranked according to their impact on the weight of a reference system. Upon considering other non-thermal criteria (flammability, toxicity and chemical stability) a final set of 10 preferred fluids is obtained. The effects of variations in system parameters is investigated for these 10 fluids by means of a factorial design.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

cold plate, fluid properties, heat transport, refrigerants, working fluids

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