Trifluoromethyl Iodide and its Blends as High-Performance, Environmentally Sound Halon 1301 Replacements

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Abstract

This paper describes the selection, properties, and current status of validation of trifluoromethyl iodide (CF_3I) and its blends as attractive candidate Halon 1301 replacements. In an effort sponsored by the U.S. Air Force, five groups of chemicals were investigated fluoroiodocarbons (FICs), geminal hydrodibromides (GHDBs), fluoroethers, hydrofluorocarbons (HFCs), and perfluorocarbons. Neat CF_3I and selected blends of CF_3I with HFCs 125, 134a, and 227ea were identified as outstanding candidate Halon 1301 replacements. These agents appear to meet all the desired criteria, including cleanliness, high firefighting effectiveness, very low toxicity and environmental impact, and acceptable stability and compatibility with engineering materials. The reasoning behind the selection of CF_3I and its blends with selected HFCs, known information on these chemicals, and computer modeling of properties of blends are discussed. Information is given on physical properties, firefighting effectiveness, toxicities of the agents and combustion products, environmental properties (including ozone-depletion potential, global warming potential, and possible reactivity as volatile organic compounds), stability on storage, cost, and availability. The likely concentrations of optimal blends are presented. Properties predicted for attractive blends are discussed. Predicted optimal agents and their weighted rankings are given, with recommendations for the remaining validation work required.

Introduction

Last year at the Halon Alternatives Technical Working conference a poster paper was presented entitled "The Ultimate Halon Replacements are in Sight" (Ref. 1). This paper uniquely described the class of chemicals most likely to provide outstanding long-term halon replacements for both flooding and streaming agents. This group consists of fluoroiodocarbons (FICs), chemicals containing fluorine, iodine, and carbon. FICs possess all the desirable properties of high firefighting effectiveness, negligible environmental impacts, and (in most cases) very low toxicities. The desirable properties of FICs have been described in some detail in publications during the past year (Refs. 2-4)

Observations on Groups of Chemicals Examined

Five groups **of** chemicals were originally investigated as potential long-term halon replacements: fluoroiodocarbons (FICs), geminal hydrodibromides (GHDBs), fluoroethers, hydrofluorocarbons (HFCs), and perfluorocarhons.

FICs are extinguishants that perform similarly to halons, in both laboratory and field tests (Refs. 2-4). Results of thermal stability testing at the New Mexico Engineering

Research Institute (NMERI) indicate that CF_3I is stable at 180°F for at least 60 days. When released into the atmosphere, the C-I bond undergoes rapid photolysis in sunlight, and the atmospheric lifetime of CF_3I has been estimated at 1.15 days (Ref. 5). Because of this short atmospheric lifetime, the fraction surviving to reach the stratosphere will be vanishingly small. For example, if a 60-day average transit time is assumed, the fraction surviving to reach the stratosphere would be $e^{-60/1.15}$ or about 10^{-23}. This calculation does not account for any rapid mixing that may occur between the troposphere and stratosphere by tropical storms. It has been speculated that such mixing could conceivably raise the ODP for surface release to approximately 0.01. The author estimates that the actual ODP for tropospheric release will be somewhere between these values, perhaps somewhere between 1×10^{-5} and 1×10^{-10}. In any case the effects on stratospheric ozone are likely to be negligible and the improvement over the ODPs of current halons will be many orders of magnitude. If FICs are released directly into the stratosphere (from aircraft in flight above the tropopause) the ODP will be much higher, probably comparable to that of Halon 1301. However, the quantities of halons released annually directly into the stratosphere worldwide appear to be very small, on the order of only 1,000 or 2,000 lbs.

Toxicity data on FICs are highly encouraging (Refs. 2-4). Incomplete reports in the older literature indicate low acute toxicities for CF_3I and $CF_3CF_2CF_2I$. Recent results from Armstrong Labs for CF_3I indicate very low acute toxicity and rapid elimination from the body (Ref. 6). The only FIC for which adverse toxicity data has been found is the two-carbon FIC, perfluoroethyl iodide, CF_3CF_2I, which is reported to be a strong cardiac sensitizer (Ref. 4). For this reason perfluoroethyl iodide has not been pursued as a streaming agent, despite attractive physical properties and extinguishment ability.

GHDBs are outstanding extinguishants (considerably superior to halons and FICs) but even the most volatile GHDBs ($CHFBr_2$ and CF_3CHBr_2) are liquids and do not possess attractive physical properties for total flooding agents. In addition, because of the nonzero ODP (estimated by the author at 0.05 to 0.2), restrictions on hydrobromofluorocarbons under the Montreal Protocol, and concerns about toxicity, geminal hydrobromides are considered much less attractive than FICs.

HFCs are the most attractive group of blending agents to mix with FICs for firefighting. They have several advantages over fluoroethers and perfluorocarbons. HFCs have moderate firefighting ability, low toxicity, low cost, good stability, and good physical properties as total flooding agents. They have zero ODP and moderate GWPs. The only environmental factor of concern is the GWP, which might possibly lead to future regulations on releases of HFCs. However, if the HFCs used are the ones with shorter atmospheric lifetimes and as much as possible is trapped and recycled, their use may be acceptable. In examination of HFCs as potential blending agents, HFCs 32 and 143a were eliminated from consideration because of their flammability and scarcity, and perfluoropropane because of its high GWP. This left as the top candidates pure CF_3I and blends of CF_3I with HFCs 134a or 227ea. Blends of CF_3I with HFC-134a or 227ea are predicted to be near-azeotropic or azeotropic. Any of these agents could also include the slightly higher-pressure agent HFC-125, which would assist as a propellant and is an effective extinguishant in it own right. In summary, the HFCs appearing most attractive for blending with CF_3I are HFCs 125, 134a, and 227ea.

Because of their very limited availability, unexceptional extinguishing ability, relatively high GWPs, and, in some cases, thermal instabilities, fluoroethers appear to hold

no advantages over HFCs and were ruled out as attractive components of firefighting agents at this time.

Although perfluorocarbons are very attractive from the standpoints of low toxicity, high firefighting effectiveness, and current availability in bulk at reasonable cost, their high GWPs make them less attractive than HFCs.

Table 1 shows that, on all bases of measurement (gas volume percent, relative weight, and relative volume), CF_3I is a much more effective firefighting agent than any of the HFCs listed. Whereas HFCs in general require two to three times the weight and volume of Halon 1301, trifluoromethyl iodide requires less volume and only about 40% more weight.

Table 1. Relative Weights and Volumes of Total Flooding Agents Compared to Halon 1301.

Agent Name	Formula	MW	Liq. Dens.	Cup burner %	Rel. Wt.	Rel. Vol.
Halon 1301	CF_3Br	148.91	1.50	2.90	1.00	1.00
trifluoromethyl iodide	CF_3I	195.91	2.36	3.00	1.36	0.87
HFC-125	CF_3CHF_2	120.00	1.23	9.40	2.61	3.19
HFC-134a	CF_3CH_2F	102.00	1.20	10.50	2.48	3.10
HFC-227ea	CF_3CHCF_3	170.00	1.42	5.90	2.32	2.45

Property	Value
boiling point at 1 atm pressure	-22.5 °C = -8.5 °F
bond dissociation energy	54 kcal/mole
CAS number	2314-97-8
critical pressure	4.04 MPa
critical temperature	395 K
critical volume	225 cm^3/mole
dipole moment	0.92
electron affinity	150 ± 20 kJ/mol
heat of formation	-141 kcal/mole
heat of vaporization	22 kJ/mol
liquid density	2.36 at -32.5°C
molecular weight	195
refractive index (liquid)	1.379 at -42°C
vapor heat capacity, C_p	70.9 J/mol-K
vapor pressure at 20°C	85 psia

The combustion products of CF_3I are HF, CO_2, and HI. The only qualitative difference between combustion products of halons and FICs is the production of HI instead of HBr (and, for Halon 1211, HCl). Although the data on toxicity of HI are limited, it appears to be comparable in acute toxicity to other acid gases (such as HF, HBr, and HCl). The facts that the human body requires iodine and can use and excrete it effectively indicate that the long-term effects of HI may be less than those of HBr. It is possible that, because of the lower bond strength in CF_3I compared to CF_3Br, the quantities of combustion products under given conditions may be greater from FICs than halons. However, given the limited human exposure and the large quantities of toxic gases produced from fuels without any extinguishing agent, combustion products of FICs are not expected to pose a problem. In addition, the lower C-I bond strength in FICs compared to the C-Br bond strength in halons may mean that a larger percentage breaks down in the fire and a smaller amount of agent may be required. The relative ease of decomposition of FICs in flames may especially aid extinguishment of large, hot fires.

Advantages of Blends

Military specifications require an effective temperature range of -65°F (-54°C) to 165°F (74°C). The low end of range is encountered in airborne aircraft and at ground level at higher latitudes. The boiling point of CF_3I (-22.5°C or -8.5°F) is much higher than that of Halon 1301 (-56°C or -72°F). This higher boiling point means CF_3I is much less volatile than Halon 1301; below -22.5°C CF_3I will be discharged as a liquid and will remain as a liquid. Although a liquid can be dispersed finely, it does not fill quickly around obstacles. If a fast response time is required (*e.g.*, a few milliseconds as in tanks and aircraft *dry* bays) it might not be possible to obtain the necessary inertion speed with a liquid agent. Although it is possible that appropriate engineering (nozzles, pressures) can deliver pure CF_3I effectively at low temperatures, adding a blending agent may increase the vapor pressure and improve performance at low temperatures. The ideal blend would be a low-boiling azeotrope in which the components have synergistic suppressant effects (better than expected extinguishment from the combined effects of the components).

Optimal Blends

It is possible to design blends that are expected to have the same performance per unit volume as (are isovolumic with) Halon 1301. Examples of such blends are shown in Table 3.

Table 3. Blends Isovolumic with Halon 1301

Blending Agent	Mole Fraction CF_3I	Mole Fraction Blending Agent	Rel. Wt.
HFC-125	0.93	0.07	1.44
HFC-134a	0.87	0.13	1.50
HFC-227ea	0.93	0.07	1.42

As shown in Table 3, it appears possible to formulate agents with the same performance per unit liquid volume as Halon 1301, with a gain in agent weight of 40% to 50%. It should be noted that these are not necessarily the most attractive blends possible.

Some additional properties of CF_3I and top candidate blending agents are given in Table **4.**

Table 4. Additional Properties of CF_3I and Top Candidate Blending Agents

Agent	GWP (CFC-11 = 1.0)	Toxicity (2-hr LC_{50}, ppm)	Est. Cost ($/lb in 1995)
CF_3I	0.0027	unknown	30.00
HFC-125	0.58	>700,000	11.00
HFC-134a	0.27	>500,000	7.50
HFC-227ea	0.45	>800,000	12.00

Candidate agents were ranked on the basis of the following criteria (with weightings): extinguishing efficiency (25%), toxicity (25%), materials compatibility (10%), ODP (20%), **GWP** (10%), and cost (10%). Since all candidates considered have zero or extremely close to zero ODP, all were given full scores in this area. All candidates were also given full scores for materials compatibility on the basis of reported information indicating that all are probably compatible with an acceptably wide range of materials. The areas where agents differed were in extinguishing efficiency, toxicity, **GWP,** and cost. Weighted rankings for all factors considered are given in Table 5. In Table 5 for simplicity blends are considered to be equal parts of each component.

Table 5. Weighted Rankings of Candidate Halon 1301 Replacements

		Ext. Eff.	Toxicity	Mat. Comp.	ODP	GWP	Cost	Total
	% Weighting	25	25	10	20	10	10	100
Rank	Candidate							
1	CF_3I/HFC-227ea	24	23	10	20	8	8	**93**
2	CF_3I/HFC-134a/HFC-125	21	25	10	20	7	9	**92**
3	CF_3I/HFC-134a	20	21	10	20	9	10	**90**
4	CF_3I/HFC-227ea/HFC-125	23	24	10	20	6	7	**90**
5	neat CF_3I	25	20	10	20	10	5	**90**
6	CF_3I/HFC-125	22	22	10	20	5	6	**85**

The top blends finally recommended for testing are shown in Table **6.** All of these blends could also contain a small amount of HFC-125 (perhaps 10% to 30% by moles).

Table 6. Top Halon 1301 Replacement Candidates for Phase II Testing

Component1	Component2	Mole Percentages
CF_3I	none	100:0
CF_3I	HFC-134a	50:50 to 80:20
CF_3I	HFC-227ea	20:80 to 80:20

The AZEO Program

ETEC has developed a proprietary computer program, called AZEO, that calculates properties of mixtures and predicts azeotrope formation and composition. Mathematical modeling in this program is based upon the theory of corresponding states using a third order virial equation of state (Refs. 1-3). AZEO uses the well-documented Soave modification of the Redlich-Kwong equation of state, specifically fitted to small halogenated hydrocarbons. The Pitzer-Curl method is used to calculate mixture cross-correlation coefficients. The required inputs for each chemical are the molecular weight, normal boiling point, critical temperature, and critical pressure.

The AZEO program correctly calculates properties of all known azeotropes tested (including R-500 and R-502) within 1% accuracy. AZEO runs on a PC, works for up to five-component mixtures, and allows a choice of units. It identifies probable azeotropes, near-azeotropes, and non-azeotropes. For azeotropes and near-azeotropes, it gives the approximate azeotropic composition. It calculates vapor pressure curves and gives enthalpies of vaporization and specific heats of liquid and vapor as functions of temperature. AZEO provides pressure-volume-temperature data with an accuracy within 1% and enthalpies of vaporization within 2%. AZEO is only a tool for initial screening to identify attractive blends and possible azeotropes; all results obtained from AZEO must be validated by laboratory measurements.

In the most recent version of the AZEO program, the equation of state can be optionally fitted to experimental vapor pressure data. For pure substances this allows highly accurate modeling, and for mixtures it decreases the error below 5%. This greatly improves the accuracy of modeling without the need for binary interaction coefficients as required in Carnahan-Starling-deSantis (CSD) modeling. If binary interaction coefficients are available and CSD modeling is used, the error can be reduced to about 1%.

Calculated properties from AZEO for pure CF_3I and for blends of 60:40 by moles CF_3I:HFC-134a and CF_3I:HFC-227ea are given in Tables 7 through 9.

Table 7. Calculated **Properties** of Pure CF_3I

THERMODYNAMIC DATA FOR FILE NAME PURECF3I

DATE: 05-01-1994 TIME: 16:02:18

Temp.	Press	Volume Vapor	Density Liquid	Enthalpy Liquid	Latent	Vapor	Entropy Liquid	Vapor
		Vg	1./Vf	Hf	Hfg	Hg	Sf	Sg
Degrees	Psia	Ft3/lbm	Lb/cu.ft	BTU/Lb			BTU/Lbm-Deg R	
-40.0	6.544	3.414	148.701	0.000	47.10	47.10	0.0000	0.1114
-30.0	8.526	2.676	147.422	0.416	47.23	47.64	0.0010	0.1111
-20.0	11.013	2.105	146.067	1.332	47.34	48.67	0.0032	0.1108
-10.0	14.087	1.671	144.632	2.325	47.33	49.66	0.0053	0.1104
0.0	17.850	1.339	143.112	3.396	47.21	50.61	0.0076	0.1100
10.0	22.412	1.081	141.507	4.544	46.98	51.52	0.0099	0.1096
20.0	27.892	0.880	139.803	5.770	46.62	52.39	0.0122	0.1091
30.0	34.416	0.722	137.999	7.073	46.15	53.22	0.0146	0.1086
40.0	42.117	0.596	136.091	8.454	45.56	54.02	0.0171	0.1080
50.0	51.132	0.495	134.071	9.912	44.86	54.77	0.0196	0.1074
60.0	61.603	0.413	131.934	11.448	44.04	55.49	0.0222	0.1068
70.0	73.674	0.347	129.629	13.062	43.10	56.17	0.0248	0.1061
80.0	87.490	0.293	127.242	14.752	42.05	56.80	0.0275	0.1054
90.0	103.198	0.248	124.743	16.521	40.88	57.40	0.0302	0.1047
100.0	120.942	0.211	122.055	18.367	39.60	57.96	0.0330	0.1039
110.0	140.866	0.180	119.206	20.290	38.20	58.49	0.0359	0.1031
120.0	163.114	0.154	116.181	22,291	36.68	58.97	0.0388	0.1023
130.0	187.828	0.132	112.963	24.370	35.04	59.41	0.0418	0.1014
140.0	215.152	0.113	109.531	26.526	33.29	59.82	0.0448	0.1005
150.0	245.230	0.097	105.853	28.759	31.42	60.18	0.0479	0.0995
160.0	278.214	0.084	101.878	31.070	29.44	60.51	0.0510	0.0985
170.0	314.260	0.072	97.503	33.459	27.34	60.79	0.0542	0.0975
180.0	353.538	0.062	92.417	35.925	25.12	61.04	0.0575	0.0964

Property =	Constant +	...* Tr +	...* Tr**2 +	...* Tr** 3 +	..* Tr** 4
Psat	-1.11762E+03	55.125E+02	-8.6197E+03	3.2065E+03	1.7630E+03
Vg	5.35592E+02	-26.599E+02	4.9648E+03	-4.1228E+03	1.2840E+03
Ldens	4.61149E+01	40.060E+01	-3.8695E+02	0.0000E+00	0.0000E+00
Hf	3.58612E+01	-17.867E+01	1.9881E+02	0.0000E+00	0.0000E+00
Hfg	-6.73910E+01	36.760E+01	-2.9439E+02	0.0000E+00	0.0000E+00
Hg	-1.45298E+01	11.945E+01	-1.8495E+00	-4.1762E+01	0.0000E+00
Sf	-3.34955E-02	-32.272E-03	1.4844E-01	0.0000E+00	0.0000E+00
Sg	9.08407E-02	89.762E-03	-9.2948E-02	0.0000E+00	0.0000E+00

Tmin = -40 Tmax = 185 Degrees F
USE CAUTION EXTRAPOLATING ABOVE AND BELOW ENDPOINTS

Cpv = .1037254 **Cp/Cv** = **1.172219** **Cpliq** = .1768405 **at** *300* (K)

Tr = T abs(I) / T(crit) **Tc** = **711.7493 (R) or 395.4163 (K)**

Table 8. **Calculated Properties** of a 60:40 **(by** moles) **Blend** of CF_3I and HFC-134a

THERMODYNAMIC DATA FOR FILE NAME **22196040**

DATE: **05-02-1994** **TIME:** 22:03:00

Temp.	Press	Volume Vapor	Density Liquid	Enthalpy Liquid	Enthalpy Latent	Enthalpy Vapor	Entropy Liquid	Entropy Vapor
		Vg	1./Vf	Hf	Hfg	Hg	Sf	Sg
Degrees	Psia	Ft3/lbm	Lb/cu.ft	BTU/Lb			BTU/Lbm-Deg R	
-40.0	6.912	3.998	122.133	0.000	56.84	56.84	0.0000	0.1345
-30.0	8.963	3.145	121.687	0.490	57.02	57.51	0.0012	0.1341
-20.0	11.505	2.493	120.582	1.490	57.26	58.75	0.0035	0.1337
-10.0	14.634	1.992	119.414	2.587	57.36	59.95	0.0060	0.1333
0.0	18.451	1.604	118.178	3.783	57.32	61.11	0.0085	0.1329
10.0	23.066	1.302	116.871	5.076	57.14	62.21	0.0110	0.1324
20.0	28.597	1.064	115.489	6.467	56.81	63.28	0.0137	0.1318
30.0	35.172	0.875	114.027	7.956	56.34	64.30	0.0165	0.1312
40.0	42.924	0.724	112.480	9.543	55.73	65.27	0.0193	0.1306
50.0	51.997	0.602	110.843	11.228	54.98	66.20	0.0222	0.1299
60.0	62.535	0.504	108.937	13.011	54.08	67.09	0.0252	0.1292
70.0	74.691	0.424	107.273	14.891	53.04	67.93	0.0283	0.1284
80.0	88.617	0.358	105.324	16.869	51.86	68.73	0.0314	0.1276
90.0	104.470	0.303	103.133	18.945	50.53	69.48	0.0347	0.1267
100.0	122.409	0.258	100.945	21.119	49.07	70.19	0.0380	0.1258
110.0	142.592	0.220	98.718	23.391	47.46	70.85	0.0414	0.1249
120.0	165.179	0.188	96.222	25.760	45.71	71.47	0.0449	0.1239
130.0	190.332	0.161	93.555	28.228	43.81	72.04	0.0484	0.1229
140.0	218.213	0.139	90.640	30.793	41.78	72.57	0.0521	0.1218
150.0	248.990	0.119	87.576	33.456	39.60	73.06	0.0558	0.1207
160.0	282.833	0.103	84.258	36.217	37.28	73.50	0.0596	0.1195
170.0	319.920	0.088	80.628	39.075	34.82	73.89	0.0635	0.1183

Property = constant + ...* Tr + ...* Tr**2 + ...* Tr** 3 + ..* Tr** 4

Psat	-7.18695E+02	30.371E+02	-3.0516E+03	-2.0749E+03	3.4690E+03
Vg	6.65970E+02	-32.686E+02	6.0349E+03	-4.9612E+03	1.5308E+03
Ldens	5.08014E+01	28.717E+01	-2.7981E+02	0.0000E+00	0.0000E+00
Hf	5.17715E+01	-23.104E+01	2.3979E+02	0.0000E+00	0.0000E+00
Hfg	-8.73097E+01	44.596E+01	-3.4362E+02	0.0000E+00	0.0000E+00
Hg	-1.07300E+01	11.455E+01	3.0355E+01	-5.9297E+01	0.0000E+00
Sf	-1.79342E-02	-95.279E-03	2.0476E-01	0.0000E+00	0.0000E+00
Sg	1.09118E-01	10.557E-02	-1.0539E-01	0.0000E+00	0.0000E+00

Tmin = **-40** **Tmax** = **170** Degrees **F**

USE CAUTION EXTRAPOLATING ABOVE AND BELOW ENDPOINTS

Cpv = **.1254605** Cp/Cv = **1.179785** Cpliq = **.2076032** at **300** (K)

Tr = T abs(I) / T(crit) Tc = **696.024** (R) **or** **386.68** (K)

Table 9. Calculated Properties of a 60:40 (by moles) Blend of CF_3I and HFC-227ea

THERMODYNAMIC DATA FOR FILS NAME 22936040

DATE: 05-02-1994 TIME: 22:07:16

Temp.	Press	Volume Vapor	Density Liquid	Enthalpy Liquid	Latent	Vapor	Entropy Liquid	Vapor
		Vg	1./Vf	Hf	Hfg	Hg	Sf	Sg
Degrees	Psia	Ft3/lbm	Lb/cu.ft	BTU/Lb			BTU/Lbm-Deg R	
-40.0	6.087	3.871	129.146	0.000	51.34	51.34	0.0000	0.1214
-30.0	7.985	3.014	123.383	0.576	51.34	51.91	0.0013	0.1211
-20.0	10.405	2.347	122.182	1.553	51.49	53.04	0.0036	0.1208
-10.0	13.419	1.846	120.901	2.634	51.49	54.12	0.0060	0.1204
0.0	17.134	1.466	119.536	3.817	51.34	55.16	0.0085	0.1199
10.0	21.669	1.175	118.089	5.104	51.04	56.15	0.0111	0.1194
20.0	27.150	0.949	116.538	6.493	50.60	57.09	0.0136	0.1189
30.0	33.714	0.773	114.887	7.986	50.00	57.99	0.0165	0.1183
40.0	41.508	0.633	113.139	9.582	49.26	56.84	0.0194	0.1177
50.0	50.683	0.522	111.267	11.280	46.37	59.65	0.0223	0.1170
60.0	61.397	0.433	109.288	13.082	47.33	60.41	0.0253	0.1163
70.0	73.815	0.361	107.163	14.987	46.14	61.13	0.0285	0.1156
80.0	88.104	0.302	104.915	16.994	44.80	61.80	0.0317	0.1148
90.0	104.436	0.254	102.523	19.105	43.32	62.42	0.0350	0.1139
100.0	122.988	0.214	99.973	21.319	41.68	63.00	0.0384	0.1130
110.0	143.937	0.181	97.246	23.636	39.90	63.53	0.0418	0.1121
120.0	167.468	0.153	94.309	26.056	37.97	64.02	0.0454	0.1111
130.0	193.771	0.129	91.071	28.578	35.89	64.46	0.0491	0.1101
140.0	223.044	0.109	87.565	31.204	33.66	64.86	0.0526	0.1091
150.0	255.497	0.093	83.705	33.933	31.28	65.21	0.0566	0.1080
160.0	291.354	0.078	79.166	36.765	28.75	65.52	0.0606	0.1068
170.0	330.862	0.066	73.149	39.700	26.07	65.77	0.0646	0.1056

Property =	Constant +	...* Tr +	...* Tr**2 +	...* Tr** 3 +	..* Tr** 4
Psat	-3.27640E+02	70.061E+01	2.2604E+03	-7.5292E+03	5.5982E+03
Vg	6.89689E+02	-33.907E+02	6.2645E+03	-5.1489E+03	1.5872E+03
Ldens	1.59034E+01	40.715E+01	-3.7728E+02	0.0000E+00	0.0000E+00
Hf	5.71950E+01	-24.710E+01	2.5181E+02	0.0000E+00	0.0000E+00
Hfg	-9.46044E+01	45.798E+01	-3.5881E+02	0.0000E+00	0.0000E+00
Hg	-1.51102E+01	12.098E+01	1.2752E+01	-5.2703E+01	0.0000E+00
Sf	-9.43388E-03	-12.044E-02	2.2368E-01	0.0000E+00	0.0000E+00
Sg	9.51206E-02	10.772E-02	-1.0626E-01	0.0000E+00	0.0000E+00

Tmin = -40 Tmax = 175 Degrees F

USE CAUTION EXTRAPOLATING ABOVE AND BELOW ENDPOINTS

cpv = .1127048 Cp/Cv = 1.170613 Cpliq = .2110773 at 300 (K)

Tr = T abs(I) / T(crit) Tc = 696.1921 (R) or 386.94 (K)

Streaming Agents

The observation that perfluoropropyl iodide should be an excellent Halon 1211 replacement has been published (Refs. 2 and 3) . Table 10 shows properties of selected streaming agents. Table 10 shows that perfluoro-n-propyl iodide is a much more effective firefighting agent than HCFC-123 or perfluorohexane. While HCFC-123 and perfluorohexane require about two to three times the weight and volume of Halon 1211, perfluoro-n-propyl iodtde is predicted to require only about 80% more weight and 60% more volume. These estimates are of necessity very crude because they cannot take into account deliverability factors or effects of larger, hotter fires. There are several reasons why FICs are expected to be even more effective on larger, hotter fires. The weaker C-I bond will result in a higher fraction decomposing in the flames, and some may undergo photolysis. Heat also makes C-I bonds more susceptible to photolysis.

Table 10. Relative Weights and Volumes of Streaming Agents Compared to Halon 1211.

Agent Name	Formula	MW	Liq. Dens.	Cup burner %	Rel. Wt.	Rel. Vol.
Halon 1211	CF_2ClBr	165.37	1.85	3.2	1.00	1.00
Halon 2402	CF_2BrCF_2Br	259.82	2.16	2.1	1.03	0.88
HCFC-123	$CHCl_2CF_3$	152.93	1.46	6.3	1.81	2.29
perfluorohexane	C_6F_{14}	338.06	1.70	4.4	2.82	3.07
perfluoro-*n*-propyl iodide	$CF_3CF_2CF_2I$	295.93	2.10	3.2	1.79	1.58
dibromofluoromethane	$CHBr_2F$	191.80	2.42	1.8	0.65	0.50

Other Uses of FICs

Although the effort described in this paper was limited to the examination of total-flooding firefighting agents, the potential usefulness of FICs is not limited to this area. As described above, 1-C_3F_7I shows strong potential as a streaming agent. FICs and blends containing FICs also show excellent potential as general CFC replacements in many applications. The author and his co-inventor Lance Lankford have successfully demonstrated several other promising uses of FICs. For example, a mixture of 52% by moles CF_3I and 48% HFC-152a has been shown to be a nonflammc e, high-performance drop-in replacement for CFC-12 in refrigeration without changing t e mineral oil lubricant (Ref. 7). Trifluoromethyl iodide, both alone and in blends, has been successfully demonstrated as a foam blowing agent (Ref. 8). Calculations predict that rigid foams blown with FICs will have insulating abilities 10% to 40% greater than those blown with conventional agents, and will have a payback period of less than one year for refrigerators. Tests by the author using two FICs (perfluoro-*n*-butyl iodide and perfluoro-n-hexyl iodide) as solvents have shown that they are effective cleaners for oils and greases, are miscible with a wide range of common solvents, and can render mixtures with other common solvents nonflammable (Ref. 9).

The Ikon Corporation has been formed to promote testing, development, manufacture, and use of FIC technologies, provide know-how and technical support, license FIC technologies, and make available the benefits of FIC technologies worldwide.

Additional Validation Work Required

Since the first and second interim reports for this effort were submitted in March and June 1993 (Refs. 10 and 11) and a paper and talk were presented on the subject (Ref. 1), several of the recommendations made have already been implemented. Laboratory testing of the thermal stability of CF_3I is underway at both the National Institute of Standards and Technology (NIST) and NMERI. Acute toxicity tests of CF_3I have been completed by the U.S. Air Force at Armstrong Laboratories. Two pilot plants to manufacture CF_3I have come into operation, and the price has already dropped by over 75% (from over $600/lb to less than $150/lb). It is estimated that bulk costs of production of CF_3I will be in the range of **$5** to $10/lb.

It is recommended that cup-burner tests on the top-ranking blends identified in this effort begin immediately. The purpose of these tests will be to determine the optimum concentrations of components in the recommended blends for greatest ease of delivery and firefighting effectiveness at the lowest cost. Each pair or triad of agents should be tested at the range of concentrations specified, with special attention paid to detecting possible synergism. Tests for formation of binary and ternary azeotropes among the top recommended chemicals (CF_3I and HFCs 125, 134a, and 227ea) should also be carried out.

After the optimal blends have been identified through cup-burner and azeotrope testing, cardiotoxicity testing should he carried out on the most attractive blend(s) identified so that approval for use under the EPA SNAP program can be requested.

The concentrations of combustion products of FICs should be measured in a realistic fire scenario using established procedures, to determine possible firefighter exposures.

Additional studies of the tropospheric and stratospheric reactions of FICs should be carried out. These studies should be aimed at quantitative determination of the atmospheric lifetimes, effects of FICs on smog, and the extent of stratospheric ozone depletion that would occur if FICs were released directly into the stratosphere by high-flying aircraft.

It is recommended that $CF_3CF_2CF_2I$ and its blends be tested as streaming firefighting agents (Halon 1211 replacements). Work is underway on this through the efforts of Dr. Charles Kibert and Tyndall AFB. Dr. Kibert is also to be commended for his efforts in forming the "Ad Hoc CF_3I Working Group" to exchange information among researchers.

A comprehensive toxicity testing program, possibly a new Program for Alternative Fluorocarbon Toxicity Testing (PAFT), should be undertaken to investigate the chronic and subchronic toxicities of CF_3I and other FICs.

Because of the great promise of FICs hold as general CFC and halon replacements, it is recommended that acute toxicity testing be started as soon as possible on the other most promising FICs, including $CF_3CF_2CF_2I$, $CF_3(CF_2)_3I$, and $CF_3(CF_2)_5I$. It is recommended that additional testing and validation of FICs and FIC-containing blends as refrigerants, solvents, foam-blowing agents, aerosol propellants, and hydraulic fluids be carried out. This effort will help aid the Air Force, other Department of Defense (DoD) and government agencies, and industrial users and consumers in their efforts to phase out ozone-depleting substances quickly and with minimum disruption of operations.

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