SELECTION OF A SIMULANT OF CF_3Br FOR USE IN ENGINE NACELLE CERTIFICATION TESTS[†]

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ABSTRACT

This paper describes the selection of a simulant of CF_3Br for the purpose of certification testing engine nacelles fire suppression systems. In order to illustrate the storage, delivery, and distribution requirements of CF_3Br, relevant characteristics of engine nacelle fire suppression systems and certification tests are briefly summarized. An initial screening of over 1300 chemicals based upon the boiling point, critical temperature, and molecular weight of CF_3Br is described, and the nine potential candidate simulants that were found are listed. Three final candidates (SF_6, C_2HF_5, and $CHClF_2$) were selected for experimental testing based upon their vapor pressures, Jakob numbers, and the requirements of this application: ozone depletion potential, flammability, corrosiveness, toxicity, stability, and atmospheric lifetime. To evaluate the hydraulic properties of the simulants compared to CF_3Br, pressure traces of discharges through a piping system are compared. A second comparison using high speed movies of the spray plumes at the end of the piping system is described. Results from these comparisons of the three candidate simulants with CF_3Br are presented.

I. INTRODUCTION

The Department of Defense and the Federal Aviation Administration require certification testing of fire protection systems for each aircraft engine design to ensure their effectiveness. Historically all halon 1301 systems have been tested by the discharging of halon 1301 from an installed fire bottle into the engine nacelle. The concentration of the agent is then measured to determine whether the system passes the certification test. Increased awareness of the harmful effect of halon 1301 on the environment has brought this procedure under scrutiny.

The question was asked: can the certification test use a less harmful chemical to predict the performance of a discharge of halon 1301 in an aircraft engine fire protection system? In response, the United States Navy initiated a search for a simulant of halon 1301 that would have an acceptable (preferably zero) ozone depletion potential (ODP) which could be used during the certification process and for development testing. The Building and Fire Research Laboratory of the National Institute of Standards and Technology and Walter Kidde Aerospace were contacted to select and test

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three possible simulants and make a final recommendation to the Navy. This paper describes the requirements of a simulant, the review of thermodynamic properties to identify three candidates, and the experimental testing which lead to the selection of HFC-125 as a simulant of halon 1301 for certification and development testing.

Engine Nacelle Fire Suppression Systems. Though the details of engine nacelle fire suppression systems vary from aircraft to aircraft their fundamental configuration is basically the same. The agent is stored in a spherical or cylindrical pressure vessel with a volume as small as 0.7 liters (42 in^3) or as large as **15.5** liters (945 in^3). The N_2 pressurization is in the range of 2.5 MPa to 6.4 MPa **(375** - 925 psig). The ***percent liquid fill*** describes how much CF_3Br is present in liquid phase at room temperature divided by the total volume of the bottle, and is usually between 40 % and 75 %. When a bottle on board an aircraft is only 40 % filled with liquid there is a sizable weight and space penalty. In contrast when the bottle is filled to 75 %, less N_2 is available to propel the agent from the bottle and into the nacelle. In practice designers refer to the ***fill density***[1] of a fire bottle, which is the total mass of the agent divided by the volume of the bottle, rather than the percent liquid fill. The fill conditions **of** the bottle are determined by the size and geometry of the nacelle, the volume of air flowing through it, as well as the distance the bottle is stored from the nacelle.

Once the design parameters are selected for a particular engine and nacelle, a fire bottle is filled with the correct mass of CF_3Br and pressurized with the appropriate amount of N_2 to achieve the desired pressure at room temperature. During this process the bottle must be agitated to equilibrate the N_2 with the CF_3Br. The filled and charged bottle is mounted in the aircraft with the discharge head usually pointed downward. This is done so that when the aircraft is flying level, as it is supposed to when the engine nacelle fire protection system is triggered, the liquid agent is forced out by the gas above.

The release mechanism is typically a small explosive, called a squib, which ruptures a small closure disk and produces an opening that allows the agent-N_2 mixture to flow through the discharge head and into the tubing. The N_2, that was in solution at the higher storage pressure, begins to degas while the CF_3Br boils [its boiling point at atmospheric pressure is -57.8 °C (-72.0 °F)]. The detonation of the squib also promotes nucleation in the N2-saturated agent. This turbulent, highly transient mixture of dense vapor and evaporating liquid travels through usually less than 3 m of pipe (but up to 24 m) from the storage location to the targeted nacelle. The mixture sprays into the nacelle through tubes and/or holes mounted in the nacelle and located to distribute the CF_3Br simultaneously and evenly throughout the volume.

System Certification. Based upon years of testing and experience, a 6 % by volume concentration of **CF_3Br**, held for at least 0.5 s, is considered sufficient to extinguish a fire in an engine nacelle under most conditions. Any new design of an engine nacelle or fire suppression system requires that tests be run to re-certify that the 6 % level can still be maintained throughout the nacelle for the 0.5 seconds. Military aircraft are tested according to the Military Specification MIL-E-22285, while the Federal Aviation Administration **is** responsible for the certifying of commercial aircraft. The FAA test requires that a 6 % concentration be achieved with the bottle cooled to -54 °C (-65 °F) (Advisory Circular Number 20-100). For the military certification process, the discharge of the calculated amount of agent must occur in one second or less, timed from the entrance of the agent into the nacelle.

The concentration of agent is usually measured using twelve probes located throughout the nacelle while in flight or with simulated-flight air flow conditions. These probes are attached to an

[1] The fill density, when given in pounds per cubic foot, is nearly identical to the percent liquid fill because the density of CF_3Br at saturation pressure and room temperature **is 97.3 lb/ft^3 (1.56 x 10^3 kg/m^3)**.

instrument called a halon analyzer, which measures the change in concentration of the air-agent mixture. Any change in concentration affects the fluid properties of the mixture and causes a pressure variation that is detected by a strain gauge mounted on a bellows. The strain gauge resistance is calibrated against a known concentration of CF_3Br. The required concentration must be reached at all twelve probes and held for 0.5 seconds simultaneously for the system to pass the certification test.

During the process of certifying an aircraft, as many as fifty fire bottles of CF_3Br can be discharged to the atmosphere. The specific number discharged depends on the type of aircraft, the different flight attitudes, velocities, altitudes, and bottle temperatures that the certifying agency requires, as well as the amount of design modification required to achieve a successful certification test. The Environmental Protection Agency has described the certification process as a "non-essential" atmospheric discharge of the very high ozone depletion potential chemical, CF_3Br. Because of the significant amounts of CF3Br used, its deleterious effect on the environment, and resultant regulations, it is important that simulants which do not exceed an ODP of 0.2 be identified for modeling CF_3Br during future certification procedures.

II. THERMOPHYSICAL SCREENING OF CANDIDATE SIMULANTS

Given the dynamic phase change, from a liquid saturated with N_2 to a gas detected by a halon analyzer, any simulant must match as many of CF_3Br's thermophysical characteristics as possible. Previous studies have examined $CHClF_2$ and other halocarbons and refrigerants to determine their suitability as a CF_3Br simulant (Moore 1989; DiNenno *et al.* 1990). Satisfactory results have been found with SF_6 because of its comparable molecular weight and strong flashing characteristics. In an effort to broaden the search and focus on essential physical properties, NIST selected explicit criteria for a large scale search. These criteria were molecular weight, normal boiling point, and critical temperature. The molecular weight was selected as the broadest of screening tools to eliminate those chemical compounds that were less suitable than the two previously tested simulants: SF_6 and $CHClF_2$. A range of ± 65 kg/kmol about the molecular weight of CF_3Br was selected, based upon the difference between the molecular weights of CF_3Br (148.9 kg/kmol) and $CHClF_2$ (86.5 kg/kmol). The normal boiling point (-57.8 "C) and the critical temperature (67.05 "C) of CF_3Br were selected as the other two criteria based on their contributions to the phase change process. The acceptable range about both these temperatures was ± 25 ˚C. A survey of over 1,300 chemicals (REFPROP 1993; DIPPR 1993) based on these criteria revealed only nine chemicals: $CHClF_2$, C_2ClF_5, C_2HF_5, $C_2H_3F_3$, C_3F_6, C_3OF_6, C_3F_8, ClO_3F, and SF_6. Properties are summarized in Table 1.

For a candidate to be discharged into the atmosphere, it must possess an ozone depletion potential less than 0.2, preferably zero. C_2ClF_5 was removed from consideration because it has an ODP of 0.4. For discharge into the nacelle of a running aircraft engine, it is important that the chemical be non-flammable. $C_2H_3F_3$ is not suitable because it has a lower flammability limit of 13 % by volume in air, and as such it would be a fire hazard during testing. In addition, the chemical must not be corrosive, unstable, or very toxic. Both C_3OF_6 and ClO_3F fail on these points because of the ease with which they hydrolyze into highly toxic and corrosive acids: HF and HCI. The five remaining candidates were evaluated based on vapor pressure, Jakob number, experimental history, and atmospheric lifetime.

Vapor pressure is an indicator of the relative pressure reached during a discharge in the pipeline and the energy that will expel the chemical in addition to the nitrogen. Both C_3F_6 and C_3F_8 have vapor pressures more than **46** % lower than CF_3Br. **As** a result, these candidates may not achieve the same pipeline pressures as CF_3Br. At the other extreme, SF_6 has a vapor pressure 50 % greater than

CF_3Br. This may result in SF_6 dispensing more quickly than CF_3Br. Of all the five possible candidates, C_2HF_5 has the vapor pressure closest to CF_3Br.

The Jakob number (*Ja*) (Pitts ***et al.*** 1994) is the difference in enthalpy of a liquid between the normal boiling point and the ambient temperature (evaluated by the integral of the liquid heat capacity over that temperature range), divided by the heat of vaporization at the boiling point:

$$Ja = \frac{\int_{T_{bp}}^{T_{ambient}} C_p^{liq}\, dT}{H_{vap}(T_{bp})}$$

This dimensionless number is a measure of the fraction of a pure liquid that will flash to vapor when depressurized instantaneously. The ***Ja's*** for these candidates at 22 °C vary from 0.31 for $CHClF_2$ to ***0.66*** for SF_6, compared to a value of 0.51 for CF_3Br.

$CHClF_2$ and SF_6 have both been tested previously for simulating CF_3Br in shipboard room flooding applications by the Navy (DiNenno 1989, 1990). SF_6 outperformed $CHClF_2$ in these applications because, in addition to flashing characteristics, SF_6**'s** molecular weight, 146.06, is nearly ideal for testing suspension-in-air characteristics, particularly when compared to $CHClF_2$ with a molecular weight of 86.47. Though $CHClF_2$ was not selected, the Navy tests showed that it did perform satisfactorily with regards to its pipe flow characteristics. For an engine nacelle certification test, the dynamic flow characteristics are more important than the suspension in air characteristics because of the much shorter time scales involved (less than two seconds versus greater than 30 seconds). Of the remaining potential candidates, only C_2HF_5 was tested as a simulant; it was not selected (BA^{e}SEMA 1992).

Another consideration was the environmental impact of the chemicals based upon their atmospheric lifetime (ALT). Ideally, the selected candidate should have a very short atmospheric lifetime, or very low global warming potential (GWP). Global warming gases have been identified by the Environmental Protection Agency as an area of serious concern, although chemicals are not yet regulated based on a high GWP. The values in Table 1 show that SF_6 and C_3F_8 have ALTs greater than a millennium, and their S-F and C-F chemical bonds indicate that they will absorb infrared effectively (Ravishankara 1993). The possible advantages of any of these global warming gases must be balanced against their potential cost and possible regulation.

Based on the above criteria, C_2HF_5 (also known as HFC-125 or R125), $CHClF_2$ (HCFC-22 or R22), and SF_6 were selected as the three candidate simulants for experimental testing. None of these candidates is flammable, corrosive, toxic, or unstable, and there is sufficient commercial availability of each. Their basic thermodynamical properties are tabulated in Table 1. Only $CHClF_2$ has a non-zero ozone depletion potential, at 0.05. And only the atmospheric lifetime of SF_6 is greater than 50 years. Of the three, C_2HF_5 is the strongest candidate based on this thermodynamic analysis.

III. EXPERIMENTAL TESTING OF CANDIDATE SIMULANTS

Though evaluation of the chemical compounds based upon their thermophysical properties is a strong indicator of their suitability as simulants for CF_3Br in the certification testing process, the relative importance of the thermophysical differences between the candidates and CF_3Br was not known. Accordingly, comparative discharge experiments were performed. NIST and **WKA** performed tests that focused on distinct aspects of the process. WKA testing analyzed the hydraulic characteristics of the chemicals during their discharge in a fire suppression system configuration conforming to the test setup guidelines of MIL-M-22284 for the evaluation of the discharge characteristics of CF_3Br fire suppression systems. NIST analyzed the flashing characteristics of the chemicals through a T-fitting from a simulated fire suppression system using high speed movies. Pressure measurements were also taken by NIST during the spray discharge filming. In the discussion below, the general test methodology and initial conditions will be presented. The results of the pressure traces of the WKA and NIST tests and the NIST spray tests will follow.

Test Methodology. As in an actual aircraft fire suppression system, both the WKA and the NIST baseline tests consisted of a storage vessel charged with a specified mass of CF_3Br and pressurized with N_2. The vessels were attached to a 3 m long piping system to model a typical aircraft delivery system. During the experiments the agent-N_2 mixture was discharged and the pressures in the vessel and along the piping were measured by strain-gauge pressure transducers. The three pressure transducer locations were selected to evaluate the pressure decay within the vessel, the pressure response in the pipeline approximately 0.2 m (0.13 m for WKA) downstream from the discharge outlet, and pressure response at the end of the 3 m pipe. Refer to Figure 1 and Table 2.

In the case of the WKA tests, the discharge vessel used was a spherical fire bottle of 3.67 liters (224 in^3). The bottle was filled with agent and pressurized with N_2 to 4.41 MPa (640 psia). During the pressurization process the bottle was shaken to fully equilibrate the system with N_2 in solution and achieve a stable 4.41 MPa at standard temperature. The discharged CF_3Br was recovered in a 900 liter (31.8 ft^3) container. Other WKA tests were discharged to atmosphere. The pressure transducers used by WKA were of the strain gauge bridge-type. WKA pressure transducers were scanned every 20 ms. The WKA apparatus utilized a rupture disk with a squib as the discharge actuator, as is found in most aircraft systems. The agent was released through a discharge head into a piping system with a 17 mm (0.675 in) diameter, terminating in a T-fitting with two outlets of 13.4 mm (0.531 in) in diameter.

NIST performed discharges using agent recycled from cooled recovery tanks. The recycled agent was weighed and transferred to a 4.19 liter (256 in^3) fixed cylindrical vessel. N_2 was slowly bubbled through the liquid agent to maximize the dissolution of N_2 and to pressurize the vessel to 4.41 MPa (640 psia). The pressure transducers used by NIST were Wheatstone-bridge strain gauge pressure transducers. The sampling rate for each transducer was 1000 Hz. The NIST discharge apparatus consisted of a manually engaged, plunger-type valve with a solenoid trigger. Once the plunger was released, the agent-N_2 mixture traveled through the discharge head into the pipeline through a smooth section, reducing down to the 15.9 mm (0.625 in) pipe (Figure 1 and Table 2).

The spray discharge was filmed exiting the 3 m piping through a T-fitting with 7 mm (0.275 in) diameter outlets. This fitting is an actual discharge nozzle that can be found in some aircraft fire suppression systems. Figure 1 illustrates the location of the pressure transducers and the discharge T-fitting. The upward plume of each agent was filmed using a 16 mm high speed movie camera at 500 frames per second. The width and duration of these plumes indicate how the chemicals will distribute, relative to CF_3Br, when discharged into a nacelle.

Fill Conditions. Previous simulant work for use in shipboard testing by both the Naval Research Laboratory (DiNenno *et al.* 1989, 1990) and the British Ministry of Defense (BA[e]SEMA 1992) matched the mass of the potential simulants with the initial mass of CF_3Br. In these tests, only SF_6 showed strongly favorable results. This can be attributed to the fact that SF_6 has nearly the same molecular weight as CF_3Br, and its liquid density is less by only 13 %. Other candidate simulants have significantly lower liquid densities, which resulted in a decrease in compressed nitrogen available for the discharge process. For example, a one liter bottle with 0.78 kg of CF_3Br at 4.41 MPa has roughly half a liter of liquid and an equal volume of gas. The same bottle filled with 0.78 kg of

$CHClF_2$ will have approximately two-thirds liter of liquid and only one third gaseous N_2, due to the different liquid densities (neglecting agent in vapor and nitrogen in solution). This can significantly impact the discharge force as the liquid agent exits. If one matches the percent liquid fill rather than the mass of CF_3Br, the amount of gaseous N_2 is most nearly conserved.

During the tests reported here, NIST and WKA consistently reproduced the liquid fill conditions of CF_3Br for each of the different candidates. As a result, the volume of N_2 gas available to force the agent through the pipes was the same for each agent. Both vessels were filled with 51 % liquid agent, and N_2 provided the pressurization to 4.41 MPa (625 psig). For each chemical the 51 % liquid fill required a different amount of mass, based on the chemical's liquid density calculated at saturation pressure and 22 °C, and neglecting the small contribution of the nitrogen in solution and the agent in vapor. Specific fill conditions are described in Table 3.

IV. RESULTS

The plots of the pressure traces versus time from discharge of CF_3Br and candidate simulants are presented in Figures 2(a)-(c) and 3(a)-(c). The pairs of curves in descending order correspond to the pressure transducers as they occur downstream. The highest curves (solid markers) represent the pressure in the storage vessels as a function of time. The initial condition is always 4.41 MPa and the final pressure depends upon the value in the atmosphere or the recovery tank. The middle pressure traces represent the pressure measured just past the discharge head, at 0.2 m. There is a steep rise in the pressure along these traces just after the discharge is initiated when they approach the vessel pressures. For the rest of the discharge the curves follow the trend of the vessel pressures, with a reduction in pressure. The lowest pair of curves are those taken near the end of the piping system, roughly 3 m downstream. In general they follow the other two pairs of curves at a lower pressure due to friction losses.

Pressure Response of Candidates and CF_3Br. The six figures [Figures 2(a)-(c) and 3(a)-(c)] show the results of tests performed by WKA and NIST. WKA performed three discharges with each agent in order to insure repeatability and data validity. Within each agent's data group WKA found no more than 5 % deviation in pressure trace or discharge time between any two discharges. NIST performed one or two tests of each agent, and based on these and numerous tests with the same apparatus, there is less than 5 % uncertainty in the values presented.

As two sets of data, both Figure 2 and Figure 3 show the same general results. SF_6 has a higher value than CF_3Br at all three pressure transducers for at least the first 750 ms of the discharge. $CHClF_2$ is significantly lower than CF_3Br throughout. And the pressure trace of C_2HF_5 is the closest to that of CF_3Br, as was predicted by the thermodynamical analysis.

The discharge duration of ail of the candidates is less than that of CF_3Br. Comparison of the 3.0 m pressure curves shows that in the WKA data, $CHClF_2$ and C_2HF_5 have closest to the same discharge time as CF_3Br; the NIST data show that the closest replication of the discharge occurs with SF_6, with C_2HF_5 a close second.

There is a notable difference between the WKA and NIST data during the first 200 ms. The WKA trace at the 0.2 m transducer has a dip for all the compounds, while the NIST data does not. This can be attributed to the difference in discharge heads. NIST used a reducing section after their plunger release valve, while WKA used a standard fire bottle discharge head with a squib and rupture disk release mechanism. This issue does not impact the conclusion that based upon the pressure curves of the WKA and NIST tests, C_2HF_5 most closely models the behavior of the CF_3Br.

Spray Discharge Results. The primary part of the NIST experiment was designed to compare the spray characteristics of the different candidate simulants, as a predictor of the different agents' distribution when discharged into a nacelle. In this part of the NIST test the upward outlet of the T-fitting was filmed using a high speed movie camera for each candidate, and CF_3Br as a reference. Prints of frames taken at 200 ms and 900 ms after exiting the T-fitting are shown in Figures 4(a)-(d) and Figures 5(a)-(d).

At 200 ms [Figures 4(a)-(d)] the sprays of C_2HF_5 and SF_6 are nearly the same as that of CF_3Br, with C_2HF_5 slightly wider and SF_6 somewhat narrower. The spray discharge of $CHClF_2$ is significantly wider than the CF_3Br discharge. If one recalls the values of the Jakob number for each of these chemicals (*Ja* equals 0.51 for CF_3Br, 0.66 for SF_6, 0.52 for C_2HF_5, and 0.31 for $CHClF_2$) the wider spread of $CHClF_2$ and the narrower spread of SF_6 at first appears inconsistent. A reasonable explanation is that the chemicals with the higher *Ja* are flashing primarily inside the piping. The $CHClF_2$, on the other hand, does not possess the internal energy to flash (like the CF_3Br) in the confined environment of the pipe, and not until it is freed to atmospheric pressure at the end of the pipe can it fully expand.

At 900 ms [Figures 5(a)-(d)] it is evident that the stronger flashing of SF_6 has either emptied the bottle faster or it has gasified the agent so that we can not see it still exiting the T-fitting. Either way the dense vapor cloud of CF_3Br is not well represented by the SF_6. The $CHClF_2$ still has a fairly large cloud, but its conical shape indicates a weaker jet than that of either the CF_3Br or the C_2HF_5. Finally, the jet from the C_2HF_5, though smaller than the CF_3Br, best represents the flashing spray characteristics of the CF_3Br.

V. CONCLUSION

C_2HF_5 overall has the thermophysical properties that indicate that it will best simulate CF_3Br of the many possible simulants considered. Though its molecular weight is not the closest to CF_3Br, in this application suspension in a calm environment does not matter. Here the properties that best predict its dynamical behavior (the Jakob number and vapor pressure) are both closest to those of CF_3Br.

The NIST and **WKA** pressure traces confirm that C_2HF_5 best simulates the dynamic pressures achieved by CF_3Br for two different configurations of piping systems. This is a strong indicator that the fluid mechanical and thermodynamical behavior of C_2HF_5 will exhibit close similarities with that of CF_3Br in other discharge configurations. Though the pressure of C_2HF_5 falls off approximately 100 ms earlier than CF_3Br, in the engine nacelle certification testing which this simulant will be used, the latter part of the certification test is the less critical. Therefore, it is likely that this will not impact the overall results. If, however, in field tests this is found to be an issue, scaling the timing requirement could compensate for this difference.

The spray discharge tests conducted by NIST further verify that C_2HF_5 is the candidate of choice. The duration and extent of its spray at the end of a **3** m piping system show it has much in common with CF_3Br.

In conclusion, results of tests on SF_6, $CHClF_2$, and C_2HF_5 from two different laboratories demonstrate that C_2HF_5 consistently acts most like CF_3Br in both pressure response and spray width. It is, therefore, the recommendation of both the National Institute of Standards and Technology and Walter Kidde Aerospace that C_2HF_5, also known as HFC-125, be selected for full scale testing as the simulant of CF_3Br for the purpose of engine nacelle certification testing and development.

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Chemical Compounds	Chemical Formulas	Molecular Weight (kg/kmol)	Normal Boiling Point[R,D] (°C)	Critical Temperature[R,D] (°C)	Reasons for Exclusion	Vapor Pressure[R,D] (kPa) at 22 °C	Jakob Number[P]	Ozone Depletion Potential[N]	Atmospheric Lifetime[B] (years)
Bromotrifluoromethane	CF_3Br	148.9	-57.8	67.1		1496	0.51	16	110
Chlorodifluoromethane	$CHClF_2$	86.5	-40.9	96.2	***	957	0.31	0.05	16
Chloropentafluoroethane	C_2ClF_5	154.5	-39.2	79.9	0.4 ODP	NFC			
Pentafluoroethane	C_2HF_5	120.0	-48.6	66.2	***	1271	0.52	0	41
1,1,1-Trifluoroethane	$C_2H_3F_3$	84.0	-47.4	73.1	Flammable	NFC			
Hexafluoropropene	C_3F_6	150.0	-29.7‡	94.8	Low VP & Low Jakob	603‡	0.40	0	< 1†
Hexafluoroacetone	C_3OF_6	166.0	-27.3	83.9	Ex.Toxic[M]	NFC			
Octafluoropropane	C_3F_8	188.0	-36.8	72.0	Low VP & High ALT	805	0.59	0	10,000
Perchloryl Fluoride	ClO_3F	102.5	-46.7	95.2	V. Toxic[M]	NFC			
Sulfur Hexafluoride	SF_6	146.1	-64.0	45.5	***	2268	0.66[A]	0	3200

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R REFPROP - NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures, Version 4.0, J. Gallagher, *et al.* 1993.
P Pitts *et al.* 1994.
B Braun *et al.* 1994.
D DIPPR - Data Compilation of Pure Compound Properties, Version 8.01, The American Institute of Chemical Engineers, 1985.
M Material Safety Data Sheet from MDL Information Systems, Inc.
A Jakob Number was calculated by the author using data from AlliedSignal Chemicals.
*** Selected Candidate
ODP Ozone Depletion Potential
VP Vapor Pressure
ALT Atmospheric Lifetime. For these chemicals ALT is a good predictor of global warming effects.
NFC No Further Comparison because of ODP, flammability, or high toxicity.
† Correspondence with Scott Thomas, 3M Specialty Chemicals Division, from an analysis by Robert Huie, NIST.
‡ Accuracy quoted in reference as ± 10 %, all other values are accurate to ± 5 % or better.

Table 1: Thermophysical, environmental, and other properties of potential candidate simulants.

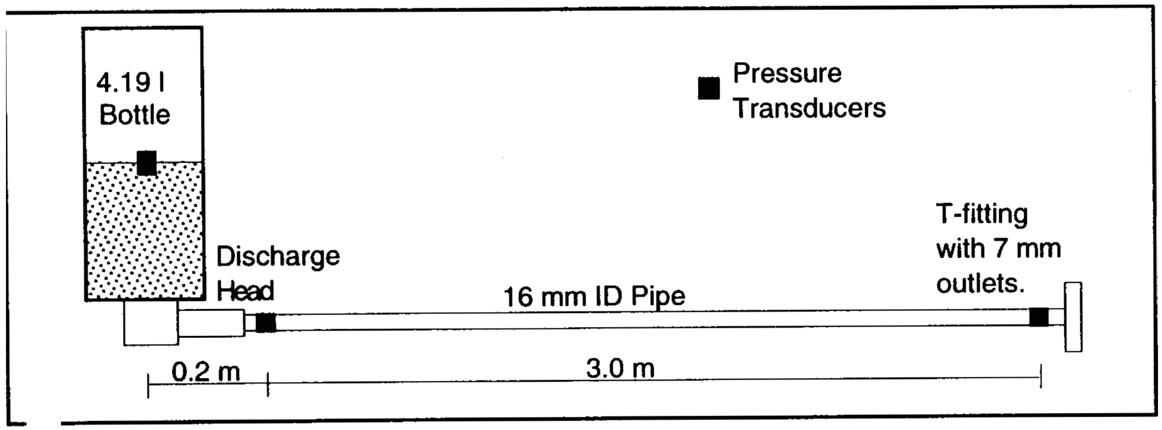


Figure 1: NIST discharge bottle, piping system, pressure transducers, and T-fitting discharge nozzle. The WKA system is similar, except that the storage vessel is spherical and dimensions are different. Dimensions for both systems are in Table 2.

	Vessel volume	Upstream PT (distance from head)	Downstream PT (distance from head)	Pipe ID diameter	Piping length	Piping volume
WKA	3.67 liter	13 cm	323 cm	17.0 mm	3.3 m	1.0 liter
NIST	4.19 liters	20 cm	318 cm	15.9 mm	3.3 m	0.7 liters

Table 2: Dimensions of WKA and NIST test apparatuses.

	CF_3Br	SF_6	C_2HF_5	$CHClF_2$
Liquid density, (kg/m^3) at sat. pressure, 22 °C	1574	1354	1207	1204
Mass fraction of CF_3Br	1.00	0.87	0.77	0.76
WKA Mass used to match 51% liquid fill. (kg)	2.95	2.59	2.27	2.27
NIST Mass used to match 51% liquid fill. (kg)	3.36	2.93	2.58	2.57

Table 3: Initial conditions for WKA and NIST tests.

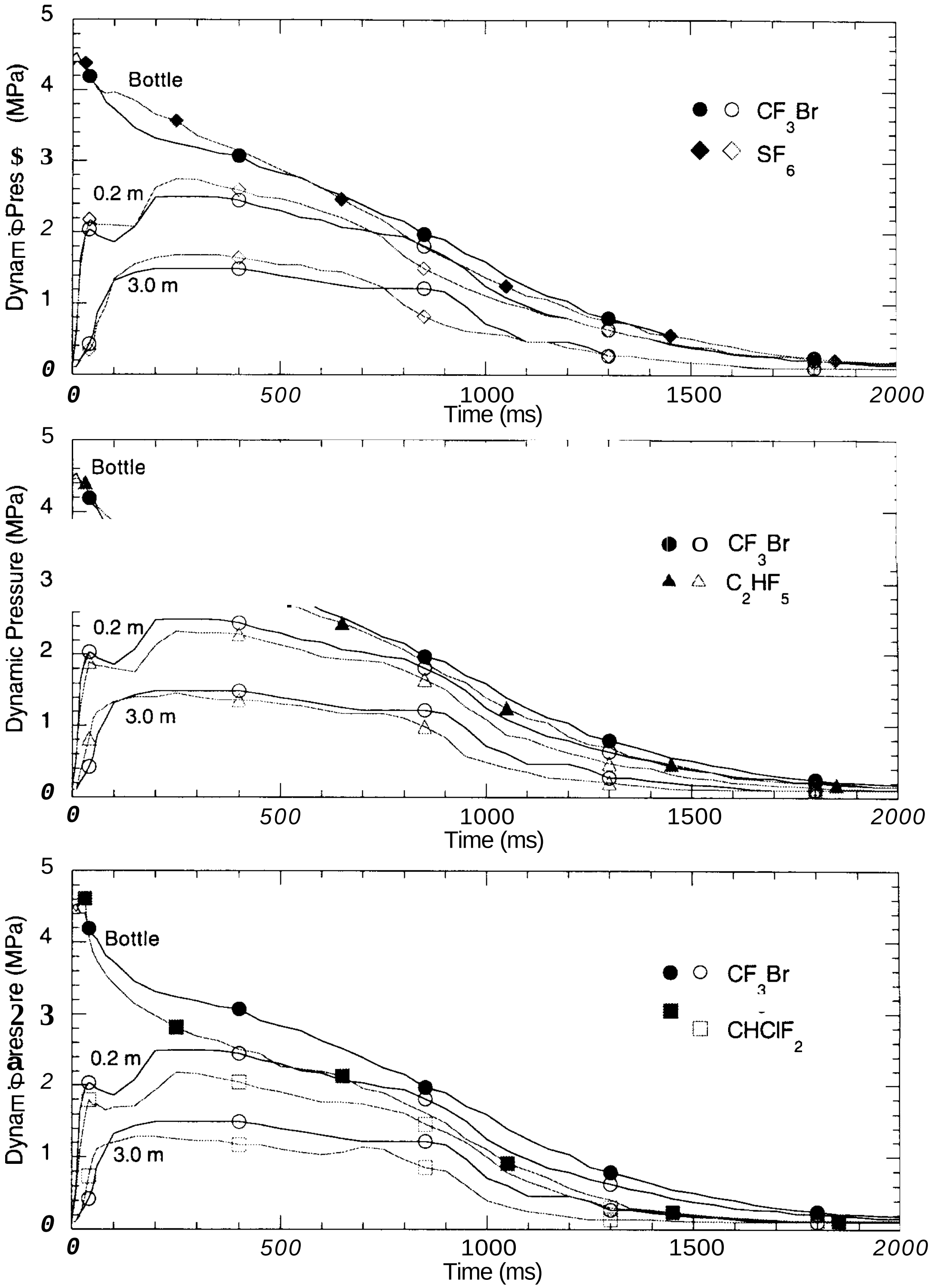


Figure **2:** Pressure traces in the vessel (solid markers) and located **0.2** m and 3.0 m downstream (outline markers) of WKA discharges to atmosphere: (a) SF_6 and CF_3Br and (b) C_2HF_5 and CF_3Br; and into a 900 liter recovery tank: *(c)* $CHClF_2$ and CF_3Br.

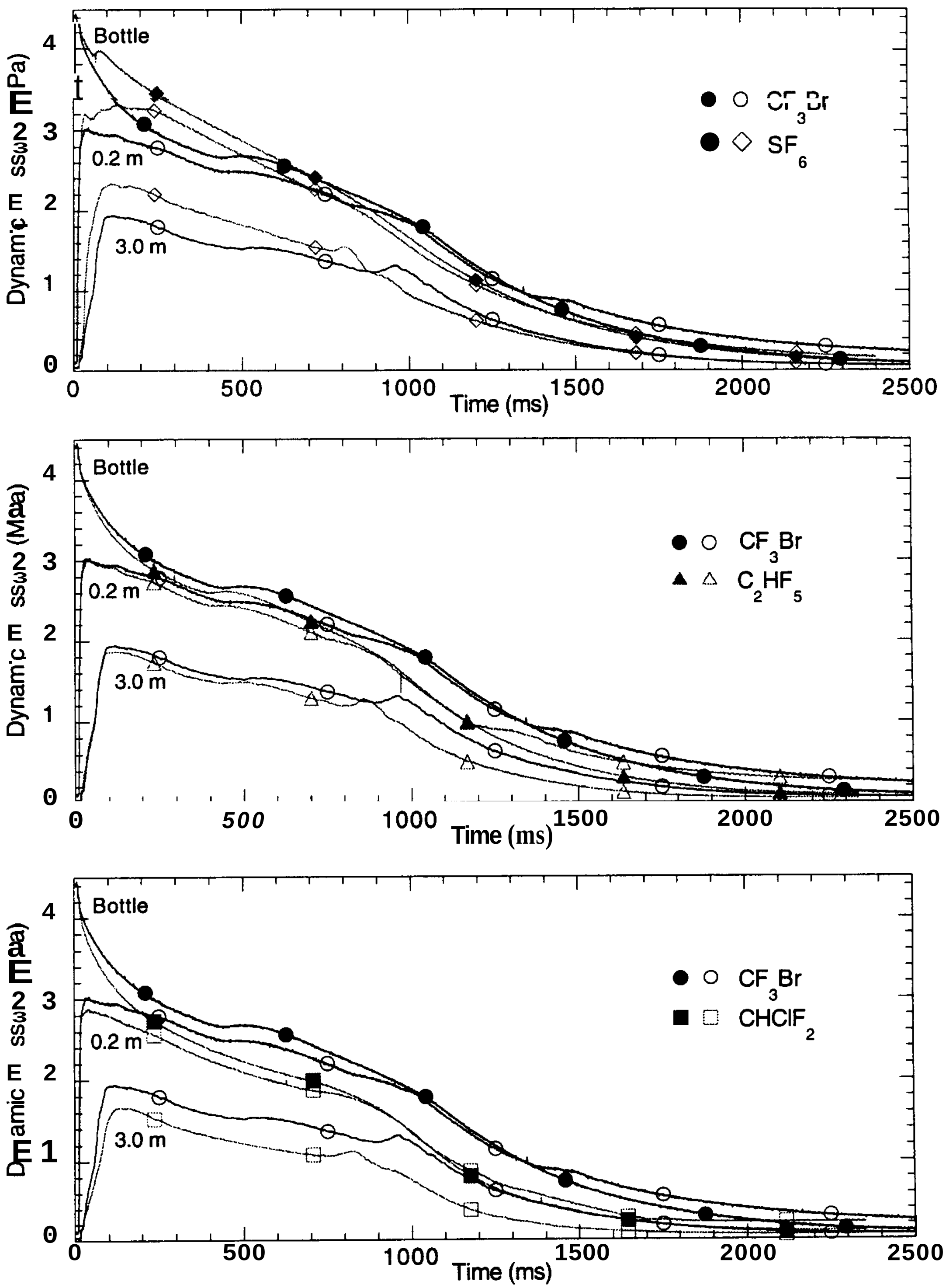
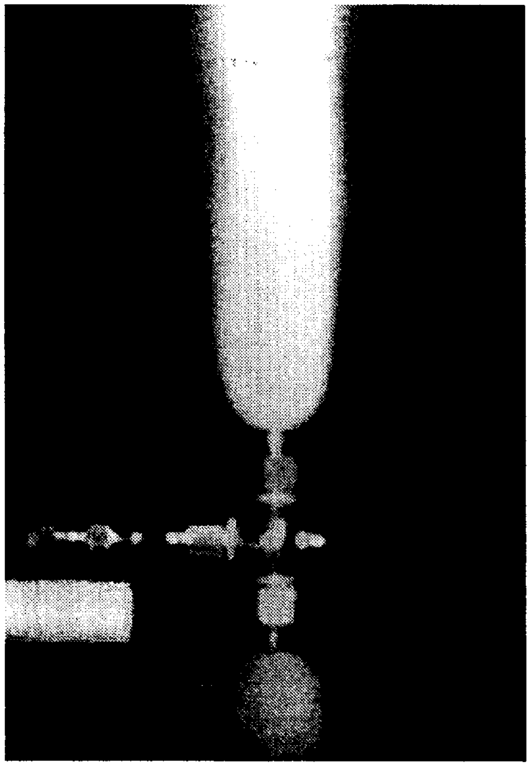
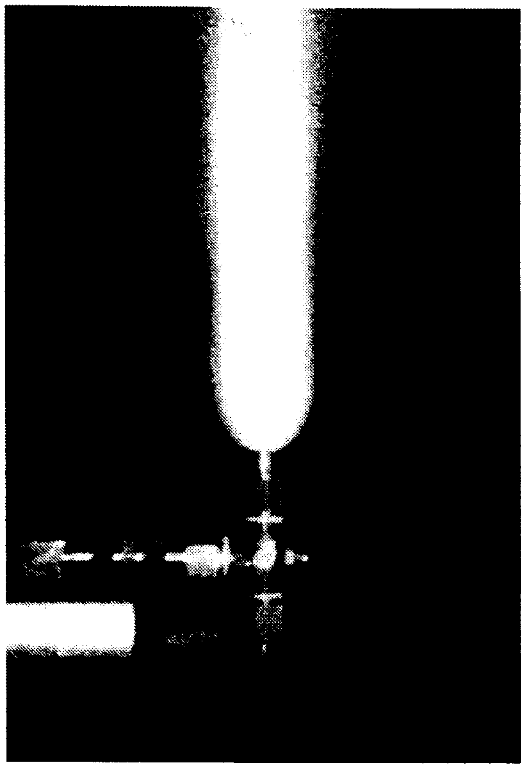


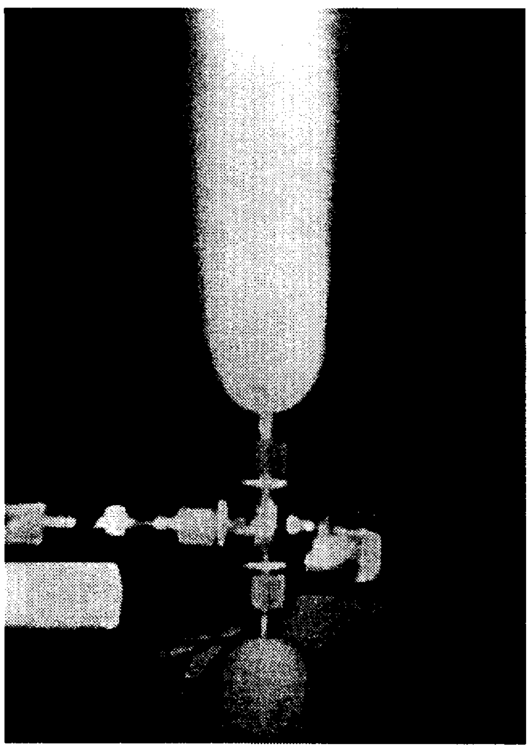
Figure 3: Pressure traces in the vessel (solid markers) and located 0.2 m and 3.0 m downstream (outline markers) of NIST discharges to atmosphere: (a) SF_6 and CF_3Br, (b) C_2HF_5 and CF_3Br, and (c) $CHClF_2$ and CF_3Br.



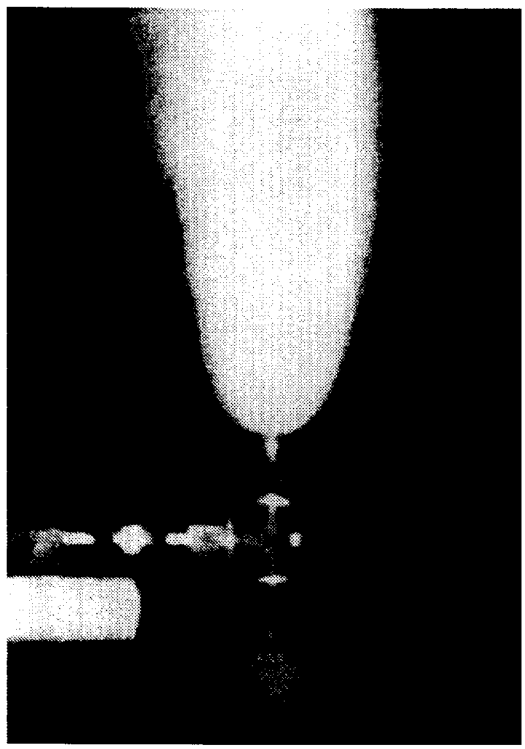
(a) CF_3Br



(b) SF_6

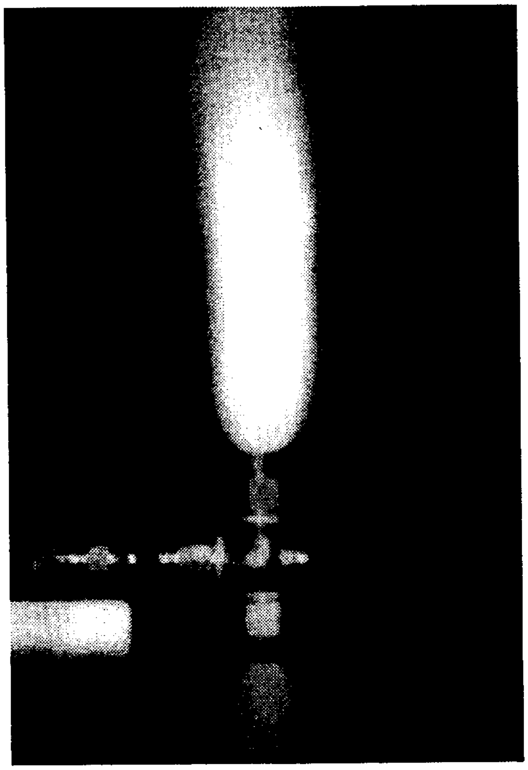


(c) C_2HF_5

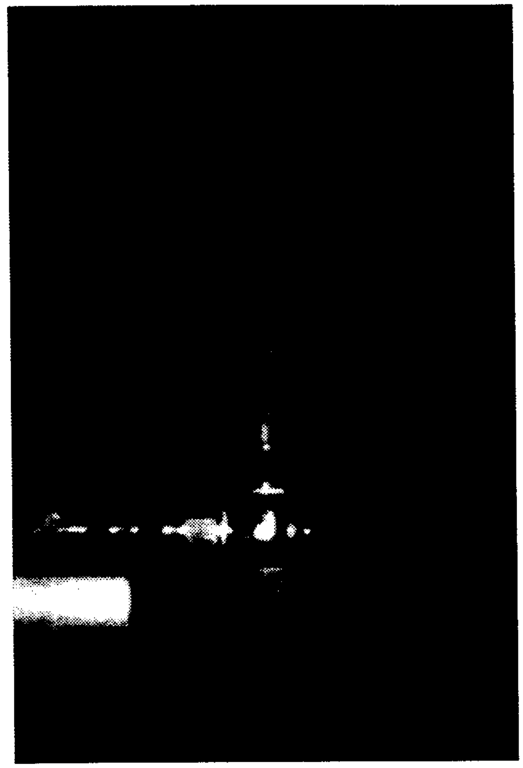


(d) $CHClF_2$

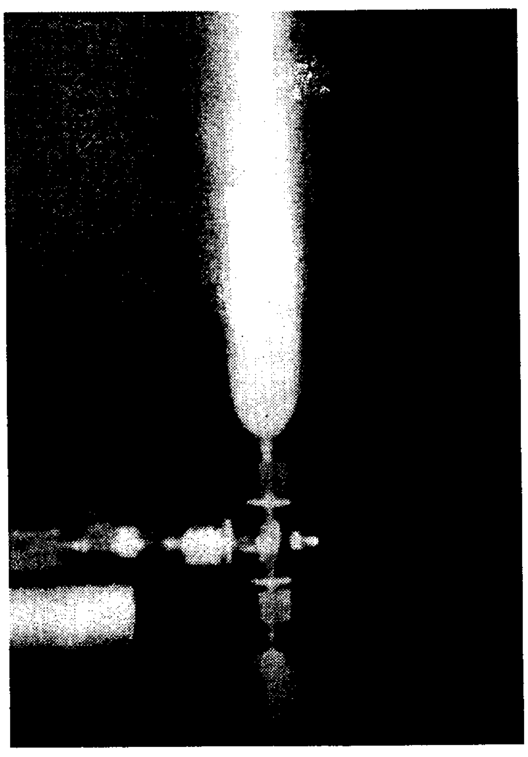
Figure 4(a)-(d): Photographs of NIST discharges to atmosphere through T-fitting at 200 ms for (a) CF_3Br, (b) SF_6, (c) C_2HF_5, and (d) $CHClF_2$.



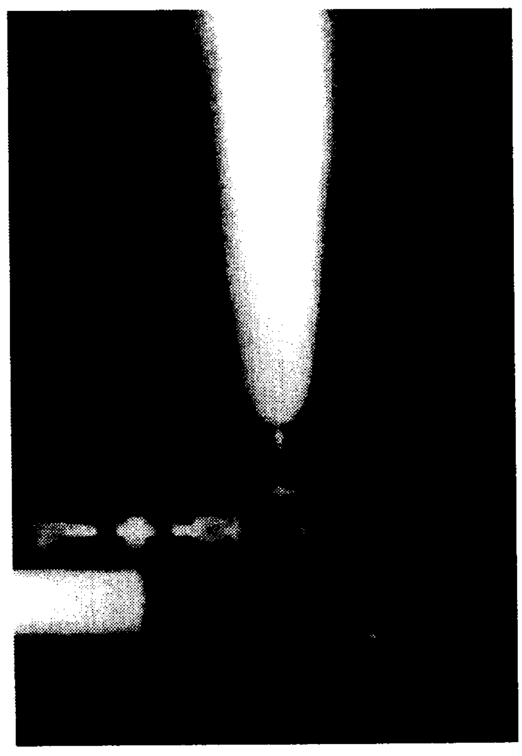
(a) CF_3Br



(b) SF_6



(c) C_2HF_5



(d) $CHClF_2$

Figure 5(a)-(d): Photographs **of** NIST discharges to atmosphere through T-fitting at 900 **ms for** (a) CF_3Br, **(b)** SF_6, (c) C_2HF_5, and (d) $CHClF_2$.