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Comparison of liquid coolants suitable for single-phase detector cooling

Abstract

Three different classes of commercial heat transfer fluids (PFCs, HFEs and FK) are selected as candidates for the single-phase liquid cooling system of the SciFi Tracker photodetectors. None of them is perfect, though. PFCs are strong greenhouse gases. C6F14, the popular PFCcoolant widely used at CERN because of its outstanding inertness and radiation resistance, has GWP of 9300. The heavier PFC fluid C7F16 with a wider liquid range has GWP of 7930. The 3M Novec fluids, designed as alternatives to PFCs and having sharply lower GWP, include a range of HFE liquids with GWP=60-300 and FK liquids, Novec 649 and 774, with GWP=1. These fluids are less inert and, arguably, less radiation resistant than PFCs. The 649, having the thermo-physical properties quite close to C6F14, had been tentatively selected as the baseline option for the SiPM cooling. HFE liquids Novec 7100 and 7200 can also be considered as alternatives. Environmental, safety and performance profiles of all above mentioned fluids are compared.

Abbreviations and acronyms

HTF	heat transfer fluid
HC	hydrocarbon(s)
HFC	hydrofluorocarbon(s)
PFC	perfluorocarbon(s)
GWP	global warming potential
C6F14	perfluorohexane C_6F_{14}
FK	fluoroketone(s)
C6K	C6-Fluoroketone, aka 3M Novec 649
HFE	hydrofluoroether(s)

1. Introduction

A single-phase liquid cooling for the SciFi tracker photodetectors [TDR 2014, TIPP 2014] was preferred to 2-phase cooling because of its lower cost, robustness, wider choice of coolants, more "off-the-shelf" cooling plant components (e.g., pumps). There were no compelling reasons to choose the more complex and demanding 2-phase technology, given the mostly passive thermal load of the SiPM read-out modules and the absence of severe material budget restrictions in this application. The freedom to choose the module connection topology[1] and reluctance to deal with high-pressure inside a fairly extensive system also favored the mono-phase choice. The environment-friendliness requirement alone was insufficient to opt, for example, for the "green" 2PACL CO2 cooling [Verlaat 2012].

The implicit idea was to use C6F14 as the coolant. This popular PFC fluid had been validated for the LHC [Battistin 2006] and used in many detector cooling systems at CERN. Its unique combination of properties (inertness, non-flammability, excellent dielectricity, safety, radiation resistance, water-like pumpability at low temperatures usually outweighs its main drawbacks:

[1] The more economical serial connection was assumed at the TDR time.

poor heat transfer characteristics, the relatively low boiling point (57°C) and, most importantly, a very high greenhouse potential (GWP = 9300 [Ivy 2012]), typical of all PFCs.

The environmental impact of C6F14 and other PFCs were tacitly disregarded compared to their obvious benefits for the design of the LHC detectors in early 2000. Now, ahead of the LHC detector upgrades, this situation has changed. With globally growing environmental awareness, the environmental impact aspects cannot be ignored anymore (at least at the official CERN level) and gradually become competitive with physics performance aspects. PFC emissions are now closely monitored at CERN []. There are two strategies to reduce them: by anticipating and preventing the losses and by replacing PFCs with "greener" fluids.

Given the big size of the SciFi Tracker and the complexity of manifolding, the inner cooling structures of ROBs and their interconnections[2], it will be difficult to make the SiPM cooling system totally "non-emissive" over the long term. Even in industrial applications [Tuma 2001], there are unavoidable operational losses related to the PFC's volatility and high thermal expansion (~ 1% per 10K). Thus, as long as we stay with liquid cooling, we have to count on a "green" solution as the baseline, while possibly keeping the cooling system (both detector and cooling plant sides) compatible with liquid PFCs, as a backup.

This memo summarizes our efforts to identify possible alternatives to C6F14 among modern commercially available fluids suitable for operation at -50C. Unfortunately, no perfect reconciliation of environment- and application-friendliness seems possible for the SciFi application, so some sort of compromise is unavoidable[3]. With C6F14 representing the extreme case of such a compromise, two other fluids have been shortlisted: the "TDR candidate" fluid 3M Novec 649, a FK with GWP=1, and the HFE fluid 3M Novec 7100.

For completeness, we also consider close alternatives to each of the candidate, within the same class: the FK Novec 774 and the HFE Novec 7200. Even the PFC class contains liquids that are somewhat superior to C6F14, e.g. 3M FC-84 (C7F16) which has a bit lower GWP and a bit better thermal properties, while having a higher boiling point (80C) and, hence, lower evaporation losses.

2. Alternative coolants

2.1 What do we want?

The requirements for the fluid in indirect cooling systems are nicely summarized in Refs [Cengel 2007] and [Mohapatra 2006]. In general, the best coolant is an inexpensive nontoxic liquid with excellent thermo-physical properties, a long service life and minimal regulatory constraints. It should be non-corrosive to the materials it comes in contact with. A high flash point and auto-ignition temperature are desired for safety reasons. Good thermo-physical properties (high thermal conductivity and specific heat; low viscosity) are required for the optimal heat transfer and low required pumping power.

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[2] Especially now that we are drifting to parallel, rather than serial, ROB connections and the 3D-printed cooling bars will be likely split into two halves.

[3] "The boundary conditions we have are contradictory, since a stable substance is by definition bad for the environment, since it remains long time in the atmosphere and something unstable is bad for the detectors. The only hope is … to find something which is not very stable to radiation, but non-corrosive. It will not be possible to apply it to the radiation area, but it will not be harmful for the atmosphere." [Taborelli 2014]

Water, one of the best HTFs available, is an obvious example of a good approximation to the ideal. However, liquids intended for electronics cooling are also required to be electrically non-conductive ("dielectric") and clean.

Electrical conductivity becomes important if the coolant may leak out of a cooling loop or be spilled during maintenance and come in contact with sensitive electronics. By the "cleanness", the ability to evaporate without leaving a residue that might attract dirt, deteriorate insulation or just irreversibly stain the setup is usually implied. DI water serves well for above-zero applications, though DI water based systems are usually quite expensive. DI water/glycol solutions are questionable because of their toxicity and "cleanness". The best attainable volume resistivities for DI water and DI/glycol are about 10^7 and 10^8 ohm-cm, respectively [T&K 2003]. We shall mark this level as the reference.

To that we have to add the application-specific requirements. The required operating temperature range should be well within the total coolant's liquid range[4]. For the SciFi cooling, the operating range is between -50C (the lowest foreseeable working SiPM temperature) and +40C (the SiPM annealing temperature).

The fluids for HEP detector cooling should be appropriate for working in the radiation environment specific to the application. This is not simply equivalent to requiring a superior radiation resistance for the coolant. In practice, it rather means that the radiolysis products appearing in the coolant should not adversely impact the cooling system integrity and efficiency over the project's life time. When assessing this factor for indirect cooling, apart from the total dose and the radiation type, one has to take into account the pipe materials (metals, plastics, elastomers), their geometry (e.g., wall thickness), the presence and efficiency of the filtering elements in the cooling loop.

Traditionally, the radiation-related effects (especially for neutrons) were associated with the presence of hydrogen (H) in the coolant [Battistin 2010] – because of the combined effect of the high neutron cross-section of H and potential hazards of acids produced by the radiolysis. For example, in fluorinated liquids the radiolysis chain involving hydrogen will result in formation of fluor-containing acids, e.g. HF or PFPA, which might cause corrosion of the metallic cooling system elements. Hydrogen can be present either in the coolant's molecule (like in HFEs), or in HC impurities, or in water dissolved in the coolant.

Obviously, the radiation-related requirements will be quite different for cooling of inner LHC detectors (with high radiation doses and thinnest possible heat exchanger walls) and for out-of-acceptance electronics (relatively thick-wall heat exchangers and low radiation doses, like in the SciFi tracker case). In [PG 2014 irrad memo] it is shown that, even under exaggerated pessimistic assumptions, the radiolysis effect for a fluoroketone fluid in SiPM cooling system will be microscopic – simply because of the low expected ionization dose and neutron fluence. The resulting concentration of acids will be low and the dominant radiation damage in this case will be associated with the impurities, rather than with the coolant itself. Similar arguments are applicable to any other fluid with no or low H content. Thus, the "no hydrogen" requirement can be tentatively lifted, as one of possible compromises.

[4] The range between the pour and boiling points at the operating pressure.

Our search for the SiPM coolant follows this hierarchy of criteria:

1. Commercial dielectric liquids
2. CERN regulations: non-flammable (no or high flash point[5]), non-toxic
3. Clean (no pollution of the workplace)
4. Operating temperature range: -50…40°C
5. Stable, non-corrosive (according to MSDN)

The shortlisted candidates are ranked according to their environmental, thermal transfer properties, pumpability, cost and safety, as well as material compatibility and reactivity.

2.2 What do we have?

A concise overview by S. Mohapatra (Mohapatra 2006) described the main classes of commercial liquids for electronics cooling. Current catalogues of leading coolant manufacturers, like 3M, DuPont, Solway Solexis, Exxon, indicate that the industry did not offer qualitatively new classes of fluids since the last major environmental policy shift which occurred after the Kyoto protocol entered into force in 2005. The industrial R&D efforts, quite expectedly, aimed at gaining the market for the mainstream applications, like air conditioning, power electronics and data center cooling, semiconductor manufacturing, home heating etc, which mostly belong to the above-zero °C and/or 2-phase cooling domains. A renaissance of interest to CO2 cooling is also observed, especially in the mobile air-conditioning sector [CO2-AC]. As to low-temperature single-phase applications, the only visible new "development" since mid-2000s was the addition of FK fluids, originally positioned as fire-fighting agents, to the HTF category, under new trade names (e.g. Novec 649, formerly known as Novec 1230).

Here are the main classes of stable dielectric coolants[6] that are liquids at a room temperature, with remarks on their safety, environmental and operational profiles:

- **Aromatics (HC):** Synthetic hydrocarbons of aromatic chemistry. These compounds are usually highly flammable and cannot be classified as non-toxic. Often they have strong odours, which can be irritating to the personnel. Temperature range: at or above room temperature, but some, like (diethylbenzene-based?) [Paratherm] CR, [Dynalene] MV, [Dowtherm] J, are good down to below -80C.
- **Silicate-ester (SE):** These synthetic liquids (i.e., [Coolanol] 20, 25R) were widely used as a dielectric coolant in military radar and missile systems. SEs have caused significant and sometimes catastrophic problems due to their hygroscopic nature and subsequent formation of flammable alcohols and silica gel. They are being replaced by aliphatic chemistry (polyalphaolefins or PAO).
- **Aliphatics (PAO):** Aliphatic hydrocarbons of paraffinic and iso-paraffinic type (including mineral oils) are petroleum-based fluids. They are non-toxic, have a non-discernible odour, and do not form hazardous degradation by-products. PAOs directly replaced the silicate-ester fluids in a variety of military and avionic applications. Example: Dynalene HF-LO (according to data sheet, is good down to -73C but combustible and toxic). Most PAO fluids have prohibitively high viscosity below 0C [Tuma 2009].

[5] The temperature at which the vapors produced from a fluid will ignite (flash-off) with the presence of an ignition source (the fluid will not burn at this point).
[6] DI water and DI-glycol mixtures are excluded because of poor stability of their dielectric properties and limited usability below -25C.

- **Silicones:** A popular coolant chemistry is a liquid polymerized siloxane (e.g.,dimethyl(or ethyl, or phenyl) polysiloxane) commonly known as *silicone oil*. The molecular weight and the thermo-physical properties (freezing point and viscosity) of this synthetic polymer can be adjusted by varying the chain length and configuration. Silicone fluids are used, as lubricants and HTFs, at temperatures as low as -100°C and as high as 400°C. They are excellent dielectrics, have low odour, are nontoxic and stable within the design temperature range. Dimethylsiloxanes feature relatively good radiation resistance (up to ~10 kGy) and phenylsiloxanes withstand up to 1 MGy. Julabo recommends silicone oils as standard coolants [Julabo Fluids] for their open-bath chillers. However, low-temperature silicone oils are expensive, flammable and, because of low surface tension and low vapour pressure, very polluting liquids. Examples: Dow Syltherm XLT, Julabo Thermal HY, Gelest Silicone Fluids.
- **Fluorinated liquids[7] (PFC, PFE, HFE, FK)** have certain unique properties: first of all, unlike all other dielectric fluids, some of them are non-combustible, non-toxic and very inert. Secondly, some of these fluids have low freezing points and low viscosities at very low temperatures. In addition, unlike silicone oils, they are "clean" (in the sense discussed above). On the negative side, all these liquids are very expensive, have quite poor thermal properties as single-phase coolants. PFCs and PFEs are greenhouse gases. Due to the extremely low surface tension and incompatibility with fluoroplastics, floirinated liquids will easily develop leaks in the systems that are not specifically designed for their use. Their volatility may result in high operation costs.

The only truly non-flammable dielectric fluids are found among fluorinated compounds. Silicones could be considered, as well, because their flammability is quite low and the low flash point (e.g., 42C for Syltherm XLT) is offset by extremely poor volatility. However, silicon oils are famous for their property to badly pollute the workplace in case of unintended spill. This is the main reason that prohibits their use in large-scale systems. The aggregate heat transfer performance of silicone oils at low temperatures is not better that that of PFCs (see Section…), while the pumpability is by order of magnitude worse.

Thus, we are left with a handful of fluorinated heat transfer liquids suitable for operation at -50C. At first look, they are quite similar, all having zero ODP and being much heavier than water, stable, inert, very fluid and volatile. They all have rather poor heat transfer properties and do not differ much from each other in that respect (see Section …). The first and main difference between them is in their GWP:

- PFC: C6F14 and heavier linear or branched perfluoroalcanes (from 3M Company, F2 Chemicals, several other minor suppliers) are potent greenhouse gases with GWP of 8000…9300 (very bad);
- HFE: segregated HFE fluids produced exclusively by 3M Company as Novec 7000-series are environmentally safe with GWP from ~50 to ~330 (good);
- FK: C6- (3M Novec 649, Novec 1230) and C7- (3M Novec 774) fluoroketones both have GWP ≈ 1 (excellent).

The huge spread in GWP does not come for free: unlike really inert PFCs, both HFE and FK fluids have minor issues at the chemistry level. In addition, they have lower electrical resistivity compared to PFCs and, arguably, lower radiation resistance. However, these drawbacks are not dramatic and leave freedom for compromises, as will be discussed in the following Sections.

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[7] Commercial HFC (e.g. HFC-134a) and HFO (e.g. HFO-1234yf) fluids massively used in 2-phase A/C systems are gases at normal conditions.

All these fluids are available from the same supplier, 3M Company [3M HTF], and the rest of this memo is based on the 3M documentation (Product Information brochures, MSDSs, articles and reviews) available from open internet sources.

2.3 PFC fluids: C6F14 and C7F16

C6F14 and other PFC fluids are supplied by 3M under the brand name Fluoroinert Electronic Fluids. C6F14 comes as FC-72[8] [3M FC72]. Other Fluoroinerts suitable for SiPM cooling are FC-84 (C7F16 and isomers, [3M FC84]) and FC-770 [3M FC770]. We shall consider only FC-84 as an alternative to C6F14 in this class, as no sufficient amount of technical data is available for FC-770. PFC liquids, as a class, have extremely high electrical resistivity, ~10^{15} Ohm·cm – better than air and comparable with FR4 (<$3.3 \cdot 10^{14}$ and ~$10^{14} \ldots 10^{15}$ Ohm·cm, respectively).

2.4 Hydrofluoroether fluids

Segregated hydrofluoroethers (HFEs), supplied by the 3M Company [3M HTF] as Novec 7000-series fluids, have an excellent blend of thermal transport, safety, and environmental properties that make them good candidates for a secondary heat transfer system. They share many of the valuable performance properties of PFCs and are positioned by 3M as sustainable alternatives to PFCs, with much lower GWPs. Concise reviews of these fluids can be found in Refs [Tuma 2001] and [Tuma 2009].

For practical purposes relevant to heat transfer, Novec HFE fluids differ from Fluorinert fluids in their chemical structure, hydrocarbon solubility and electrical properties [3M FAQ]. Unlike PFC, the HFE molecules contain one oxygen and a few hydrogen atoms. In segregated HFEs, patented by the 3M, the perfluorinated portion of the molecule is “segregated” from a fully hydrogenated portion by oxigen atom (an ether linkage). The presence of hydrogen in the molecule makes this compound susceptible to OH radicals that break it in the troposphere, which predetermines their short atmospheric lifetime and the lower GWP. It also makes the molecule a good solvent for hydrogenated materials, in particular – for HC-based pasticizers in elastomers. Like PFCs, the HFE fluids can also dissolve other fluorochemicals, while featuring a good compatibility with metals, hard plastics and unplasticized elastomers.

Novec HFEs are good dielectrics but their resistivity (10^8-10^9 Ohm·cm) may fall short in some HV applications with direct cooling, where PFCs would be eligible.

Finally, Novec HFEs are very stable, do not hydrolize, have no flash point and are non-toxic. No open information about radiation resistance of HFE is available.

We shall consider two Novec HFE liquids suitable for the operating temperature range between -100C and 50C: Novec 7100 [3M 7100] and Novec 7200 [3M 7200], having GWPs of ~300 and ~60 and boiling points of ……respectively.

2.5 Fluoroketone fluids

C6-fluoroketone (C6K) fluid 3M Novec 649, featuring a record low GWP=1 and the thermo-physical properties quite similar to C6F14, had been tentatively selected as the baseline solution for the SiPM cooling in SciFi. One known issue with this fluid is its weak reactivity with liquid water (i.e., a separate water phase): it hydrolizes producing an organic acid (PFPA). This is not the immediate issue for the intended application because of the sub-zero working temperature, the

[8] It is also available as one of 3M Performance Fluids, the PF-5060; CERN purchases PF-5060, which is, essentially, identical to FC-72.

presence of moisture and acids filters and the use of corrosion-resistant materials (e.g. SS or titanium alloy) for tubing and cooling structures in the future system. The system design will also aim at avoiding water condensation or frost deposition on the inner and outer surfaces of the cooling system, thereby reducing the risks of direct contact with moisture in case of minor leaks. These risks are further reduced by a very high volatility of the C6K at above 0C. An in-depth study of C6K (as 3M Novec 649) at CERN is foreseen [CERN WP2015].

As a fire-suppressing agent 3M Novec 1230, C6K was present on the market long before joining the HFT category. The vast available literature about C6K is reviewed in Ref [PG 2014 C6K]. As a HTF, C6K is primarily recommended for immersion cooling (pool boiling) applications, because of its relatively low normal boiling point (49C). In about 2012, 3M introduced another FK fluid, Novec 774 [3M C7K], which is a mix of isomers with 7 carbons (C7K). It features a higher boilng point, 74C[9], and, otherwise, is quite similar to C6K (in particular, has GWP≈1). FKs are very good dielectrics (~10^{12} Ohm·cm).

Unfortunately, there is no published data about their radiation resistance. The low GWP is due to a photolysis at a near UV (with the absorption peak at 307 nm). The relatively weak O=C bond might cause a reduced resistance to ionizing radiation [Taborelli 2014], which, if confirmed, will limit the use of FKs to low-dose detector cooling applications.

3. Comparison of selected coolants

3.1 Heat transfer properties

3.2 Material compatibility

3.2 The summary

4. Conclusion

References

[Ivy2012] D.J.Ivy et al., Global emission estimates and radiative impact of C4F10, C5F12, C6F14, C7F16 and C8F18, Atmos. Chem. Phys., 12, 7635–7645, 2012,

[Verlaat 2012] e.g., B. Verlaat, Evaporative CO2 cooling for thermal control of scientific equipments, at SLAC Advanced Instrumentation Seminars March 2012, https://www-group.slac.stanford.edu/ais/publicDocs/presentation152.pdf , and other B. Verlaat's publications on CO2 cooling

[Tuma 2001] Ph. Tuma and L. Tousignant, Reducing Emissions of PFC Heat Transfer Fluids, at SEMCON West, July 2001, http://multimedia.3m.com/mws/media/122381O/reducing-emissions-of-pfc-heat-transfer-fluids.pdf?fn=tech_pfc.pdf

[T&K 2003] Tuma, P.E. and Knoll, S., "A comparison of fluorinated and DI/glycol heat transfer fluids", Solid State Technology, 9 May 2003

[9] The boiling point values are reflected in the trade names of the 3M FK fluids. The prefix "6" or "7" stands for the number of carbons in the molecule.

[Tuma 2009] Ph. Tuma, D. Hesselroth, Th. Brodbeck, Next-generation dielectric heat transfer fluids for cooling military electronics, Military Enbedded Systems, July 2009

[Taborelli 2014] M. Taborelli, CERN TE-VSC-SCC, private communication, December 2014

[Cengel 2007] Y.A. Çengel, Heat and Mass Transfer: a practical approach, McGraw-Hill, 2007. Ch. 15: Electronics Cooling ; Section 15-9: Liquid cooling

[Mohapatra 2006] S.Mohapatra, An Overview of Liquid Coolants for Electronics Cooling, Electronics Cooling Magasin, May 2006

[Battistin 2010] M. Battistin et al. Technical Specification for the Supply of Perfluorocarbon fluids C3F8 and C6F14 for ATLAS, CMS and LHCb cooling system, EN-CV, 2010, EDMS 10595563

[Battistin 2006] BM.Battistin, S.Ilie, R.Setnescu, B. Teissandier "Chemical and radiolytical characterization of some perfluorocarbon fluids used as coolants for LHC experiments", TS-Note-2006-010, EDMS 804849

[Julabo Fluids] JULABO Catalog, Julabo Thermal Bath Fluids, Thermal HY fluid (MSDS) = Bayer Baysilone M3 fluid

[PG 2014 Novec649] P. Gorbounov, 3M Novec 649 as a replacement of C_6F_{14} in liquid coolingsystems, https://twiki.cern.ch/twiki/pub/LHCb/C6K/NOvec_Memo_2.pdf and EDMS 1421023 , Internal PH-LBO Memo , October 2014

[PG 2014 irrad] P.Gorbounov, Assessment of the radiation damage to the coolant in SciFi tracker, https://twiki.cern.ch/twiki/pub/LHCb/C6K/Memo_on_irradiation_damage_for_C6K.pdf and EDMS 1421023.

[3M HTF] 3M Thermal Management Fluids, Brochure 2009, Brochure 2008

[3M C7K] 3M Novec 774 Engineering Fluid, 3M Product Information, 3M Safety data sheet, 2014

[3M FC84] Fluoroinert Electronic Liquid FC-84, Product Information, Safety data sheet, 2000

[PAO]

Fully saturated perfluorocarbon (PFC) liquids have been traditionally used as refrigerants and coolants [1]. Despite their relatively low thermal conductivity compared to water and common heat transfer fluids (HTFs), they possess other properties that make them very useful for electronics and detector cooling: a wide range of boiling points, high densities, low viscosities, low pour points, low surface tension, high thermal and chemical stability, non-flammability and perfect dielectricity. They evaporate cleanly and are practically non-toxic. To notable representatives of that class of fluids used at CERN are C3F8 and C6F14, the first - as the primary refrigerant in 2-phace systems, the second – as the secondary HTF in monophase systems.

The biggest trouble with PFC liquids, however, is their very high Global Warming Potentials (GWPs)[10]: 5,000 to 10,000 times that of CO2. 1 liter of C6F14 released into the environment[11] is equivalent to emission of >13 tons of CO2. The CERN management begins to care about it and, therefore, the new developments at CERN are encouraged the use of more environmentally friendly cooling methods and materials, for example, CO2 cooling based on 2PACL cycle [2] and monophase cooling with synthetic low-GWP liquids.

The utility of hydrocarbon alternatives to PFC, like Polyalphaolefines (PAO), is limited by their flammability and high viscosity at low temperature. Silicone oils are flammable and, most nastily, do not evaporate when spilled and contaminate the cooled area. HFCs, despite their wide-spread use as refrigerants, are super-greenhouse gases. An additional limitation for HCs and HFCs is specific for CERN applications. The high content of hydrogen renders the coolant less resistant to radiation, especially to neutrons. This limitation is critical for 2-phase cooling applications in high-dose environments, where the acids produced as the result of radiolysis can cause deterioration of fine cooling structures. Monophase cooling systems with proper filtering and in mild radiation environment are by far less sensitive to the radiolysis-induced effects.

Segregated hydrofluoroether (HFE)[12] and fluoroketone (FK) fluids are non-flammable, have low (or zero in FK) hydrogen content and feature orders of magnitude lower GWPs than PFCs. They compare favorably with other classes of coolants for single phase applications, and may be suitable also for evaporative (2-phase) applications. Table 1 shows properties of representative PFC, PAO, FK and segregated HFE fluids.

My memo [] describes the C6K (C6F12O, FK) liquid recently proposed for the SiPM photo-detectors cooling in the future SciFi Tracker of LHCb. C6K had been chosen because of its record low GWP combined with the close similarity, by thermo-physical properties, to C6F14. The extensive validation of this fluid is foreseen [] and will focus on its radiation resistance and suspected reactivity with water. C6F14 remains the backup solution for this application.

In Section 2 some considerations specific for CERN applications are exposed. In Section 3, two HFE fluids, Novec 7100 and Novec 7200 are presented in more detail, as possible alternative backup solutions. In Section 4 the thermal, hydraulic and safety properties of all candidate liquids are compared and discussed.

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[10] The concept of GWP provides a common scale to compare the ability of different gases to trap heat in the atmosphere, relative to carbon dioxide.

[11] It is hard to be contained once released, because of the extreme fluidity and volatility.

[12] The term “segregated” refers to HFEs that possess a PFC segment separated or “segregated” from a fully HC segment by an ether oxygen, like in C4F9-O-CH3 (Novec 7100) and C4F9-O-C2H5 (Novec 7200) discussed in this note.

Table 1 A comparison of properties of representative heat transfer fluids (from [3])

Molecular Formula[1]	C_6F_{14}	R_FOR_H	$R_FC(O)R_F$	$CH_3(CH_2)_nCH_3$
Fluid Type	PFC	HFE	FK	PAO
Tradename	Fluorinert FC-77	Novec 7200	Novec 649	Various
Normal Boiling Point [°C]	100	76	49	>200
Freezing Point [°C]	<-100	<-100	<-100	<-60
Flashpoint [°C]	None	None	None	163
Thermal Conductivity [W/m-K]	0.057	0.063-0.075	0.059	0.136
Liquid Specific Heat [J/kg-K]	1050	1130-1320	1100	2200
Liquid Density [kg/m^3]	1680	1400-1660	1610	785
Kinematic Viscosity, 25°C [cSt]	0.40	0.32-1.1	0.42	8.8
Kinematic Viscosity, -40°C [cSt]	0.90	0.6-2.5	1.3	>300
Vapor Pressure at 25°C [kPa]	30.9	0.96-65	40	<1
Resistivity [Gohm-cm]	1,000,000	0.1	10,000	
Dielectric Constant	1.76	7.4	1.84	2.1
Dielectric Strength [kV@2.54mm]	~40	~40	~40	~40

[1] R_F and R_H refer to fully fluorinated and fully hydrogenated alkyl groups, respectively.

5. Alternatives to PFC fluids for CERN cooling applications

I compiled the following list of somewhat contradictory statements from the internet sources on reducing emissions of PFC HTFs (esp. Refs []) and my recent discussions at CERN with E. Thomas (PH-LBO-DO), M. Battistin (EN-CV-PJ), M.Taborelli (TE-VSC-SCC) and other colleagues:

1. The environment "friendliness" aspect cannot be ignored anymore when projects are discussed at CERN management level. It gradually becomes competitive with physics performance aspects.
2. PFC emissions are closely monitored at CERN.
3. PFC liquid losses can be prevented: "a properly designed cooling system won't leak!"[]. Causes of liquid leaks include inappropriate or damaged connections, inappropriate valves or pumps and others.
4. An often overlooked mechanism is evaporative loss resulting from the normal cooling system operation, e.g. in the expansion tank. An understanding of this mechanism can significantly reduce the losses [F.Tuma].
5. Because of 3) and 4), we can, probably, stay with C6F14 which had been thoroughly validated [M.T.]
6. Real system does loose coolants. Preventive measures, on average, reduce losses by ~20%
7. C6F is bad because it may react with condensation moisture and become corrosive. This contradicts with 3) and also the fact that DI water is routinely used for detector electronics and accelerator magnets cooling.[]
8. The requirements for coolant are contradictory: the "stable" substance is bad for the environment, while the "unstable" will be bad for the detectors. *Conclusion: some sort of compromise should be reached.*

In my opinion, given the size of the SciFi Tracker and expected complexity of manifolding, the inner cooling structures of ROBs and interconnections (especially now that we are drifting to parallel, rather than serial, ROB connections and the 3D-printed cooling bars will be likely split into two halves), it will be difficult to ensure perfect leak-tightness of the SiPM cooling system. Because of 1) and 2) we have to, at least formally, count on and validate the "green" coolant as the baseline, while tacitly keeping the cooling plant compatible with C6F14.

One immediate compromise which I see is to relax the "zero hydrogen" limitation, taking into account a relatively low expected radiation dose at the SiPM level in SCiFi Tracker and the robust monophase nature of the system. In my memo [] I showed that, under very pessimistic assumptions, the radiolysis effect for the C6K coolant will be microscopic, so the dominant radiation damage will be associated with the impurities (O(0.2%) for C6K). Similar arguments can be applied to fluids with a small hydrogen content, in which the radiolysis will not result in formation of HF or other acids containing fluor. Segregated HFE fluids seem to match this category. They do not hydrolize and have just a few hydrogen atoms confined to the segregated HC part of the molecule. Novec 7100 has a molecular weight of 250 and only 3 H atoms per molecule, Novec 7200 – 264 and 5, respectively.

2.2 Materials compatibility of FKs

FKs will often function as drop-in replacements for PFCs and are compatible with all metals, hard plastics, and a variety of inexpensive hydrocarbon elastomers like Ethylene Propylene

(EP) and butyl. All fluorocarbon fluids feature some hydrocarbon solvency, so heavily plasicized elastomeres may shrink or become brittle while relatively pure elastomeric polymers perform well. For this reason, no sweeping statements can be made about the compatibility of FKs with different materials. FKs far are less studied than PFCs in that respect, therefore general recommendations are based on the experience with PFCs [3, 11]:

a) O-rings and seals should be made of elastomers previously used successfully in a PFC systems (i.e. butyl, nitrile, EPDM, silicone, etc.) or hydrocarbon elastomers specifically tested or otherwise known to be low in extractable material. 3M maintains databases of compatible materials and also *provide free testing services* (to be confirmed!)

b) FC fluids, including C6K, are incompatible with fluoroelastomers, because they are similar in composition and have an affinity for each other. Thus, Teflon and Viton should be avoided.

c) Thermoplastic hoses that have been used in PFC systems generally perform well with HFEs. Elastomeric or "rubbery" tubing/hoses should be low in extractable material and, preferably graded as "no-plasticizer" products (examples: ….).

2.3 FK stability

Though FKs hydrolise to form an organic acid when dissolved in liquid water, they are very stable in its absence. FK fluids (like PFCs) are only minimally soluble in water and, due to the big difference in the density and surface tension, are very difficult to mix with it. This limits the potential hazards. Nonetheless, this "FK hydrolysis factor" should be kept in mind, together with the unknown radiation hardness, for cooling applications in HEP. See more in Section 3.

2.4 FK safety and handling

FK fluids are non-flammable and have no flash point. They are nonirritating, have low acute toxicity, and high inhalation exposure guidelines as would be expected for materials used in fire extinguishing applications. Like with PFCs (and unlike PAO and silicon oils), FK fluids evaporate cleanly and quickly if spilled and will not trap grime that must be cleaned from hardware components.

3. C6-fluoroketone (C6K) fluid (3M Novec 1230 and 3M Novec 649)

The rest of this memo is devoted to C6-fluoroketone, or *Perfluoro (2-methyl-3pentan-one, CAS 756-13-8)*, the chemical with the molecular formula $C_2F_5C(O)CF(CF_3)_2$ ($C_6F_{12}O$ for short) and the structure illustrated by Figure 2. It is sold by 3M Corp. as Novec 1230 (since 2003) and Novec 649 (since ??). The Ref. [9] gives links to all relevant 3M documents about these fluids. Ref. [12] contains a very complete compilation of documents related to the environmental and health safety issues. Ref. [10] discusses the aspects of C6K applications as a HTF for 2-phase applications and contains a comprehensive general description of this fluid.

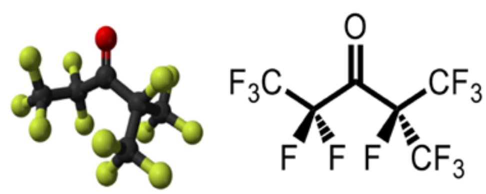

Figure 1 The molecular structure of C6-fluoroketone (from [9e] and [13e]).

Novec 1230 and Novec 649 are different brand names of the *same chemical* (further referred to as C6K), intended for different industrial applications: the 1230 – as a clean fire extinguishing agent, the 649 - as a *thermal management fluid*. According to the MSDSs [14], they have different purity grades (>99% and >99.9%, respectively) and are sold via different channels. The literature on the 1230, mostly focused on the environmental and health safety aspects, is fully applicable to the 649. The 649 is covered mostly with thermal applications in mind, especially for

ORC and "open bath immersion" (or "pool boiling") cooling [10], because of its relatively low normal boiling point (49°C).

Table 2 gives a more detailed overview of C6K (3M Novec 649) properties in comparison with C6F14 (3M Fluorinert FC-72, aka PF-5060 [8]). Apart from a strikingly different GWP, the two fluids have very similar physical properties. In particular, both have relatively low boiling points and very low vaporization heat (25 times lower than that of water), which makes them *extremely volatile* under normal conditions[13]. There is, however, an important difference at the level of chemistry: the reactivity with water that is reportedly much higher with C6K than with pFCs. Further aspect in which C6K might potentially differ is its compatibility with different materials, especially elastomers. Finally, of particular interest for CERN applications is the radiation hardness of the C6K itself and the contaminants present in the commercial fluid.

3.1 Atmospheric chemistry, GWP

The atmospheric chemistry and the environmental fate of C6F have been extensively studied because of the massive application of Novec-1230 as one of "next-generation" alternatives to halon. All relevant publications are assembled in Ref. [13]. Containing no clorine or bromine, C6K, like PFCs, has no effect on the atmospheric ozone (its direct and indirect Ozone Depletion Potential is zero). The striking difference between C6K and PFCs regards the atmospheric lifetime. It is very short for C6K, only 1-2 weeks, because of strong UV absorption at ~307 nm and photolysis in the lower atmosphere. The photolysis results in cleavage of one the *C-C* bonds alpha to the carbonyl group [13c]. The carbonyl group remains intact through the entire C6K decomposition chain till the final incorporation into water and hydrolysation to CF3C(O)OH, CO2 and HF. The degradation products of C6F are short-lived, resulting in negligible GWP. The "indirect" GWP calculated on a mass basis, is comparable with that of CO2, because the release of 1 kg of Novec 1230 fluid to the atmosphere produces 0.56 kg of CO2 [13a].

In contrast to C6K, in PFCs all C-C bonds are strengthened by F atoms and their energies are beyond the solar UV spectrum at lower atmosphere, which makes these fluids potent greenhouse gases.

[13] The ability to evaporate without a residue is regarded as a desirable property in detector cooling applications, even for dielectric liquids. For example, silicon oils, which contaminate the leak area and do not evaporate, are not good.

Table 2 : Comparison of C6K and C6F14 properties (from [7a]).

Molecular Formula	$C_2F_5C(O)CF(CF_3)_2$	C_6F_{14}
Fluid Type	fluoroketone	perfluorocarbon
Abbreviation	C6K	-
Normal Boiling Point [°C]	49	56
Critical Temperature [°C]	169	178
Critical Pressure [MPa]	1.87	1.83
Freezing Point [°C]	<-100	<-100
Closed Cup Flashpoint [°C]	None	None
Open Cup Flashpoint [°C]	None	None
Surface Tension [dynes/cm]	11.4	12.0
Thermal Conductivity [W/m-K]	0.059	0.057
Liquid Specific Heat [J/kg-K]	1103	1050
Liquid Density [kg/m^3]	1610	1680
Kinematic Viscosity [cSt]	0.42	0.40
Latent Heat [kJ/kg]	88	88
Vapor Pressure at 25ºC [kPa]	40.4	30.9
Vapor Pressure at 100ºC [kPa]	441	350
Resistivity [Gohm-cm]	10,000	1,000,000
Dielectric Constant	1.84	1.76
Dielectric Strength [kV@2.54mm]	~40	~40
Solub. H_2O in Fluid [ppmw]	21	10
Atmospheric Lifetime [year]	0.014	3200
Global Warming Potential[1]	1	9300
Ozone Depletion Potential	0	0

[1)] For 100 years integrated time horizon.

3.3 Hydraulic and Cooling properties, cavitation

The thermo-physical properties of C6K and C6F14 are quite similar. Fig. 3 shows the comparison of kinematic viscosity, density, heat capacity and thermal conductivity as function of temperature. Both fluids have very small heat conductivity and though it gets higher at low temperatures, they remain rather "insulators" than heat conductors. Below -10°C, C6K has a bit better characteristics as a coolant than C6F14: a lower viscosity, a higher and more stable specific heat, a higher thermal conductivity. This means that with C6K one can expect smaller temperature drops along and across the cooling pipe and the turbulent flow regime will be achieved at smaller fluid velocities than with C6F14.

Both fluids are heavy and have high vapour pressure. An addition, their fluid/vapour density ratio is two to three orders of magnitude smaller than that of water. These factors favour erosion and cavitation [14] in the pipes, so the cooling system design should aim at lower fluid velocities and lower overall flow rate (mind the pumps!). A very high thermal expansion coefficient of these fluids (~1%/10K) must also be taken into account.

In summary, as a coolant, C6K seem to be a good drop-in replacement candidate for C6F14.

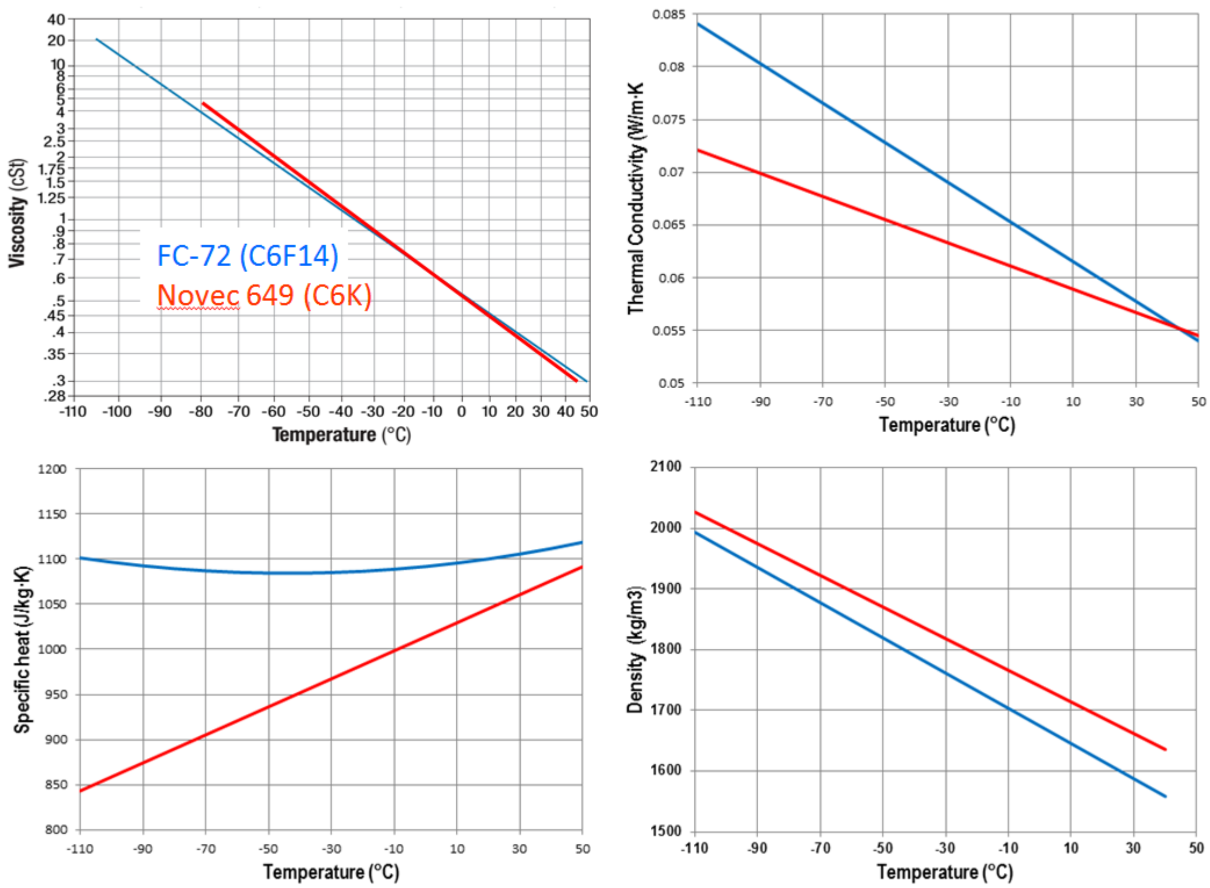

Figure 2 A comparison of some thermo-physical properties of C6K and C6F14 (from [8a] and [9c]).

3.4 Expected radiation resistance

The presence of weaker bonds in C6K molecules might imply its lower radiation resistance than with C6F14 [15], because the release of energy following the excitation by ionizing radiation will easier break the weak bonds[14]. A direct comparison of the two compounds in dedicated irradiation tests is required before considering C6K as a global replacement for C6F14. However, simple estimates [ ] for C6K as the coolant in the SciFi Tracker suggest that the radiation damage will be negligible in this application.

As to formation of long-lived isotopes by neutron radiation, there are no a priori reasons to expect a difference between C6K and C6F14.

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[14] A comparison with PEEK, the solid ketone known to be radiation hard, is not legitimate [15].

3.5 Reactivity with water

Fluorinated ketones (e.g. hexafluoroacetone) are known to hydrolyze quite vigorously. Although C6K does not exhibit this highly exothermic reaction with water, it has been found to undergo hydrolysis [13c]. It reacts with water to form heptafluoropropane (HFC-227ea) and pentafluoropropionic acid (PFPA). This fact was used by 3M opponents to criticize the Novec 1230-based fire suppression systems [9b, 16]. According to 3M [9b],

> *"Novec 1230 fluid reacts with water only when dissolved in water and it is only minimally soluble in water. Accordingly, only a very small amount of acid is formed when Novec 1230 fluid contacts liquid water and no acid is formed when Novec 1230 fluid contacts water vapor. This has been verified through numerous laboratory and full-scale tests in which Novec 1230 fluid was discharged into a humid atmosphere and monitored via methods such as FTIR. No formation of PFPA has been detected."*

Figure 3 The trace of **c**orrosion on the drain valve after running the chiller with C6F14 and C6.

The PFPA is very corrosive to a variety of metals. I can confirm this by my experience with the chiller: the visible trace of corrosion, appeared on the cold nickel-plated brass drain valve after a long period of running with C6F14, rapidly deteriorated when I switched to Novec 649. The valve suffered because it was slightly leaking when opened and the coolant met with liquid condensation water during draining.

The cooling systems used at CERN are closed circulation circuits, equipped with moisture and acid filters. Therefore, under normal running conditions there should be no risk of corrosion. Special procedures for filling and draining should be designed, similar to those applied at Novec 1230 filling stations.

However, the reactivity with water might become the principal objection by the CERN safety and the detector people, because in the case of leaks the coolant may get in contact with condensation moisture and cause the corrosion of the affected area.

3.6 Compatibility with materials

The only information about the compatibility of Novec fluids comes from 3M [16]: "Novec 649 fluid is compatible with a wide range of materials of construction and requires no special piping or handling systems, and is very stable in storage." [9d]. B. Kaiser of 3M also presented the C6K-specific summary shown in Table 3 (it also appeared in [7a]). A very good compatibility with all materials used in power electronics (including copper) can be assumed, following successful applications in immersion cooling [10]. Corrosion testing in presence of O_2 [7a] showed no significant corrosion, as well.

Elastomere compatibility in 6-month tests at 75°C showed good results for EPDM rubber. B.Kaiser [16c] claimed that the best elastomer for C6K is natural rubber, but its low-temperature performance is questionable. IMO, potential materials for flexible hoses with C6K would be ultra-pure plasicizer-free silicone rubber (e.g. Tygon formulations 2075, 2001) or PU rubber (e.g. Tygotan C-555-A, also known to be very radiation-hard and to withstand low-temperatures down to -73°C) [16d].

Table 3 Novec 649 compatibility with materials (from [16c] and [7a]).

Materials Compatibility

Compatibility of "O" Rings with Novec 649

Exposure Time: 1 Week@ 25°C, 100°C

Elastomer Type	Exposure Temperature	Change in Shore A Hardness	% Change in Weight	% Change in Volume
Neoprene	25°C	-1.8	-.06	-1.2
	100°C	-2.2	+2.3	+0.8
Butyl rubber	25°C	-2.7	+0.2	+0.1
	100°C	-4.0	+4.3	+4.2
Fluoroelastomer	25°C	-6.2	+0.7	+0.6
	100°C	-12.6	+9.5	+10.6
EPDM	25°C	-4.7	+0.6	+0.3
	100°C	-5.7	+3.3	+2.4
Silicone	25°C	N/A	+3.1	+2.8
	100°C	-5.4	+6.0	+5.1
Nitrile	25°C	-0.7	-0.3	-0.5
	100°C	+2.5	+4.6	+0.7

3.7 Safety

This topic, especially in application to Novec 1230, had been extensively addressed by the 3M Company [18,19]. Novec 1230 fluid is very low in toxicity, with NOAEL[15] of >10% v/v, and is acceptable for use in occupied areas It has shown a very low potential for irritation to the eyes, skin, and mucous membranes. The acute and repeat dose toxicity of Novec 1230 fluid are also very low. The toxicity of Novec 1230 fluid has been also independently assessed by several competent institutions and consulting firms [19h]. There is general consensus that Novec 1230 Fire Protection Fluid is not only safe for its intended use but provides a large margin of safety relative to anticipated design concentrations of fire protection systems and during the manufacture of those systems [19c]. All this, of course, regards a massive release of C6K in the event of fire. Given the intended applications in close-circuit cooling systems at CERN, only minor release in case of leaks can be anticipated. In any case, the safety arrangements for C6K should be similar to those for C6F14.

Leak detection: C6K is easy to detect (WL for IR measurement is 6.84 um).

3.8 Suppliers, commercial availability

C6K is immediately available from 3M and its dealers, always with the certificate of analysis. Novec 1230 is exclusively shipped to OEMs specializing in fire protection[16], so for CERN applications we are, essentially, limited to Novec 649. The current list price of Novec 649 is 62-66 CHF/kg (from 3M Switzerland, quotation of 22.10.2014). As “CAS 756-13-8”, this compound is available from numerous Chinese suppliers [20a], in quantities from 1 kg to tons (??), with

[15] No-Observed-Adverse-Effect Level.

[16] On 5.11.2014 I received a rectification from B.Kaiser of 3M, quoting the following statement of the European 3M management: "Novec 1230 fluid application can only be restricted to fire protection. *No other application is allowed.* If the test is required for fire protection, than a supply is possible. For the fire fighting installation you have to go to an official OEM. It would make sense to go to one of them also for the test's. For any other application, *we have to decline the supply of this material*. The price is the same as for 3M Novec 649.”

relatively low (≤ 98%) purity. A research-grade "756-13-8" is also available from standard pure chemicals suppliers, but the price can be astronomical (thousands CHF/kg).

3.9 Purification methods and other information from B.Kaiser of 3M

B.K. claimed that molecular sieve (adsorber) types are not good, because the fluid will be in contact with the increasing amount of H2O molecules, which will react with fluoroketone. He said that the *absorber type* filters (sodium sulphate or similar anhydrous stuff) are more appropriate and can be even cheaper[17].

4. Draft plan for testing C6K at CERN

The EN-CV and TE-VSC-SCC groups were involved in the C6F14 validation project at CERN [6c]; their experience is indispensable for this study. At a preliminary discussion with M.Battistin he also suggested to involve R. Setnescu (currently, a PJAS at TE-VSC-SCC).

Mauro and Michele proposed to perform a quick pilot study to make sure that C6K has a *reasonable* radiation resistance. Should it turn out to be incompatible with the doses in excess of 100 Gy, than the scope of this study will be limited to the SciFi application [5]. Otherwise, a new full-blast Detector Cooling project can be launched to qualify the fluid properly; all LHC experiments can be involved in its funding.

After the first brainstorming meeting with TE-VSC-SCC (November 4, 2014), a more detailed plan will be presented. Topics to be discussed:

- Where to irradiate; the amount of fluid required for irradiations, rough cost estimate for the pilot study?
- Containers: make new or re-use the old one?
- Shall we irradiate C6F14 together with C6K, to compare the effects of the same dose?
- Whether to continue attempts to purchase Novec 1230?
- C6K reactivity with water: can it be a show-stopper for applications at CERN?
- Additional aspects to be studied: rectification methods, compatibility with elastomers.
- Rectification of commercial samples at CERN or elsewhere?

The principal study could be quite similar to the one for C6F14: we take a fresh commercial sample (>99% pure C6K + some unknown impurities), irradiate discrete portions with a wide range of doses and watch the fluid for the appearance of undesirable products of the C6K decomposition products, like acids and water. Appropriate purification methods should be proposed.

Mauro remarked that the price for such an irradiation test in an external firm would be the same for one of more samples if we can irradiate them in the same run. Therefore, it would be

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[17] I think that zeolite adsorbents should work with Novec, as well: the pore size is too small for C6K molecules (comparable in size with C6F14) to reach H2O. C6K can be chemically reactive with activated alumina adsorbers, though [7a], to be verified experimentally.

beneficial to irradiate samples of different fluids, including C6F14 (and Novec 1230, should we be able to get it).

One factor that differs C6F from heavy fluorocarbons (apart from GWP) is its reported reactivity with liquid water phase (Section 3.5). Though this factor has a lower importance in the closed-loop applications, especially at below-zero temperatures, water-removal methods should be addressed with particular attention in this study.

The time frame is quite limited: from now through May 2015 we want to get some initial results, at least for low-dose irradiation (relevant for the SciFi application.

References and quoted materials

1. *Uses and Emissions of Liquid PFC Heat Transfer Fluids From the Electronics Sector* EPA-430-R-06-901, http://www.epa.gov/semiconductor-pfc/documents/pfc_heat_tranfer_fluid_emission.pdff and Refs therein
2. *2PACL CO2 cooling*
3. *F. Tuma et al. on PFC emissions:*
   a. Reducing Emissions of PFC Heat Transfer Fluids, at SEMCOM July 2001, http://multimedia.3m.com/mws/mediawebserver?mwsId=66666UgxGCuNyXTtlXfVM8TtEVtQEcuZgVs6EVs6E666666--&fn=tech_pfc.pdf
   b. Next-generation dielectric heat transfer fluids for cooling military electronics, 2009 http://mil-embedded.com/articles/next-generation-fluids-cooling-military-electronics/
4. *Use of PFC coolants at CERN*
   a. Technical Specification for the Supply of Perfluorocarbon fluids C3F8and C6F14 for ATLAS, CMS and LHCb cooling systems, IT-3673/EN, EDMS: 1059563, http://indico.cern.ch/event/91119/material/0/12?contribId=3;
   b. M. Pimenta dos Santos, USE OF FLUOROCARBONS IN THE COOLING OF LHC EXPERIMENTS ST-Note-2003-019, http://cds.cern.ch/record/1140764/files/st-note-2003-019.pdf
   c. F.Lehner, M.Stoulski , "The liquid cooling system of the LHCb Inner Tracker…" http://multimedia.3m.com/mws/media/64892O/fluorinert-electronic-liquid-fc-72.pdf?fn=prodinfo_FC72.pdf; LHCb Inner Tracker TDR, Section 5.7.1 http://lhcb.web.cern.ch/lhcb/TDR/front%20cover/LHCb-IT-TDR.pdf
   d. LHCb RICH, EDMS 781457, https://edms.cern.ch/document/781457/1
   e. CERN is a significant source of PFC emissions: ILK review for PFC (2005) EDMS 634952, M.Battistin (2006) EDMS 774749; E. Thomas (LHCb 2013) EDMS 1311056 (LHCb 2013), All other CERN registers of PFC: EDMS search (greenhouse)
5. *LHCb Tracker Upgrade Technical Design Report* CERN-LHCC-2014-001 ; LHCB-TDR-015 (SciFi tracker = Chapter 3) https://cds.cern.ch/record/1647400/files/LHCB-TDR-015.pdf
6. *PFC fluids for HEP applications*
   a. V. Vacek et al. "Perfluorocarbons and their use in cooling systems for semiconductor particle detectors", https://cds.cern.ch/record/681439/files/indet-2000-025.pdf

b. G. Hallewell et al. "Properties of saturated fluorocarbons: Experimental data and … ", http://phdtree.org/pdf/33128674-properties-of-saturated-fluorocarbons-experimental-data-and-modeling-using-perturbed-chain-saft/
c. M.Battistin, S.Ilie, R.Setnescu, B. Teissandier "Chemical and radiolytical characterization of some perfluorocarbon fluids used as coolants for LHC experiments", TS-Note-2006-010, EDMS 804849 https://edms.cern.ch/file/804849/1/TS-Note-2006-010.pdf

7. *Fluoroketones, C6K general properties*
   a. P.E. Tuma, Fluoroketone C2F5C(O)CF(CF3)2 as a Heat Transfer Fluid for Passive and Pumped 2-Phase Applications, 24th SEMI-THERM Symposium, 2008 http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=04509386
   b. E. Forrest et al. Pool Boiling Performance of Novec 649 Engineered Fluid, ECI International Conference on Boiling Heat Transfer, 2009 http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/40/079/40079220.pdf
   c. C7K = Novec 774 http://www.gpo.gov/fdsys/pkg/FR-2012-08-10/html/2012-19688.htm; 3M Product Information
   d. NIST REFPROP Version 9.1 includes Novec 649. http://www.nist.gov/srd/nist23.cfm
   e. J. Gustavsson, C. Segal , "Characterization of a Perfluorinated Ketone" for LIF Applications, 46^{th} AIAA Aerospace Sciences Meeting, 2008, http://plaza.ufl.edu/jgu/public_html/UF/AIAA-2008-259-527FKchar.pdf

8. *Perfluorohexane C6F14*
   a. 3M Fluoroinert Electronic Liquid FC-72, Product information http://multimedia.3m.com/mws/media/64892O/fluorinert-electronic-liquid-fc-72.pdf?fn=prodinfo_FC72.pdf
   b. 3M Fluoroinert Performance Fluid PF-5060, Product information, http://multimedia.3m.com/mws/media/244056O/performance-fluid-pf-5060-product-information.pdf?fn=prodinfo_pf5060.pdf
   a. CERN EN-CV, Detector Cooling Section, Fluids data: http://detector-cooling.web.cern.ch/detector-cooling/fluidmaterial.html
   b. Molecular structure (3D): http://commons.wikimedia.org/wiki/File:Perfluorohexane_3D_ball.png

9. *C6K, general*
   a. **3M Novec 1230 fire protection fluid:** http://solutions.3m.com/wps/portal/3M/en_US/3MNovec/Home/ProductCatalog/?PC_Z7_RJH9U5230OOA50IEKHCMDN11H0000000_nid=D7B0VRPJHSbeJ7332M26RCgl and all Refs. therein, in particular
   b. Product Bulletin "**What you need to know about "Novec 1230**…" http://multimedia.3m.com/mws/mediawebserver?mwsId=66666UgxGCuNyXTtMxT_nXTVEVtQEcuZgVs6EVs6E666666--&fn=5050ECAROComparison.pdf
   c. **3M Novec 649 Engineering fluid:** http://solutions.3m.com/wps/portal/3M/en_US/3MNovec/Home/ProductCatalog/?PC_Z7_RJH9U5230OOA50IEKHCMDN11H0000000_nid=F55Z1XTKWXbeQQBXSJ1LVVgl and Refs therein, in particular
   d. **Novec 649 Product Information:** http://solutions.3mmagyar.hu/3MContentRetrievalAPI/BlobServlet?lmd=1351678101000&locale=hu_HU&assetType=MMM_Image&assetId=1319241050803&blobAttribute=ImageFile
   e. **Novec 1230,** Wikipedia http://en.wikipedia.org/wiki/Novec_1230

10. *C6K: Immersion cooling applications*
    a. P.E. Tuma, US Patent , Publ. # WO 2010123671 A1, http://www.google.nl/patents/WO2010123671A1?cl=en
    b. 3M Novec Data Center Cooling Project https://www.facebook.com/3MNovecdatacentercooling
    c. See [7b]
    d. R. Bharath, Thesis "Viability of…", http://etd.auburn.edu/handle/10415/4203

11. *3M Fluorochemicals in Heat Transfer Applications (Frequently asked questions)*
    NB: in this document only Novec HFE fluids (7000 series) are described !
    http://detector-cooling.web.cern.ch/detector-cooling/data/3M_FAQ_Fluorinert.pdf

12. *A 3M collection of documents on Novec 1230 environmental and health safety, including the GWP study.* http://www.tceq.texas.gov/assets/public/legal/rules/rule_lib/petitions/13028PET_petex.pdf
In particular:
    a. Taniguchi, N. et al. "Atmospheric chemistry of …" *J. of Phys. Chem. A*, 107(15), 2674-2679, 2003.
    b. D. Jackson et al., "Atmospheric degradation of …", Environ. SCi. Technol., 2011, 45(19), 8030-8036
    c. 3M Technical briefs etc

13. *Environmental fate of C6K (PFMP) and its decomposition products.*
    a. 3M Environmental Properties of Novec 1230 Fluid, Technichal Brief (includes a comment on indirect GWP) http://multimedia.3m.com/mws/mediawebserver?mwsId=SSSSSuH8gc7nZxtUmx_UOx21evUqe17zHvTSevTSeSSSSSS--&fn=technvc1230_enviroprop.pdf
    b. See [7a,b]
    c. J. Owens (3M Performance Materials, ~2003) "Understanding the stability and environmental characteristics of a sustainable halon alternative" (very clear and good summary of pre -2003 studies) http://www.nist.gov/el/fire_research/upload/R0301570.pdf and Refs. therein, esp..Ref. 2: J.Owens, "Physical and Environmental Properties of a Next Generation Extinguishing Agent" http://www.nist.gov/el/fire_research/upload/R0201323.pdf (explains the logic behind the C6K choice as a halon replacement)
    d. T.Stein et al. "Atmospheric chemistry of C6K…", J. Phys. Chem A 1999, 103, 5705 http://pubs.acs.org/doi/pdf/10.1021/jp990599t
    e. D. Jackson Thesis "Hydrolysis and Atmospheric …", U. of Toronto, 2013. Chapter 2 = reprint of [7b]: https://tspace.library.utoronto.ca/bitstream/1807/35854/3/Jackson_Derek_A_201306_PhD_thesis.pdf
    f. D'Anna et al. , Environ. Sci. Technol., 39, 8708, 2005, http://pubs.acs.org/doi/full/10.1021/es048088u

14. *Cavitation:*
    a. Fluoroketone: by far higher propensity to cavition than in water: S.Kelly and S.Segal "Simulation of Cryogenics Cavitation" http://enu.kz/repository/2011/AIAA-2011-808.pdf
    b. http://plaza.ufl.edu/jgu/public_html/UF/AIAA-2008-576-232FKcav.pdf
    c. C6F14 speed of sound: ~480 m/s http://web.physics.ryerson.ca/mkolios/publications/strohm-ius11.pdf

15. *C6K radiation resistance*
    a. R. Setnescu, private communication

16. *Novec fluids: Compatibility with Materials. 3M compatibility testing*
    a. See [9d]
    b. 3M Brochure "3M Thermal Management Fluids" http://multimedia.3m.com/mws/mediawe....
    c. Private communication by B. Kaiser (3M Switzerland) TWIKI link
    d. Plasticizer-free silicone Tygon hoses http://www.piedmontplastics.com/media/275605/tygon%20catalog%20t-110r%208-06.pdf)

17. *C6K and water*
    a. See [9b]
    b. Polemics with DuPont expert: https://www.linkedin.com/groups/Please-suggest-which-Gas-suppression-3216235.S.177437534
    c. !!! [19f] test is described http://www.nicnas.gov.au/__data/assets/pdf_file/0011/10361/STD1019FR.pdf

18. *MSDS Documents for C6K*
    a. Novec 649: http://www.mgchemicals.com/downloads/3m/649-msds.pdf
    b. Novec 1230: http://www.remtec.net/docs/msds-novec-1230.pdf
    d.

19. *Novec 1230/649 safety issues*
    a. See [9b], "3M "What you need to know about Novec 1230"
    b. EPA: "Acceptable Exposure Limit (AEL) Memo for Novec 649", … 250 ppm http://docketwrench.sunlightfoundation.com/document/EPA-HQ-OAR-2003-0118-0228

c. 3M Technical Brief: NOvec 1230 Safety Assessment (also in [7]) http://multimedia.3m.com/mws/mediawebserver?mwsId=SSSSSuH8gc7nZxtUmx_UOx2ZevUqe17zHvTSevTSeSSSSSS--&fn=nvc1230_sftyaccssmnt.pdf
d. NOAEL http://www.gielle.it/gielle.pdf
e. Good summary table http://www.sevosystems.com/3Products%20and%20Services/8Novec%201230/Novec.html
f. National Occupational Health and Safety Commission, 3M Novec Fire Protection Fluid 1230 - Full Public Report (STD/1019), 2002 http://www.nicnas.gov.au/__data/assets/pdf_file/0011/10361/STD1019FR.pdf
g. pentafluoropropionic acid: CF_3CF_2C=O-OH (PFPA) http://www.chemspider.com/Chemical-Structure.56147.html
h. Novec 1230 Regulatory and Industry Approvals: http://solutions.3m.com/wps/portal/3M/en_US/3MNovec/Home/ProductCatalog/1230/Regulatory/

20. *C6K suppliers*
   a. LOOKCHEM.COM: http://www.chemicalbook.com/ProdSupplierGWCB2238274_EN.htm; MOLBASE.COM: http://www.molbase.com/en/search.html?search_keyword=756-13-8&gclid=CjwKEAiAj-KiBRC48YzhnLSg0D0SJAClOhK3d4VTo95XX99nkJGtk90DH_rizzAIkP1utpYIj-ViqhoCsILw_wcB&page=4
   b. GIELLE Fire Protection http://www.novec1230systems.info/
   c. AMEREX (DuPont FM-200 and 3M Novec 1230 systems) http://amerex-fire.com/products/clean-agent-system-with-fm200-or-3m-novec-1230/
   d. Synthesis of FKs http://www.organic-chemistry.org/synthesis/C1F/fluorocarbonylcompounds.shtm

21. Irradiation at CERN:
   a. GIF: https://gif-irrad.web.cern.ch/gif-irrad/; GIFF++ facility is expected to be fully operational by spring 2015 https://espace.cern.ch/sba-workspace/gifpp/SitePages/Home.aspx
   a. Neutron irradiation (IRRAD-2 facility): http://testing-irradiation.web.cern.ch/testing-irradiation/irrad2.htm; CERN irradiation facility: http://ph-news.web.cern.ch/content/new-proton-mixed-field-irradiation-facility-cern-ps-1