

EP-DT Detector Technologies

### Towards more eco-friendly gaseous detectors

### Beatrice Mandelli on behalf of CERN EP-DT Gas Team

### CERN

CEA Seminar 28<sup>th</sup> March 2023

# Outline

#### **GHGs for particle detectors**

GHG emissions from particle detection at LHC experimentsEU F-gas regulationGHG studies in ECFA Roadmap and DRD collaboration

### **Strategies for reduction of GHG emissions**

Gas recirculation Gas recuperation Eco-friendly gas mixtures

### Conclusions

# GHGs for particle detection (at LHC experiments)

GHGs are used in several gaseous detectors mainly due to their properties necessary for optimal detector performance and long term operation



- ~ ~20-30 years ago, it was the time to get rid of ODP gases
- There was not the awareness on the use of GHGs
- Many gaseous detectors were conceived with use of GHGs
- Now it is time to address the usage of GHG worldwide, including particle detectors

3

# **GHG emissions at CERN**

Greenhouse gas emissions at CERN arise from the operation of the Laboratory's research facilities. The majority of emissions come from CERN's core experiments and more than 78% are fluorinated gases



The CERN's objective is to reduce its scope emissions by 28% by the end of 2024

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# GHGs for particle detection at LHC: Run 2



- -40% GHG emissions from Run 1 to Run 2 excluding ATLAS and CMS RPC systems
- ATLAS and CMS RPC systems: +35% increase of GHG emissions due to development of new leaks
- All other detector systems: decrease of GHG emissions from -20% to -80% from Run 1 to Run2
  - Thanks to the different gas system upgrades and a major attention on the use of GHGs
- GHG emissions during LS2 reduced by 75% with respect to Run 2

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# The EU HFC Phase down policy

#### **European Union "F-gas regulation"**

- Limiting the total amount of the most important F-gases that can be sold in the EU from 2015 onwards and phasing them down in steps to one-fifth of 2014 sales in 2030.
- **Banning the use** of F-gases in many new types of equipment where less harmful alternatives are widely available.
- **Preventing emissions** of F-gases from existing equipment by requiring checks, proper servicing and recovery of the gases at the end of the equipment's life.



Prices are increasing in EU and availability in the future is not known. Reduction of the use of F-gases is fundamental for future particle detector applications

# The ECFA Roadmap and DRD1 collaboration

#### **Detector Research and Development Themes (DRDT)**

**DRDT 1.1** - Improve time and spatial resolution for gaseous detectors with long-term stability

**DRDT 1.2** - Achieve tracking in gaseous detectors with dE/dx and dN/dx capability in large volumes with very low material budget and different read-out schemes.

**DRDT 1.3** - Develop environmentally friendly gaseous detectors for very large areas with high-rate capability.

**DRTD 1.4** - Achieve high sensitivity in both low and high-pressure TPCs.



These main activity areas correspond to the major drivers from future facilities

DRD1:<br/>Gaseous DetectorsWG1: Technologies<br/>WG2: Applications<br/>WG3: Gas and material studies<br/>WG4: Detector physics, simulation and software tools<br/>WG5: Electronics for gaseous detectors<br/>WG6: Detector production<br/>WG7: Common test facilities<br/>WG8: Training and disseminationWithin the topics, also the<br/>eco-gases searches

# The ECFA roadmap and DRD1 collaboration

	NAGO	J.				
	Mag.		inents.			Rad-hard/longevity
	Contraction of the second	() () () () () () () () () () () () () (	etoe,	/	Muon system	Time resolution
		later in the second	<sup>eutrin</sup> o	¢.	Bronosod technologies	Fine granularity
	The Construction of the Co	Con Second	L'és és 4	the second	RPC, Multi-GEM, resistive GEM,	Gas properties (eco-gas)
d			370 02 02 02 02 02 02 02 02 02 02 02 02 02	Lio Loc	Micromegas, micropixel Micromegas, µRwell, µPIC	Spatial resolution
DRDT	< 2030	2030-2035	2035- 2040 2040-2045	>2045		Rate capability
1.1	•	•••		• • • /		Rad-hard/longevity
1.1	•	•••			Inner/central	Low X <sub>o</sub>
1.3					tracking with PID	IBF (TPC only)
1.3				ě ě ě	Provide the sheet strends	Time resolution
1.1					TPC+(multi-GEM, Micromegas,	Pate capability
1.2		I			Gridpix), drift chambers, cylindrical lavers of MPGD, straw chambers	
1.1						
1.2		2				Fine granularity
1.1					Dreath annan/	Rad-hard/longevity
1.1 1.3					Calorimeters	Low power
1.1					Catorinicters	Gas properties (eco-gas)
1.1					Proposed technologies: BPC, MBPC, Micromegas and	Fast timing
1.3			$\bullet \bullet \bullet$		GEM, µRwell, InGrid (integrated	Fine granularity
1.2		ĕ			readout), Pico-sec, FTM	Rate capability
1.1	•					Large array/integration
1.2	•	I				Rad-hard (photocathode)
1.1		•			Particle ID/TOE	IBF (RICH only)
1.4		2	2		Particle ID/ FOP	Precise timing
1.4	• •	ĕ	ě		Proposed technologies: RICH+MPGD, TRD+MPGD, TOF:	Rate capability
1.4 1.4					MRPC, Picosec, FTM	dE/dx
1.4 1.4			•			Fine granularity
Mus	t happen or main physics	s goals cannot be met	Important to meet se	veral physics goals		Low power
😑 Desi	rable to enhance physics	reach 💦 🔵 R&D need	ds being met			Fine granularity
DRDT 1.1 Improve time and spatial resolution for gaseous detectors with			TPC for rare decays	Large array/volume		
	long-term s	long-term stability				Higher energy resolution
DRDT	1.2 Achieve trac	king in gaseous o	detectors with dE	low to very high pressure)	Lower energy threshold	
	in large volumes with very low material budget and different read-out schemes				$\backslash$	Optical readout
DRDT	1.3 Develop en	Develop environmentally friendly gaseous detectors for very large				Gas pressure stability
areas with high-rate capability			$\mathbf{i}$	Radiopurity		

8

DRDT 1.4 Achieve high sensitivity in both low and high-pressure TPCs

More info here: 10.17181/CERN.XDPL.W2EX

28 Mar 2023

## **CERN strategies for GHG reduction**



## **CERN strategies for GHG reduction**



# Gas systems at the LHC experiments

The gas systems are complex apparatus that have to ensure an extremely high reliability in terms of **stability** and **quality** of the gas mixture delivered to the detectors

#### **20 Gaseous Detector Systems at LHC**

- 10 different types of gaseous detector technologies
- Several gases used
- Ar, CO<sub>2</sub>, CF<sub>4</sub>, C<sub>4</sub>F<sub>10</sub>, iC<sub>4</sub>H<sub>10</sub>, SF<sub>6</sub>, C<sub>2</sub>H<sub>2</sub>F<sub>4</sub>, nC<sub>5</sub>H<sub>12</sub>, H<sub>2</sub>, O<sub>2</sub>, CH<sub>4</sub>, Xe, Ne, N<sub>2</sub>
- More than 20 gas mixtures

#### 28 Gas Systems at LHC

- 300 modules all over CERN
  - 60 PLCs, >10k sensors
  - Hundreds km of pipes
- Huge detector systems
  - Thousands of m<sup>2</sup>, up to 800 m<sup>3</sup>
- Gas recirculation up to 100%

#### If greenhouse gases used: gas recirculation system

#### Thanks to gas recirculation: GHG emission already reduced by >90%!!!

(Without gas recirculation systems, GHG emissions would be 10 times more!)



# **Complexity of gas recirculation systems**

12

#### - Gas recirculation system can be very complex

- Pressure and flow fluctuations, etc
- Gas distribution
- Stability of gas mixture composition
- Creation of impurities
  - They could accumulate in the gas system
  - Their concentration depends on luminosity and recirculation fraction
  - They could affect long-term detector operation
- Compulsory use of cleaning agents
  - Needed to absorb impurities
  - Destabilisation of gas mixture composition





Purifier: destabilisation of gas mixture

# **Recirculation systems for laboratories**

- At CERN 5-10% of emissions are coming from small experiments, testing facilities and laboratories
- In last years, it often more and more difficult to get F-gases
- F-gas prices are also increasing

#### Development of small gas recirculation systems designed for small experiments and laboratories



#### For medium/small experiments and facilities Tens of detectors, hundreds of litres, ~20 kEURO

- Control system and monitoring based on simple PLC
- Possible to have some parameters controlled remotely
- Presence of sensors for pressure, flow, humidity,  $O_2$

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#### For laboratory set-ups Few detectors, Few of litres, ~1 kEURO

- Control system based on RaspBerry PI
- Manual (optional remote) control
- Limited number of electronic sensors and cheap components
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## **CERN strategies for GHG reduction**



# Gas Recuperation systems at LHC experiments

#### Sometimes it is not possible to recirculate 100% of gas mixture due to detector constrains

- Detector air permeability, max recirculation fraction, presence of impurities, etc.
- A fraction of gas has to be renewed
- Some gas is sent to the atmosphere
- This fraction of gas mixture can be sent to a recuperation plant
- The GHG is extracted, stored and re-used
- Challenges: R&D, custom development, operation and recuperated gas quality
- Gas recuperation can also be used to **empty/fill** the detectors during long shutdown periods



#### Advantages:

- further reduction of gas consumption **Disadvantages:**
- higher level of complexity
- dedicated R&D
- gas mixture monitoring

#### Gas recuperation systems for GHGs at CERN:

#### **CF**<sub>4</sub>: CMS Cathode Strip Chambers and LHCb RICH2

- Both systems operational

#### $C_2H_2F_4$ and $SF_6$ : Resistive Plate Chambers (RPC)

- First system will be operational in ~1month
- C<sub>4</sub>F<sub>10</sub>: LHCb RICH1
  - Old system operational new under design

# The CF<sub>4</sub> recuperation system for CMS CSC

#### **CSC Gas System**

- Detector volume ~90 m<sup>3</sup>
- Gas mixture: 50% CO<sub>2</sub>, 40% Ar, **10% CF**<sub>4</sub>
- Gas recirculation: 90%
- Limited by detector permeability to Air
- ~800 l/h at exhaust: -> 80 l/h of CF<sub>4</sub> for recuperation





### **CF**<sub>4</sub> Recuperation System

- Recuperation of CF<sub>4</sub> with warm separation
- 3 phases needed and several parameters affect recuperation efficiency
- Recuperated CF<sub>4</sub> quality to monitor
- CSC detectors operated with recuperated CF<sub>4</sub> during Run 2
  - No change in the CSC performance observed
- Current recuperation efficiency ~65%

# The R134a recuperation system for RPCs

### ATLAS and CMS RPC Gas Systems

- Detector volume ~15 m<sup>3</sup>
- Gas mixture: ~95% C<sub>2</sub>H<sub>2</sub>F<sub>4</sub>, ~5% iC<sub>4</sub>H<sub>10</sub>, 0.3% SF<sub>6</sub>
- Gas recirculation: ~90%
- maximum recirculation validated for RPC detectors
- Fundamental to repair detector leaks
- To have the gas at the exhaust (600-1000 l/h)

#### **RPC** Recuperation System

- Not convenient to recuperate the gas mixture
- Cold separation for R134a
  - Thermodynamic phase transitions
- R134a and *i*C<sub>4</sub>H<sub>10</sub> form an azeotrope
  - A mixture of liquids whose proportions cannot be altered or changed by simple distillation
  - Intramolecular force of same-species is much higher than the reciprocal attraction separation by quasi-static increase of temperature



Slow heating of the liquified azeotrope allows to enrich the liquid of R134a and the vapour of  $iC_4H_{10}$ , obtaining the separation

# The R134a recuperation system for RPCs



## **CERN strategies for GHG reduction**



## **Possible alternatives to GHG gases**

New eco-friendly liquids/gases have been developed for industry as refrigerants and HV insulating medium... not straightforward for detector operation



The new eco-friendly gas mixtures have to fulfil several requirements for their use in LHC Experiments

- Detector performance similar to current ones
- ➡ No change of FEB electronics, HV system, etc
- Long-term operation (to evaluate possible aging issues)
- No flammability or toxicity of the gas mixture

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# Set-ups: laboratory and irradiation facility



#### Laboratory

- Gas mixing unit
  - Gas mixture up to 6 components
- DAQ
  - CAEN Digitizer V1730: resolution 0.24 mV, sampling 500 MS/s
- Gas analysis
  - GC, MS and ISE

### Data analysis

- pulse charge, pulse height, time, etc.
- efficiency, avalanche/streamer ratio, cluster size, time resolution

#### Gamma Irradiation Facility (GIF++)

- Gamma source
  - <sup>137</sup>Cs of 12 TBq —> 662 keV gamma
  - Lead filters to allow attenuation factors (ABS) between 1 and 46000
- Muon Beam
  - 100 GeV and 10<sup>4</sup> muons/spill (core beam size 10 x 10 cm<sup>2</sup>)
- Detectors tested up to to ~ kHz/cm<sup>2</sup>
- Very similar DAQ, gas system and gas analysis of laboratory



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# **Resistive Plate Chamber (RPC) Detectors**

#### **RPC** main features

- Planar geometry, uniform electric field - ~ 5kV/mm
- Ionisation region = multiplication region
  - No drift (good time resolution)
- Induced charge movement read on pick-up strips
- **Resistive electrodes** 
  - ~10<sup>10</sup> Ohm\*cm (High Pressure Laminate)
- Operation in avalanche mode
  - Signal of few pC, good rate capability
- Single, double or multi-gap RPC
- Used at LHC experiments
  - ALICE, ATLAS, CMS as trigger
  - ALICE as TOF system

#### Foremost parameters of an RPC

- Efficiency and efficiency plateau
- Time resolution
- Cluster size
- Avalanche to streamer (> ~16pC) ratio
- Streamer fraction
- Currents flowing through the electrodes



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from the signal:

pulse height,

time

# Addition of He or CO<sub>2</sub> to std gas mix

### 1:1 R134a substitution with HFO doesn't work for 2mm RPC

N.B. As it is today, He cannot be used in CMS and ATLAS

+10% CO<sub>2</sub> -> -200 V

+50% CO<sub>2</sub>: 15%

-500

HV<sub>eff</sub> - w.p. [V]

500

28 Mar 2023

0.4

**Streamer |** 0.2

0.1

0.0

-1000

Necessary to add a gas to lower working point (and GWP!)



- Addition of He or CO2 to lower the working point
- Streamer probability increases with addition of CO<sub>2</sub> -
  - Increase of drift velocity and decrease of attachment coefficient
- With 30% CO<sub>2</sub>, ~1% SF<sub>6</sub> needed to have same streamer probability of standard gas mixture (0.3%)
  - but detector currents increase of ~20% under high irradiation



prob.

st. Ē

Eff.

# HFO as replacement of R134a

### 70% CO<sub>2</sub> needed with HFO to keep same wp of standard gas mixture

- Streamer probability ~15% with both CO<sub>2</sub> gas mixtures
  - Already with 1% of  $SF_6$
  - It seems HFO doesn't contribute so much to streamer
- CO<sub>2</sub>/HFO gas mixture has higher currents and avalanche charge signals

R134A/IC4H10/SF6 95.2/4.5/0.3 CO2/HFO/IC4H10/SF6 69/25/5/1

CO2/R134A/IC4H10/SF6 69/25/5/1

- It seems HFO has a clear effect in detector currents
- Also visible at high gamma rates





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400

# HFO/R134a based gas mixtures with CO<sub>2</sub> or He

#### A small fraction of R134a is kept to lower currents and charge

Streamer probability

Mean avalanche and streamer charge

- To have good working point: CO<sub>2</sub> at 50% and He at 30%
  - Necessary to increase the SF<sub>6</sub> concentration to lower streamer probability
- In CO<sub>2</sub> based gas mixture: higher streamer charge and wp but lower streamer probability
- Higher charge because higher CO<sub>2</sub>
- Lower streamer because higher SF<sub>6</sub>



# Long-term studies with HFO gas mixtures

**RPC** long-term operation with eco-friendly gas mixtures under high background radiation and possible ageing effects must be investigated

#### **Creation of the ECOGAS@GIF++ collaboration:**



a joint effort between CERN Gas Team, ALICE, ATLAS, CMS, LHCb-SHIP RPC communities

- Set-up at CERN Gamma Irradiation Facility (GIF++)
  - 12.2 TBq <sup>137</sup>Cs and H4 SPS beam line
- Several RPCs under test from different experiments
- Detector performance studies
  - At different back-ground radiations
  - For different gas mixtures and for different types of RPCs
- Long-term performance studies
  - Irradiation of RPCs to accumulate an equivalent charge of the HL-LHC Phase
  - Fundamental for the validation of new eco-friendly gas mixtures
- Three gas mixtures under study
  - CO<sub>2</sub> 50-70% + <u>HFO 45-25%</u> with~5% iC<sub>4</sub>H<sub>10</sub> and 1% SF<sub>6</sub>



Muon beam, Source On, 350 Hz/cm2





# Creation of impurities under irradiation



## Alternatives to SF<sub>6</sub>



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# Performance with NOVEC gases

### **NOVEC 5110**

#### PRO



- Very low GWP: <1
- High boiling point: 27 C
- Application in industry Sensitive to UV radiation
- High dielectric strength



- High concentration (~2%) of NOVEC 5110 needed to obtain good streamer suppression
   Suspect that NOVEC 5110 breaks inside RPC
- Higher working point for concentrations > 0.3%
- Avalanche and streamer charge similar of std gas mixture from 0.9%
  - At 0.3% very large avalanche signals



- PRO
  - Good vapour pressure
  - Application in industry
  - High dielectric strength





- GWP of 2200
- It may react with H<sub>2</sub>O



- Streamer probability always lower than std gas mixture
  - 0.1% of NOVEC 4710 already enough!
- Avalanche charge and cluster size lower than std gas mixture
- Higher working point for concentrations > 0.1%

# **Comparison of all tested gases**



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## Not only detector performances....



# **HFO degradation**

Atmospheric lifetime of HFO1234yf is 11 days Atmospheric lifetime of HFO1234ze is 18 days Atmospheric lifetime of R134a is 500 years



Hydrofluoric Acid (HF)

- It has already been measured that HFO produces much more HF than R134a in RPC detectors

#### Trifluoroacetic acid (TFA)

- HFO1234ze is estimated to break down into TFA at less than 10%, whereas R-1234yf will break down into TFA at 100% (R134a at 21%)
- TFA highly soluble: no formation of insoluble salts
- Phytotoxic

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# **NOVEC degradation**



#### **NOVEC 4710**





- Bakelite HPCs use 40% relative humidity
- Production of an amide from NOVEC 4710 + H<sub>2</sub>O
  - Sub-products in the order of ppb
  - Solid at room T with a melting point of 49°C
  - The amide has appreciable vapour pressure at 60°C, it remains in gas phase at low concentrations

#### Tests on-going in laboratory

- Try to reproduce 3M tests
- Analysis at the output of an RPC

# **Possible CF**<sub>4</sub> replacements

**CF**<sub>4</sub> is used in different types of particle detectors to prevent aging, to enhance time resolution or because of its scintillation photon emission

#### CMS CSC studies

- CF<sub>4</sub> is a **source of fluorine** radicals to protect against anode ageing
  - Now 10% CF<sub>4</sub> in CSC gas mixture
- Two possibile approaches to reduce GHG consumption (beyond the recirculation and recuperation systems)
  - Decrease the CF<sub>4</sub> concentration: preliminary results show that 5% could be safe for operation
  - CF<sub>3</sub>I and HFO1234ze not best candidates
  - Look for other alternatives to CF<sub>4</sub> on-going

#### LHCb RICH studies

- RICH detectors use either CF<sub>4</sub> or C<sub>4</sub>F<sub>10</sub>
  - Necessary for good refractive index
- Replacement of C<sub>4</sub>F<sub>10</sub> with C<sub>4</sub>H<sub>10</sub>
  - Refractive index matches very well
  - But C<sub>4</sub>H<sub>10</sub> flammable
- Replacement of CF<sub>4</sub> with CO<sub>2</sub>
  - Under investigation
- Use of SiPM to reduce the chromatic error and increase the yield





# Conclusions

With climate change a growing concern and implementation of F-gas regulations, it is fundamental for existing and future particle detector application to reduce GHG emissions and search for eco-friendly gas mixtures

#### Gas recirculation systems

- Gas recirculation systems are the best way to reduce GHG consumption
- All detector systems using GHGs should work under gas recirculation
- Also small laboratories could be equipped with gas recirculation units

#### Gas recuperation plants

- Used when not possible to recirculate 100% of the gas mixture
- Very complex and different technologies depending on the GHG to recuperate
- Suitable and affordable in medium-big experiments

#### **Alternative gases**

- A lot of work especially in RPC community to search for alternatives to C<sub>2</sub>H<sub>2</sub>F<sub>4</sub>
- Not an easy task to find new eco-friendly gas mixtures for current LHC detectors
- Fundamental for future particle detectors
- Need to understand detector lifetime with new eco-friendly gases
- But often not "so friendly" as described...

# **Back-up slides**

# Minimization of flow/pressure fluctuations

#### Goal: to minimize any chamber pressure/flow fluctuations at the level of ~ 0.1 mbar

- New automated regulation valves on the return of each distribution rack to minimize any pressure changes
- To decrease the risk of developing new leaks at the detector level
- 30 distribution racks for Barrel and Endcap divided into top and bottom
- Different valve seats depending on pressure, flow, etc.
- Installation of reference volumes
  - To have a good reference for the regulation of the detectors pressure
- Addition of gas impedances
  - To smooth pressure and flow fluctuations at the output of distribution system, i.e. pressure and flow seen by the detectors







# Gas recuperation: LHCb RICH2 CF<sub>4</sub>

#### **RICH2 Gas System**

- Detector volume ~100 m<sup>3</sup>
- Gas mixture: 92% CF<sub>4</sub>, 8% CO<sub>2</sub>
- Gas recirculation: ~100%
  - Small quantity lost in leaks or for gas system operation

#### **RICH2** Recuperation System

- Two recuperation modes (warm separation)
  - During long shutdown: emptying detector
  - During Run: recuperation of small quantities otherwise lost in gas modules
- New system implemented in LS2
  - Upgrades on-going

#### Performance

- Recuperation efficiency ~60%
- About 30 m<sup>3</sup> of CF<sub>4</sub> recuperated in LS2
- CF<sub>4</sub> quality satisfactory
- CF<sub>4</sub> recuperated will be re-used for Run 3 operation





# Why it is so difficult to find good GHG alternatives

When looking for alternatives eco-friendly gases, several factors have to be taken into account

Performance

#### Safety

#### Safety first for detector operations

- Gas mixture not flammable
- Gas components cannot have high toxicity levels

#### Performance

GWP is related to IR absorption over time. Low GWP gases have short atmospheric lifetimes

- Water solubility -> rain out
- OH reactivity -> oxidation
- UV absorbance —> photolysis

RPC short and long term performance are affected

- Good quenching gases required
- Radiation-hard gas required
- Gases cannot heavily react with H<sub>2</sub>O or UV radiation

# Tradeoff between flammability and GWP

- Replacing F with Cl or H: it shortens atmospheric lifetime BUT increase flammability limit
- Adding C=C bound: it increases reaction with O<sub>2</sub>

GWP represents the main environment concern

**Environment** 

Environment

Safety

## Alternatives gases to lower RPC w.p.



# What about other HFCs?



# **NOVEC 5110**



28 Mar 2023

# **NOVEC 4710**



- Good vapour pressure
- Application in industry
- High dielectric strength

#### **CONS**

- **GWP of 2200**
- It may react with H<sub>2</sub>O



- Streamer probability always lower than std gas mixture
  - 0.1% of NOVEC 4710 already enough!
- Avalanche charge and cluster size lower than std gas mixture
- Higher working point for concentrations > 0.1%

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Gas

# HFO-1224yd



- Avalanche charge a bit higher than std gas mixture
- Higher working point for concentrations > 0.3%

## How to measure F<sup>-</sup> production in detectors

#### Ion Selective Electrode (ISE) station

- It measures fluoride ions in aqueous solutions
  - When the F<sup>-</sup> sensing element is in contact with a solution containing fluoride ions, an electrode potential develops
  - The potential depends on the level of free fluorine ions in solution (Nernst equation)
- Gas mixture is bubbled in water+TISAB II solution
  - Bubbling efficiency in trapping the HF



# Alternatives to SF<sub>6</sub>: search in HV industry

(a) 3
0 200 300 T <sub>R</sub> [K] 0 200 500

Dielectric	GWP	Lifetime (year)	<b>Tb</b> ( ° <b>C</b> )
1	23900	3200	-63.8
0.36	0	-	-198
0.3	1	300-1000	-78
0.4	6300	50000	-128
1.2	0.4	6 days	-21.8
1.2	8000	>3000	-
2	1490	30	-4.7
1.5 - 2	1	15 days	27
-	0.88	20 days	15
	Dielectric 1 0.36 0.3 0.4 1.2 1.2 2 1.5 - 2 -	DielectricGWP1239000.3600.310.463001.20.41.28000214901.5 - 21-0.88	Dielectric 1GWPLifetime (year)12390032000.360-0.31300-10000.46300500001.20.46 days1.28000>300021490301.5 - 2115 days-0.8820 days

:

1

:

group	< <i>E</i> r> [rel. SF <sub>6</sub> ]	<7 <sub>B</sub> > [K]	< <i>Z</i> >	n	
C <sub>3</sub> -Ketones	0.39	319	2.00	17	
C <sub>3</sub> -Aldehydes	0.56	320	1.89	18	
C <sub>3</sub> -Acyl Fluorides	0.98	293	3.15	13	
C₄-Ketones	0.69	352	2.58	138	
C₄-Aldehydes	0.77	345	2.39	117	
C₄-Acyl Fluorides	1.14	326	3.36	110	
C₅-Ketones	0.94	375	3.30	923	
C₅-Aldehydes	1.00	370	2.91	685	
C₅-Acyl Fluorides	1.35	356	3.85	590	
SF <sub>6</sub>	1	209 [18]	6	1	

Nr	SMILES	Er	T <sub>B</sub>	T <sub>B</sub> ∟
	$C_3$ -compounds			
(1) (2) (3) (4)	FC(=0)C(C(F)(F)F)(F)F O=C(C(F)(F)F)C(F)(F)F FC(C(C(=0)F)(F)F)F FC(=0)CC(F)(F)F	1.34 1.03 1.11 1.31	255 262 263 278	280 280 288 302
	C <sub>4</sub> -compounds			
(5) (6) (7)	FC(=0)C(C(C(F)(F)F)F)(F)F FC(C(C(F)(F)F)(C(=0)F)F)F FCC(C(F)(F)F)(C(=0)F)F	1.63 1.82 1.91	270 277 295	317
	$C_5$ -compounds			
(8) (9) (10) (11)	FC(=0)C(C(F)(F)F)(C(F)(F)F)C(F)(F)F $O=C(C(C(F)(F)F)(C(F)(F)F)F)C(F)(F)F$ $FC(C(C(C(F)(F)F)(F)F)(C(=0)F)F)F$ $O=C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)C(F)(F)F$ $FC(=0)C(C(C(F)(F)F)F)(F)F)C(F)F)F$	2.77 1.93 2.28 2.01	283 293 296 302	303 310 322

M. Rabie, C. Franck, predicting the electric strenght of proposed sf6 replacement gases by means of density functional theory

1