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Definition and optimization of a MELCOR model of the IFMIF-DONES Argon Purification Subsystem

A. Manjavacas [a,1,*], M.A. Vázquez-Barroso [a,1], C. Torregrosa-Martín [b], J. Maestre [b], F. Martín-Fuertes [c]

[a] University of Granada, Gran Vía de Colón 48, Granada, 18010, Spain
[b] IFMIF-DONES España, Gran Vía de Colón, 48, Granada, 18010, Spain
[c] Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT), Av. Complutense 40, Madrid, 28040, Spain

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ABSTRACT

IFMIF-DONES will be an experimental facility designed to irradiate material samples under conditions similar to those expected in future fusion power reactors. As a radiological facility, it requires the precise design of specific safety subsystems to ensure the protection of the public, the plant personnel and the environment. This is the case of the Argon Purification Subsystem (ArPS), which is responsible for ensuring the inertization of those rooms where liquid Li may be present, involving a risk of fire and hazardous releases. In this context, it is important to set Ar purity requirements as design input for the ArPS to ensure this inertization while being technically sound due to the large amounts of volumes involved. To support this design process, a MELCOR simulation model of the IFMIF-DONES ArPS has been developed. Using this model, we perform a parametric study to analyse the performance of this subsystem under different configurations. The goal is to keep the impurity concentrations of the inert rooms stable during a year of operation in order to minimize the risk of Li reactions, while ensuring dynamic confinement and reducing Ar consumption. In addition, the transition between maintenance and operation modes is considered, analysing the effect of different transition periods and injected Ar inventory.

1. Introduction

From the early 1990s, the fusion materials scientific community have promoted the development of a neutron source for the qualification of materials to be used in future fusion power reactors, such as the DEMOnstration power plant (DEMO) [1,2]. This research was planned to be feasible in an irradiation facility with material samples being exposed to fusion-like radiation conditions [3,4].

The International Fusion Materials Irradiation Facility-DEMO Oriented Neutron Source (IFMIF-DONES) [2] is an initial step aimed to provide relevant data for the early engineering design of DEMO [4,5]. The facility will operate a 5 MW continuous wave deuteron linear accelerator producing neutrons via deuteron-lithium target interaction, aiming at reaching a maximum dose of 20 dpa in the material specimens within its initial operation phase.

As a radiological facility, the IFMIF-DONES design must ensure the safety of the public, its personnel and environment [6,7]. On this basis, a description of the IFMIF-DONES safety functions was provided in [8], following the defense-in-depth principles, identifying reference accident scenarios, and defining barriers of protection by a prevention-detection-mitigation approach.

Several potential accidents are directly associated with the presence of a liquid Li loop in the facility. This loop supplies liquid Li under optimal conditions to the target, where the high-power beam interacts with the Li. Within the target, the speed of the Li reaches approximately 15 m/s to efficiently dissipate the energy deposited by the beam, which is subsequently removed by a heat removal system [9]. To ensure its operation under safe conditions, all the Li piping and inventory are kept in close and leak-tight rooms, filled with Ar in continuous purification.

In addition to the inertization, dynamic confinement is applied as an inherent safety measure in the IFMIF-DONES facility. This consists of keeping those areas with potential radionuclide sources under negative gauge pressure with respect to their surrounding rooms. Among the rooms that must comply these two requirements — inertization and dynamic confinement — we distinguish the so-called Lithium Loop Cell

* Corresponding author.
E-mail addresses: manjavacas@ugr.es (A. Manjavacas), manvazbar@ugr.es (M.A. Vázquez-Barroso), cltorregrosa@ifmif-dones.es (C. Torregrosa-Martín), jorge.maestre@ifmif-dones.es (J. Maestre), francisco.martin-fuertes@ciemat.es (F. Martín-Fuertes).
[1] Contributed equally to this work.

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(LLC), Hot and Cold Trap Cells (HTC, CTC), and Target Interface Room (TIR). To do so, they are filled with Ar and kept under negative gauge pressures.

For the implementation of dynamic confinement, the standards ISO 17873 [10] and ISO 10648-2 [11] have been adopted. While ISO 17873 has been used for the selection of negative gauge pressures of the rooms, ISO 10648–2 is taken as a reference for leak-tightness requirements. In addition, the Ar Purification Subsystem (ArPS) is responsible for the close-loop re-circulation and purification of Ar within the inert rooms, keeping negative dynamic confinement pressures in conjunction with the Argon Supply Subsystem (ArSS).

In this paper, we focus on the parameters influencing the IFMIF-DONES ArPS performance. Factors such as rejected and injected Ar volumes, permissible leak rates, limiting impurity concentrations reached in steady state, or proper pressure levels are some of the main aspects involved. We also consider the transition process between maintenance and operation conditions, when the re-inertization of the served rooms takes place. The goal is to perform a parametric study of these uncertain parameters by studying their influence on the system outputs. We seek to evaluate which design parameters guarantee safe inertization conditions while reducing the associated purification loop complexity. For doing so, we use the MELCOR code [12,13] performing transient simulations of the mass balances in the inert rooms and Ar purification loops for different scenarios.

On this basis, Section 2 provides an overview of the inertization measures adopted in the IFMIF-DONES facility, and the objectives addressed, followed by Section 3 where we introduce the MELCOR model of the ArPS. In Section 4, the methodology adopted in this study will be described, while the analyses and discussion on the results are presented in Section 5. Finally, Section 6 addresses the general conclusions and future work derived from this research.

2. Design considerations of the ArPS

2.1. Ar-filled rooms and operation modes

The IFMIF-DONES main building will feature several rooms with potential presence of liquid Li, which can react with air constituents producing highly exothermic reactions [14,15].

Inertization measures based on Ar-filled room atmospheres and the Li operation temperature ranges (< 300 °C), are expected to be sufficient to prevent Li ignition in the event of Li piping failure and spillage. Inert rooms will be enclosed by steel liners, covering walls, floor and ceiling [8], preventing potential reactions caused by Li in contact with concrete [16–18]. Furthermore, experimental activities are currently being developed to study Li behaviour and ignition conditions [19,20].

The rooms studied in this work are those represented in Fig. 1, which are as follows:

- The *Lithium Loop Cell* (LLC), which houses the main lithium loop, including an electromagnetic pump, heat removal equipment, and a Li dump tank. It houses a free volume of 2635 m^3.
- The *Hot* and *Cold Trap Cells* (HTC, CTC). These cells house the cold and hot hydrogen traps of the Li purification systems. Their free volumes are 532 m^3 and 546 m^3, respectively.
- The *Target Interface Room* (TIR). Includes components of the high-energy accelerator beam transport line upstream of the target. It houses a free volume of 209 m^3.

We also consider the following plant subsystems with which these rooms interface, as represented in Fig. 2:

- The *Argon Purification System* (ArPS), responsible for the removal, purification and re-injection of Ar into the inert rooms.
- The *Argon Supply Subsystem* (ArSS), which stores, distributes and injects Ar into the Ar-served rooms in sufficient quantity, purity and pressure conditions.
- The *Gaseous Radioactive Waste Treatment System* (G-RWTS), which stores and enables the proper release of gases from the facility to the external environment after strict purification processes.

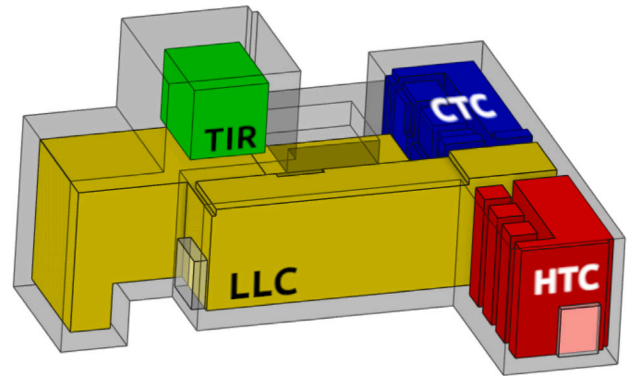

Fig. 1. Layout of the Ar-filled rooms and their physical confinement barriers (in grey).

Table 1
Assumed preliminary VPSA purification efficiencies.

Impurity	Efficiency (%)
N_2	70
O_2	80
H_2O	95

In order to ensure the dynamic confinement of the rooms, they must be maintained at a pressure of about 101065 Pa (−260 Pa relative to atmospheric pressure), according to the recommendations of ISO 17873 for rooms with high contamination and radiation risks (C4 classification [10]). In addition, two atmosphere modes are considered for these rooms: normal operation and maintenance. During normal operation, rooms will remain inertized and perform their expected function. This mode is conceived to be continuously active, provided that there are no exceptional situations or maintenance campaigns that force the interruption of the deuteron beam [2].

For maintenance scenarios, the inert atmospheres will be replaced with air to allow personnel access if necessary. No air-Li reactions are considered a risk during these periods, as Li is not in circulation and remains safely stored in a dump tank. However, the transition between air and Ar atmospheres is expected to be a complex and costly process, due to the large volumes involved and the purification requirements.

2.2. Ar purification requirements

To minimize the risk of Li fires and/or slow reactions, the ArPS must ensure the continuous removal of O_2, N_2 and H_2O from the inert rooms [8]. As in previous analyses, such as [15], this study does not take into account minority reactants — *e.g.* CO_2 —, the presence of which is considered negligible in air and therefore in inert atmospheres. The origin of impurities lies either in infiltrations from adjacent air-filled volumes, or due to the quality of the clean Ar injected. In the current design, the ArPS will be equipped with two Vacuum Pressure Swing Adsorption (VPSA) units ensuring continuous purification. At least one VPSA must be in operation at all times. However, it is also considered the possibility of multiple VPSAs working in parallel.

During ArPS operation, the system is designed for continuously extracting 80 m^3/h from the inert rooms atmospheres and being routed towards the VPSA units. The preliminary purification efficiencies currently considered are those detailed in Table 1. These efficiencies represent the percentage of impurities — *i.e.*, N_2, O_2 and H_2O — removed from the inlet flow by each VPSA unit.

Furthermore, a process to consider in the ArPS design is the transition of the rooms from maintenance to operation mode. In this air-to-Ar

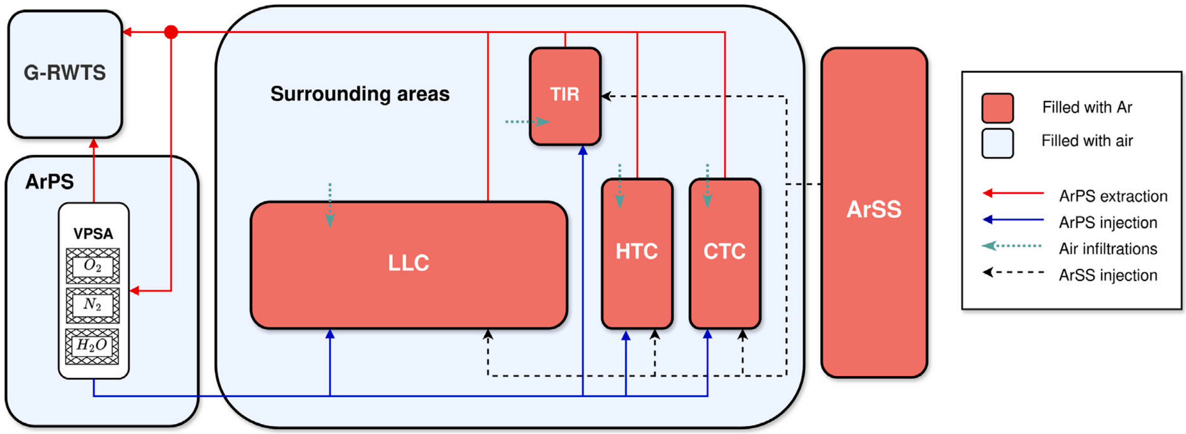

Fig. 2. Connections between the Ar-filled rooms, ArPS, ArSS, G-RWTS and surrounding areas.

Table 2
Maximum considered mass rates per VPSA unit. The water concentration is insufficient to saturate the VPSA units; therefore, no saturation values are included.

Impurity	Saturation rates (kg/h)	
	S_1	S_2
N_2	0.866	1.73
O_2	2.81	5.61
H_2O	*NA*	*NA*

exchange process, the saturation of the VPSAs could take place, thus degrading their purification performance. To account for this, we consider VPSA saturation rates, which represent the maximum mass rate of impurities that they could extract. Two possible saturation ratios are considered, as shown in Table 2, based on the maximum observed ratios of impurities removed in preliminary simulations. These are provisional inputs pending further technical information on the VPSAs performance, and are expected to be redefined in future phases of the project.

Regarding leak-tightness, we consider IFMIF-DONES inertized rooms as containment enclosures, following the terminology and classification provided by ISO 10648-2 [11]. The standard provides a classification of allowable leakage rates for different types of enclosures. These are defined in terms of Hourly Leak Rate (HLR, h^{-1}), which shall be multiplied by the total volume of the enclosure to obtain a volumetric flow of infiltration. In addition, Ar injection must compensate any room pressure variations caused by leaks/infiltrations or exhausts during the purification process, in order to remain within the defined dynamic confinement pressure ranges.

The current design of the facility considers that the ArSS injects clean Ar into the inert rooms whenever necessary. However, it is desirable to minimize these injections to optimize the amount of high purity clean Ar required by the facility operation.

2.3. Objectives of the parametric studies

In this work, we conduct a parametric study to identify the influence of different factors on the performance of the IFMIF-DONES ArPS.

During normal operation, limiting the concentration of air components — primarily O_2, N_2, and H_2O — and maintaining stable pressure levels in the inert rooms are important requirements for the safe operation of the facility. However, these measures compete with the unavoidable costs and complexities associated with maintaining large volumes of high purity Ar inventory.

Given these constraints, we seek to define an optimal and feasible configuration of the ArPS. In particular, we study the differences between an ArPS design that omits the injection of clean Ar into inert rooms, and an alternative setting where clean Ar injection is allowed. We assume an uninterrupted period of normal operation of one year, which begins once a steady state of the system is reached. From this moment on, the Li operations are considered to be operative.

Moreover, we study the maintenance-to-operation transition when a re-inerting process — with complete renewal of the inert rooms atmospheres — is performed. Specifically, we study how the number of days employed in the re-inertization process of the LLC influences this transition, also varying the number of purification units available, and their saturation rates.

Summarizing, we consider the following parameters to determine their effect on the ArPS performance:

- For the study of the ArPS in operation:
  - Ability/inability to inject clean Ar from the ArSS to the inert rooms.
  - HLR values.
  - Number of VPSA units working in parallel.
- For the study of the maintenance-operation transition:
  - Total volume of Ar injected.
  - Transition days invested in the process.
  - VPSA mass saturation rates, defined in Table 2.
  - Number of VPSA units involved in the inertization process.

Our goal is to explore different design alternatives to consequently establish definitive purity requirements. For this reason, we consider the following output metrics to compare the obtained results:

- The maximum amount of impurities reached in operation, and after the maintenance-operation transition period.
- The total volume of Ar invested.

Based on these premises, we proceed to develop a simulation model of the ArPS, being MELCOR the tool used for this purpose.

3. MELCOR model description

3.1. ArPS MELCOR model

MELCOR is an engineering-level computer code developed by Sandia National Laboratories for the U.S. Nuclear Regulatory Commission. Its main objective is the simulation of accident progression in nuclear facilities, enabling the computation of different physical phenomena, such as thermal-hydraulics, aerosol physics or heat transfer

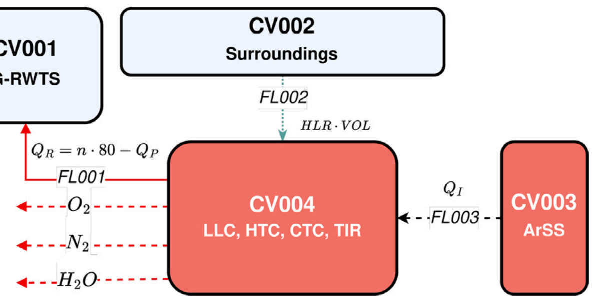

Fig. 3. Diagram of the ArPS MELCOR model. Air-filled volumes are shown in grey. Ar-filled volumes are represented in red. Mass sinks for O_2, N_2 and H_2O are represented as dashed red lines.

equations [12,13]. It has positioned itself as a relevant tool in the nuclear domain, with previous applications in a variety of outstanding projects [21–23]. Furthermore, MELCOR is currently employed in the safety modelling of IFMIF-DONES [8,15,24], which makes it an optimal choice for integration with existing models of different facility subsystems.

During a MELCOR simulation, the calculation of the conservation equations for mass, momentum and energy is performed in a series of discrete time steps. The solution to the linearized hydrodynamic equations used by MELCOR is computed by implicit finite difference methods [12,13]. Each simulation allows the monitoring of several output variables over time, such as volume pressures, temperatures, flow velocities or mass concentrations.

Based on the building blocks offered by MELCOR, a reference simulation model of the IFMIF-DONES ArPS was developed. The input data and design hypotheses considered will be described below. As shown in Fig. 3, we distinguish between four CVs representing:

- The G-RWTS, represented by CV001, being a CV with time-independent properties.
- The surrounding areas, which are represented by CV002. This volume is used as a source of air infiltrations — *i.e.*, impurities — into the Ar-filled volumes, emulating adjacent rooms. Its properties are equally time-independent.
- The ArSS, represented by CV003, is a time-independent CV filled with high purity Ar. It is used to inject clean Ar into the system's rooms, replacing rejected volumes and ensuring that the required pressure is maintained.
- The inert atmosphere rooms, filled with Ar (CV004). These are the LLC, TIR, HTC and CTC, grouped in an equivalent CV. This simplification makes it possible to reduce computation times without losing accuracy in terms of purification, as all the rooms have similar atmospheric compositions and temperatures (see Appendix A).

A control logic is implemented to ensure stable pressures within room atmospheres, as the variable values concerning total volumes over time are a consequence of the mass balance of the system and are pressure-independent.

Regarding the FLs included in the model, two types of connections were represented: leaks and duct connections.

- FL001 extracts a rejected flow rate (Q_R) from CV004 to CV001, emulating the volume extraction to the G-RWTS.
- FL002 introduces air into CV004, emulating leak paths — *e.g.*, wall penetrations, hatches, door gaps — from adjacent volumes at higher pressures, represented by CV002. The introduced volume is equal to the total volume of the CV multiplied by the corresponding HLR.
- FL003 connects CV003 to CV004, allowing the injection of pure Ar from the ArSS into the inert atmosphere rooms. The injection flow rate is represented as Q_I.

The flow rates of these FLs are controlled by control functions (CFs). In the case of FL002, it has a constant imposed flow rate corresponding to the assumed leak rate. Conversely, FL001 and FL003 have a variable flow rate, which depends on the pressure of the inert rooms —whenever the pressure rises, a minimum flow is rejected, and whenever it drops, the minimum amount of Ar required to compensate it is injected. A summary of the properties of the CVs and FLs employed in this model is provided in Appendix A.

Several factors are considered when performing the parametric study. We assume the following boundary conditions in our model:

- The volume and temperature of the rooms under study, extracted from updated project documentation.
- The initial pressures of the rooms, corresponding to their ISO 17873 classification [10].
- The initial atmospheric composition of the rooms, both in operation — Ar (99.5%), O_2 (0.105%), N_2 (0.395%) — and maintenance — Ar (1%), O_2 (21%), N_2 (78%) —.
- Initial relative humidity of 40% at existing air proportion (0.02% in operation, 40% in maintenance).
- A common source volume for infiltrations, with atmospheric air conditions. Even if in the real plant design the studied inert room are surrounded by other underpressurized spaces, our study is based on fixed infiltration rates, allowing their simplification into a common external air source.
- The purity (99.95% Ar, 0.05% air, and relative humidity of 0.02%), temperature and pressure of the injected Ar by the ArSS.
- The flow rate extracted from the rooms by the ArPS. A total flow rate of 80 m/h per VPSA is considered, according to the current system design.
- Purification efficiencies assumed for a flow rate of 80 m/h, as described in Table 1.
- A fixed HLR during the maintenance-operation transition.

3.2. Argon purification simulation

To simulate the operation of the ArPS, we distinguish between rejected and purified flows. A total flow rate of 80 m^3/h is extracted by each of the n VPSA units. As shown in Fig. 3, Q_R represents the rejected flow to the G-RWTS, while Q_P represents the remaining flow ($n \cdot 80 - Q_R$) that is purified and returned to the system.

MELCOR allows the definition of explicit sources and sinks — *i.e.*, negative sources — of mass and/or energy. Each CV mass source/sink is associated with a specific material introduced or removed from the volume according to a specific rate (kg/s). MELCOR does not specify concentration distributions within CVs, assuming homogenization of all elements. Thus, it is possible to model the extraction of impurities with mass sinks instead of using additional FLs and CVs.

The modelling of this extraction can be summarized as follows:

1. Based on the efficiencies of the VPSAs, we calculate the amount of impurities to be removed per m^3 of room atmosphere. MELCOR assumes that these atmospheres are homogeneous.
2. We scale the amount of impurities to the volume to be purified at each time step (Q_P).
3. The sinks remove directly from CV004 the mass of impurities corresponding to the calculated volume. We consider a separate sink for each impurity (O_2, N_2, H_2O).

Table 3
List of variables and abbreviations in the model.

Variable	Units	Abbreviation
Rejected/injected/purified Ar flow	m^3/h	Q_R, Q_I, Q_P
Hourly leak rate	h^{-1}	HLR
Final impurity concentrations	% (vol.)	$C_f^{O_2}$, $C_f^{N_2}$, $C_f^{H_2O}$
Initial/final Ar concentration	% (vol.)	C_0^{Ar}, C_f^{Ar}
Injected Ar volume per year	m^3	V_I
Rejected volume per year	m^3	V_R
Initial/current pressure in CV004	Pa	P_0^{CV004}, P^{CV004}

Furthermore, the rejected flow rate Q_R is extracted through FL001 to be treated by the G-RWTS (CV001). If required, this volume is refilled in the rooms atmospheres with pure Ar by the ArSS through FL003.

Finally, the volume removed from the system — including Ar and impurities — is given by the sum of Q_R and the impurities removed from CV004. If this amount results less than the infiltrations from external volumes (FL002), the pressure in the Ar-filled rooms will increase over time due to the unbalanced mass flow.

4. Methodology

In the following subsections, we will describe the simulation scenarios conducted. We first study the ArPS operation with and without Ar injection. Then, the maintenance-operation transition is analysed.

A summary of the variables referred to in the following subsections and their corresponding abbreviations can be found in Table 3.

4.1. Analysis of the ArPS in operation mode

Two different models are considered to find the optimal configuration of the ArPS in operation mode. First, we assume a model where Ar injection is suppressed ($Q_I = 0$) and determine a Q_R value that maintains stable pressures and impurity levels during a full year of operation. We then look at an alternative scenario where the injection of clean Ar from the ArSS is enabled ($Q_I \neq 0$) to evaluate if improvements are achieved over the previous scenario. We thus sought to assess whether the injection of clean Ar is strictly necessary to maintain low impurity concentrations during operation, as it is actually contemplated in the current design of the facility. We also consider the possibility of varying the number of VPSA units and leak rates, assessing its impact on the rooms' pressures and impurity concentrations.

Starting from the initial room conditions described in Appendix A, we conduct a parametric study for each HLR, looking for the configuration that:

- Ensures that the impurity concentrations are below operational safety limits during simulation time.
- Maintains stable pressures in inert atmosphere rooms, such that $P^{CV004} \in \left[P_0^{CV004} \pm 40\right]$ Pa, where oscillations of 40 Pa around 101065 Pa are assumed to provide enough margin to ensure the dynamic confinement conditions.
- Reduces V_R and V_I (when considered), and hence its associated costs.

4.1.1. Scenario without clean Ar injection

In this case, the objective is to test whether pressure increases caused by infiltrations in the inert rooms can be compensated by removing part of the Ar-filled atmosphere without any injection of clean Ar, while maintaining acceptable purity levels. In this way, the volume corresponding to Q_R is not re-injected as clean Ar, but as air purifiable by the VPSAs.

The impurities concentrations and pressures depend exclusively on: (1) the purification achieved by the VPSA units, (2) the rejected Ar flow rate, Q_R, and (3) the assumed leak rates (HLRs).

Table 4
Scenarios suppressing Ar inlet.

Scenario	HLR (h^{-1})	VPSA units
(A1)		1
(A2)	1.0E−04	2
(A3)		3
(A4)		1
(A5)	5.0E−04	2
(A6)		3
(A7)		1
(A8)	5.0E−03	2
(A9)		3

To keep the pressure of the inertized rooms stable, the value of Q_R depends on their current pressure, that is:

$$Q_R = \begin{cases} k & \text{if} \quad P^{CV004} \geq P_0^{CV004} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

where $k \in \mathbb{R}^+$. As the rejected volume is calculated by integrating Q_R over the whole year, the total rejected volume (V_R) is independent of the value of k — *i.e.*, V_R remains invariant — and it only has an effect on pressure oscillations. If k increases, then Q_R will be > 0 for a shorter period of time, but resulting in the same integral value of V_R, as it is the volume needed to level the balance of mass flows in CV004 for a full year. At the same time, the exhausted volume should compensate for the pressure rise caused by air infiltrations from the surrounding areas.

The performance of the purifiers is considered independent of the amount of impurities passing through them — *i.e.*, no saturation is assumed —, which makes the system mainly dependant on the leak sizing. In addition, the operation of multiple VPSA units working in parallel is also studied, assuming: $Q_P + Q_R = n \cdot 80$, with n being the number of operative units.

To summarize, tests omitting clean Ar injection were performed using different numbers of VPSA units and HLRs, leading to the scenarios shown in Table 4. Moreover, we consider (A4) as the baseline scenario hereafter, since it assumes an intermediate HLR and only requires the operation of a single VPSA, which corresponds to the current system design.

4.1.2. Scenario with clean Ar injection

In the second scenario, we consider alternating clean Ar injection into the system from the ArSS. Unlike the previous case, the impurity concentrations and pressures also depend on the amount of injected Ar, as there exists a relationship between it and the rejected flow: the bigger Q_R, the bigger the necessary Q_I to compensate for the consequent pressure drop, and vice versa. For this reason, we consider the values of Q_R and Q_I as function of the current pressure in the rooms, such that:

$$Q_R = \begin{cases} k & \text{if} \quad P^{CV004} \geq P_0^{CV004} \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

$$Q_I = \begin{cases} 0 & \text{if} \quad P^{CV004} \geq P_0^{CV004} \\ k & \text{otherwise} \end{cases} \tag{3}$$

where $k \in \mathbb{R}^+$. In contrast to the previous scenario, the rejected volume V_R oscillates depending on the amount of clean Ar injected V_I — *i.e.*, the higher the injected Ar volume, the higher the rejection required —. The different proposed scenarios are summarized in Table 5.

4.2. Analysis of the maintenance-operation transition

We now analyse the behaviour of the LLC when transitioning from maintenance to operation mode in a given period of time, supposing that the rest of the rooms can be independently kept in a steady state.

Table 5
Scenarios considering Ar injection.

Scenario	HLR (h^{-1})	VPSA units
(B1)	1.0E−04	
(B2)	5.0E−04	1
(B3)	5.0E−03	

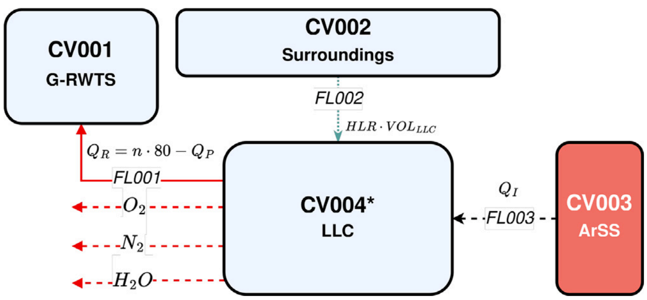

Fig. 4. Diagram of the alternative ArPS MELCOR model for the maintenance-to-operation transition, where CV004* represents the LLC with air atmosphere.

The influence of different parameters is considered, such as the number of VPSA units, their saturation, or the assumed transition days — to be minimized —. We assume that real purification units will not have the same efficiency in atmospheres composed entirely of air as in practically inert ones. Therefore, different saturation of mass rates are assumed for each impurity extraction, as shown in Table 2.

The MELCOR model employed for this experimentation is represented in Fig. 4. In this case, volume CV004* represents the air-filled LLC, as specified in Appendix A, with clean Ar injection and HLR = 5.0E−4 h^{-1}. We consider a continuous Ar injection flow rate Q_I, while the rejected one Q_R is pressure-dependent, as in the previous scenarios:

$$Q_R = \begin{cases} C_1 \cdot k & \text{if} \quad P^{CV004^*} \geq P_0^{CV004^*} \\ C_2 \cdot k & \text{otherwise} \end{cases} \tag{4}$$

$$Q_I = k \tag{5}$$

with $k, C_1, C_2 \in \mathbb{R}^+$. In this case, C_1 and C_2 values are adjusted to ensure the pressure stabilization, and may vary depending on the scenario. For most of the cases, $C_1 = 1.0125$ and $C_2 = 0.95$ meet this objective, except when the rejected flow becomes less significant compared to the purified flow ($Q_R \ll Q_P$), thus assuming $C_2 \in \{0.85, 0.9\}$.

Based on these premises, we perform a parametric study for different values of V_I — directly related to Q_I —, looking for the configuration that ensures that final impurity concentrations are below operational safety limits. We also seek to minimize V_I and V_R, while ensuring stable pressure during transition —*i.e.*, $P^{CV004^*} \in [P_0^{CV004^*} \pm 40]$ Pa.

We begin by considering a one-day transition period, varying the number of VPSA units, Ar volume injected, and saturation values. These scenarios are summarized in Table 6.

Finally, we consider additional scenarios that increase the number of days employed for the maintenance-operation transition up to 5 days. These are summarized in Table 7.

5. Results of the parametric study

5.1. Analysis of the ArPS operation mode

The following subsections present the results of the ArPS simulations under operation conditions, both omitting and considering clean Ar injection. All referenced data are included in Appendix B.

Table 6
Description of the maintenance-to-operation scenarios for one-day transition period. Saturation rates correspond to the values previously defined in Table 2.

Scenario	VPSA units	V_I (m^3)	Saturation rates
(C1)		2400	
(C2)	1	4800	S_1
(C3)		6000	
(C4)		7200	
(C5)		2400	
(C6)	2	4800	S_1
(C7)		6000	
(C8)		7200	
(C9)		2400	
(C10)	1	4800	S_2
(C11)		6000	
(C12)		7200	

Table 7
Summary of maintenance-operation transition scenarios for different time periods and injected Ar. Saturation rate correspond to the value previously defined in Table 2.

Days	VPSA units	Saturation rate	V_I (m^3)			
			2400	4800	6000	7200
1			(C1)	(C2)	(C3)	(C4)
2			(D1)	(D2)	(D3)	(D4)
3	1	S1	(D5)	(D6)	(D7)	(D8)
4			(D9)	(D10)	(D11)	(D12)
5			(D13)	(D14)	(D15)	(D16)

5.1.1. Scenarios without clean Ar injection (A1-6)

Regarding the ArPS model without clear Ar injection, the results obtained for each scenario are shown in Fig. 5, representing the final concentrations of N_2, O_2, and H_2O, as well as total volumes of Ar rejected (grey bars and bottom axis).

For scenarios (A1-6), impurity concentrations do not exceed 4% by volume, without surpassing 1% for scenarios (A1-3). As expected, when the number of VPSA units is increased, the impurity concentrations consequently decrease, reducing the Ar rejection necessary to regulate the pressure levels. Therefore, the inclusion of additional VPSA units proves useful in these scenarios.

The HLR considered is also a critical factor when determining ArPS performance. For the largest HLR scenarios (A7-9), impurity concentrations are above 10%, while pressure peaks of nearly +40 Pa are observed. This is caused by large infiltrations compared to the capacity of the purification units, resulting in massive volume rejections. In general, we observe that increasing the HLR implies bigger pressure fluctuations and volume rejected.

For the smallest HLR scenarios (A1-3) infiltration flows are not large enough to compensate the purified volumes through the VPSA units. This results in an initial pressure drop (over 200 Pa) when including additional VPSA units in (A2-3). This situation could be prevented by starting from a purer initial atmosphere, thus avoiding large purification flows. However, after this event, pressure fluctuations keep stable, and the system behaves smoothly.

5.1.2. Scenarios considering Ar injection (B1-3)

We now analyse the results obtained for the scenarios where clean Ar injection is enabled. For comparison with scenarios including Ar injection, only the case with a single VPSA unit is considered. The results obtained are represented in Fig. 6.

As it can be noted, large volumes of Ar are rejected, which will require their compensation with recurrent clean Ar injection. We observe how (B1-2) scenarios converge at impurity concentrations below 1% and 4%, respectively, while (B3) exceeds 30%. These concentrations are quite similar to the no-injection scenario with a single VPSA unit

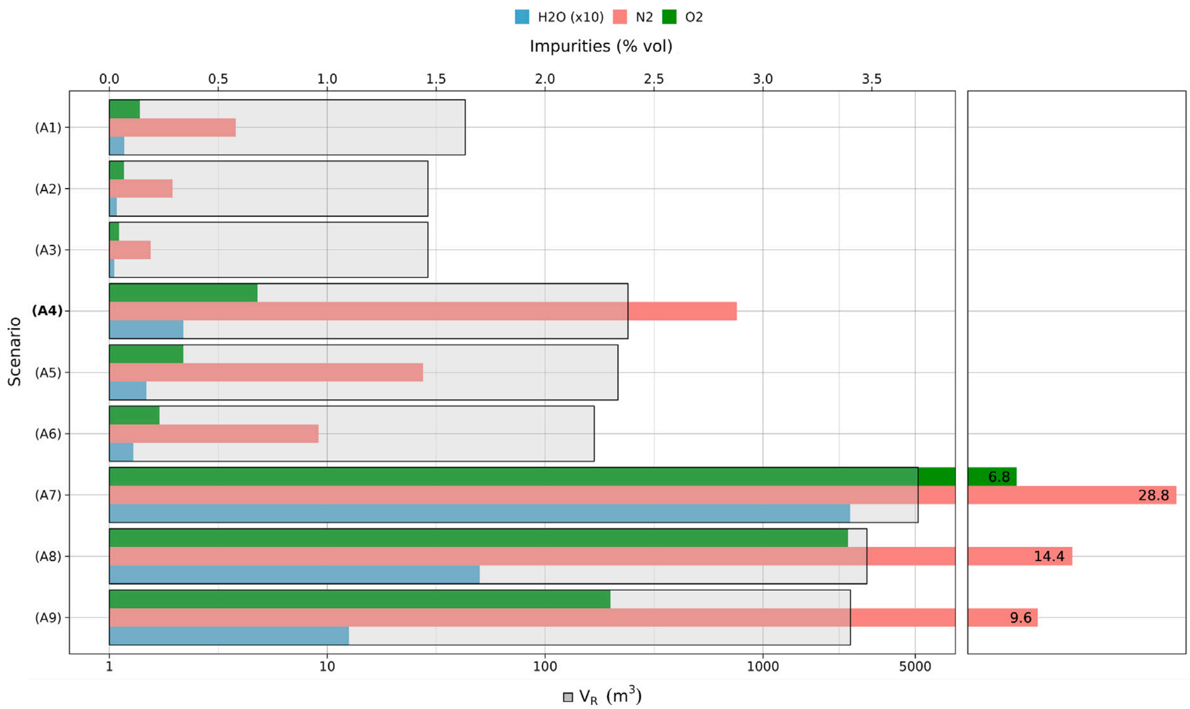

Fig. 5. Results obtained in scenarios without clean Ar injection (A1-9). Final concentrations of N_2, O_2, H_2O and total volume of rejected Ar (V_R) are represented for each scenario.

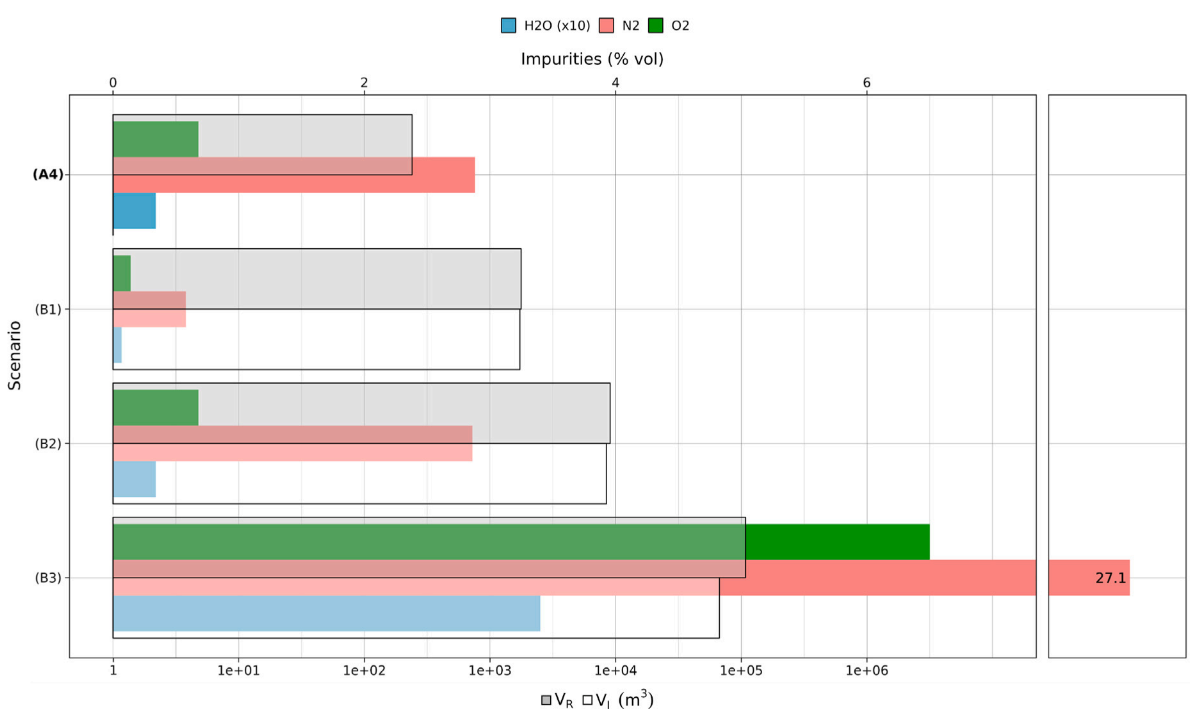

Fig. 6. Results obtained in scenarios with clean Ar injection (B1-3) compared with the baseline scenario (A4). Final concentrations of N_2, O_2, H_2O and total volume of injected (V_I) and rejected Ar (V_R) during a year of operation are represented for each scenario.

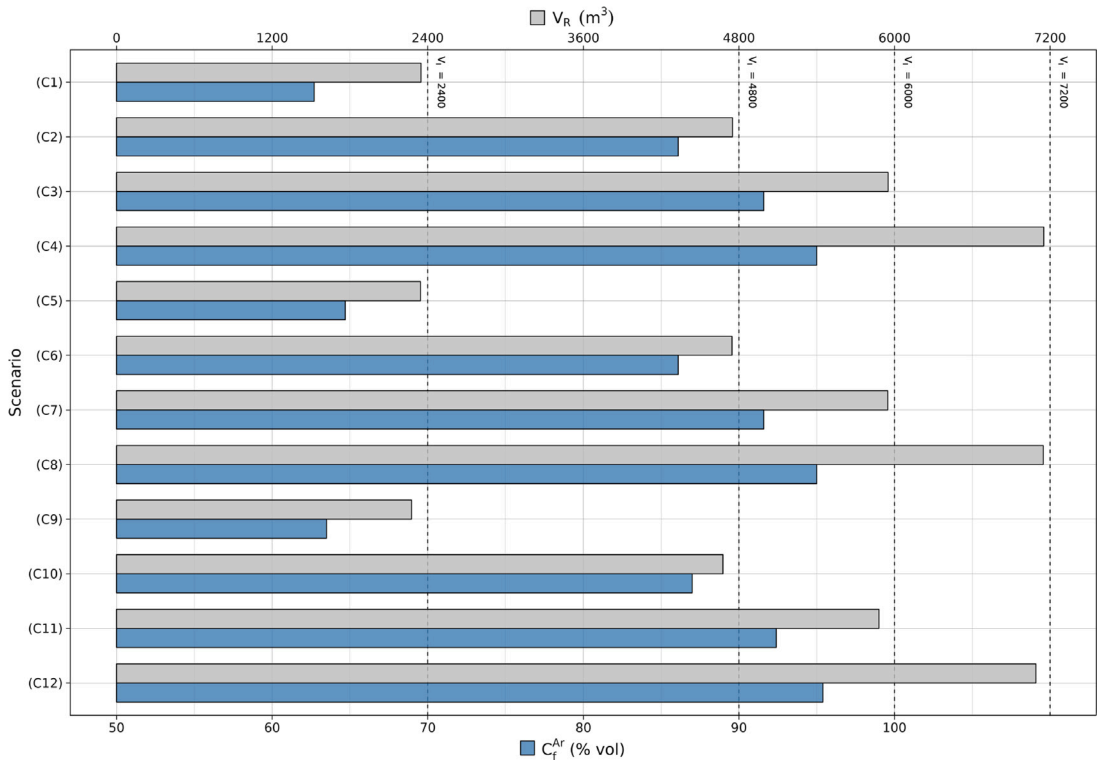

Fig. 7. Results obtained in scenarios for maintenance-operation transition (C1-12). Final concentration and total volume of rejected Ar in a whole year operating (V_R) are represented for each scenario.

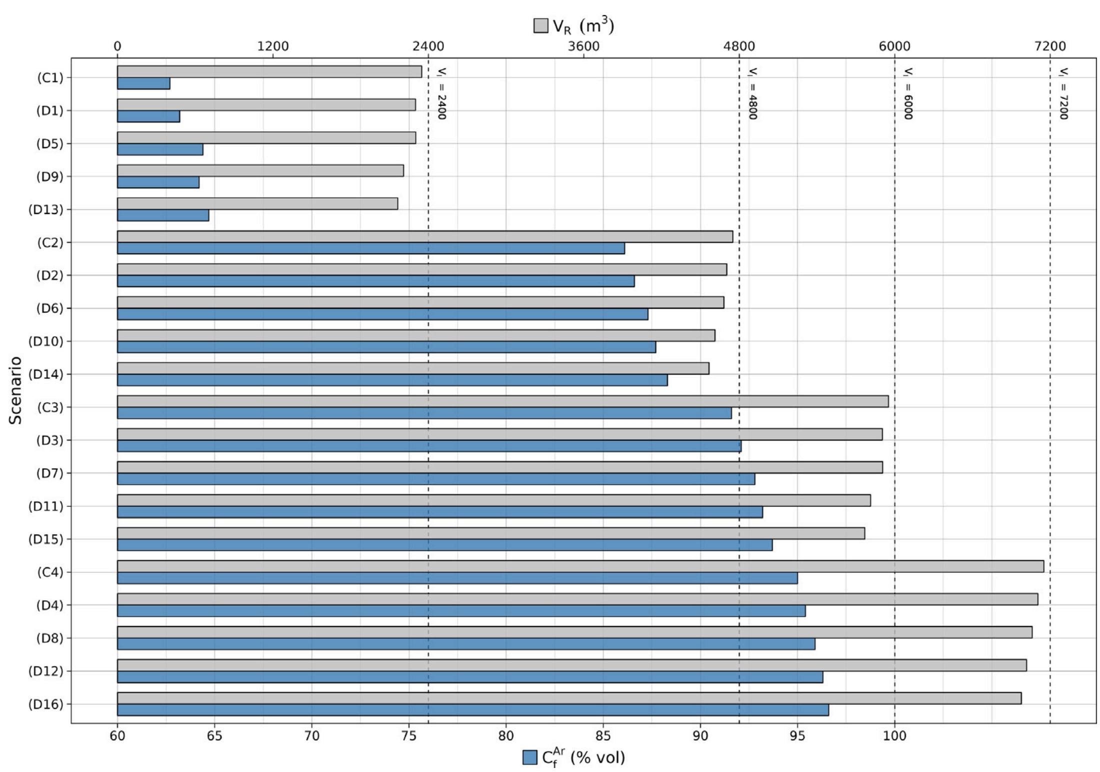

Fig. 8. Results obtained in scenarios for maintenance-operation transition (C1-4) and (D1-16). Final concentration and total volume of rejected Ar after a year of operation (V_R) are represented for each scenario.

(A1,4,7). In addition, pressure variations in the largest HLR case (B3) do not remain in the expected ±40 Pa range.

Therefore, the injection of clean Ar during operation does not significantly reduce the impurity concentrations inside inert rooms. This avoids the need to reject large volumes through the G-RWTS and replace them with clean Ar from the ArSS to maintain pressure levels. Thus, the no-injection scenario is assumed to be the most efficient and cost-effective solution while meeting safety requirements.

5.2. Analysis of the maintenance-operation transition

The results of simulating the maintenance-operation transition in the LLC under different configurations are now described. During this process, clean Ar is injected into the LLC, while a certain volume of the room atmosphere is exhausted without passing through the VPSA units.

We begin by considering a one-day transition period, varying the injected Ar volume, the saturation extraction of mass rates values, and the number of VPSA units purifying at their maximum capacity ($Q_P = n \cdot 80$ m^3/h).

Fig. 7 depicts the final Ar concentration and rejected volumes for these scenarios. As can be observed, increasing the number of VPSA units (C5-8) or their saturation capacities (C9-12) does not significantly improve the final composition of the rooms compared to the 1-VPSA scenario (C1-4), since impurity concentrations differ by less than 1% for the same injected Ar volume. Nevertheless, increasing the number of VPSA results in a greater H_2O extraction, given that no saturation is considered for this impurity.

Furthermore, a larger clean Ar injection is associated not only with a purer final state but also with a larger rejected flow and consequently with higher economic costs. It also involves larger pressure variations, although these fluctuations do not exceed +45 Pa in any scenario.

Finally, we consider several scenarios in which the number of days employed for the maintenance-operation transition is increased up to 5 days. The results are represented in Fig. 8.

For the same injected clean Ar volume, increasing the transition time forces a slower injection and, therefore, the rejection of larger volumes to obtain similar results. Hence, for a similar Ar inventory, the final composition is worse in the shortest transition time scenario. Similarly, given the same final purity, cleaner Ar is required to achieve shorter transition periods.

In conclusion, the results demonstrate that increasing the number of days employed for the air-to-Ar atmosphere transition does not result in a significant improvement in the final impurity concentrations. For those cases with similar Ar injection, variations are about 1% per additional day employed (see Appendix B). In addition, Ar final concentrations reach 90% with an injection slightly smaller than 6000 m^3, which represents more than twice the LLC volume.

6. Conclusions and future work

In this paper, we model and provide a parametric study of the IFMIF-DONES Ar purification subsystem. Based on preliminary design parameters, we analyse the purification process of the Ar-filled rooms, studying the influence of several parameters — number of purification units, Ar injection, and rejected flows — on the final concentrations of Li contaminants, as well as the assurance of dynamic confinement during one year of operation.

We observe that, in the scenarios considered, clean Ar injection is not necessary to maintain safe conditions in the inert rooms. In addition, increasing the number of purification units used by the ArPS resulted in a slight improvement regarding O_2, N_2 and H_2O concentrations. We also find that minimizing leak rates is the major governing process in order to reduce these impurities in the inert atmospheres. On this basis, the final impurities concentrations after a full year of operation are low enough to consider that Li ignition is not feasible in these atmospheres.

Finally, we analyse the maintenance-operation transition in the specific case of the LLC, demonstrating its feasibility in a period from one to five days, depending on the assumed equipment and Ar inventory. We observe that, in the case of the LLC, an injection of 4800 m^3 — approximately twice its volume — is required to meet an operation purity requirements of at least 85%. The actual amount necessary will depend on the purity requirements and the number of days invested in this transition. Additionally, a longer transition period will lead to better impurity removal by the ArPS, resulting in a lower rejected flow rate.

As future work, we intend to conduct a detailed study of reactions involving Li for the final states obtained in these simulations. Furthermore, we will continue iterating on the study of the ArPS, incorporating additional scenarios and updated design parameters, thus leading to an expanded review of its performance.

CRediT authorship contribution statement

A. Manjavacas: Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **M.A. Vázquez-Barroso:** Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **C. Torregrosa-Martín:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis. **J. Maestre:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **F. Martín-Fuertes:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The code, data and plots used in this work are available in the following repository: https://github.com/manjavacas/paper-sgs-ifmif-dones.

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Appendix A. MELCOR input data

Table A.8 summarizes the properties of the volumes represented in the ArPS MELCOR model, including their geometry, gas composition, pressure, humidity and temperature. The initial pressure of CV004 — to be kept steady during operation — corresponds to a C4 enclosure according to ISO 17873 classification, while the rest remain time-independent.

Table A.8
CVs geometries, initial properties and gas compositions in the reference model. Extracted from the Main Building, HVAC and SGS design description documents.

CV	Represents	Geometry				Initial properties			Gas composition		
		Height (m)		Volume (m^3)		Depression (Pa)	Temperature (°C)	Rel. humidity (%)	Ar (%)	O_2 (%)	N_2 (%)
CV001	*G-RWTS*	50		10^6		0	20	40	1	21	78
CV002	*Air inlet*	50		10^6		0	20	40	1	21	78
CV003	*ArSS*	30		10^6		−260	20	0.02	99.95	0.0105	0.0395
CV004	*LLC*	7.2	7.2	2635	3922	-260	20	0.2	99.5	0.105	0.395
	TIR	14.5		209							
	HTC	8.5		532							
	CTC	8.5		546							
CV004*	*LLC*	7.2		2635		−260	20	40	1	21	78

Table A.9
Model FLs.

FL	Represents	Length (m)	Flow area (m^2)
FL001	Rejected flow through ArPS	7.5	0.5
FL002	Air leak path from external volumes	0.5	0.5
FL003	Ar injection from ArSS	0.5	1.0

Table B.1
Simulation results suppressing Ar inlet. V_R is integrated over a whole year of operation.

Scenario	V_R (m^3/year)	Impurity concentrations (%)			C^f_{Ar} (%)
		$C_f^{O_2}$	$C_f^{N_2}$	$C_f^{H_2O}$	
(A1)	43	0.14	0.58	6.8E−3	99.28
(A2)	29	0.067	0.29	3.4E−3	99.64
(A3)	29	0.045	0.19	2.3E−3	99.76
(A4)	240	0.68	2.88	0.034	96.4
(A5)	216	0.34	1.44	0.017	98.2
(A6)	168	0.23	0.96	0.011	98.8
(A7)	5156	6.8	28.8	0.34	64.1
(A8)	3000	3.39	14.4	0.17	82.0
(A9)	2520	2.3	9.6	0.11	88.0

We assume the same HLRs for all rooms, which correspond to the most conservative within its ISO 10648–2 classification. In turn, if we look at the layout of the rooms in the building, the volume from which the air infiltrates into the inert rooms does not make a difference on leak simulations, as all the surrounding rooms share common characteristics and the HLR determines the total volume injected, independently of the room geometry.

Note that, even if the TIR is placed in the first floor of the building whilst the rest of the rooms are located in the base floor, we consider all of the at the same height to avoid gravitational effects. In fact, we assume a number of Ar supply considerations that are consistent with the ArSS as opposed to the ArPS studied in this work. These considerations include gravitational effects, Ar supply temperature, pressure drops in supply ducts, etc.

Finally, Table A.9 summarizes the physical properties and functions of the FLs included in the model.

Appendix B. Simulation results

This appendix includes the tables with the output data corresponding to the considered scenarios. While (A1-9) scenarios (Table B.1) represent simulations suppressing clean Ar injection, (B1-3) scenarios (Table B.2) allow it.

Tables B.3 and B.4 represent the results for different simulations of the maintenance-operation transition. In these scenarios, the former cases (C1-12) represent different configurations for a 1-day scenario, while the latter data (C1-4, D1-16) compares the results obtained for different transition periods.

Table B.2
Simulation results including Ar inlet. V_I and V_R are integrated over a whole year of operation.

Scenario	V_I (m^3/year)	V_R (m^3/year)	Impurity concentrations (%)			C^f_{Ar} (%)
			$C_f^{O_2}$	$C_f^{N_2}$	$C_f^{H_2O}$	
(B1)	1730	1770	0.14	0.58	6.8E−3	99.3
(B2)	8450	9050	0.68	2.86	0.034	96.4
(B3)	67 000	108 000	6.5	27.1	0.34	66.1

Table B.3
Results of the sensibility analysis for one-day maintenance-operation transition in the LLC, with HLR = 5.0E−4 h^{-1}.

Scenario	V_R (m^3/year)	Impurity concentrations (%)			C_f^{Ar} (%)
		$C_f^{O_2}$	$C_f^{N_2}$	$C_f^{H_2O}$	
(C1)	2348	7.87	29.2	0.18	62.7
(C2)	4750	2.93	10.9	0.070	86.1
(C3)	5951	1.77	6.58	0.044	91.6
(C4)	7151	1.06	3.95	0.029	95.0
(C5)	2344	7.88	29.3	0.088	62.7
(C6)	4747	2.93	10.9	0.035	86.1
(C7)	5948	1.77	6.59	0.023	91.6
(C8)	7148	1.06	3.95	0.015	95.0
(C9)	2275	7.70	28.6	0.18	63.5
(C10)	4677	2.74	10.2	0.072	87.0
(C11)	5880	1.60	5.98	0.046	92.4
(C12)	7090	0.95	3.61	0.029	95.4

Table B.4
Results of the sensibility analysis for different periods of maintenance-operation transition in the LLC, with HLR = 5.0E−4 h^{-1}.

Scenario	V_R (m^3/year)	Impurity concentrations (%)			C_f^{Ar} (%)
		$C_f^{O_2}$	$C_f^{N_2}$	$C_f^{H_2O}$	
(D1)	2300	7.79	28.9	0.094	63.2
(D2)	4703	2.82	10.5	0.039	86.6
(D3)	5904	1.67	6.20	0.026	92.1
(D4)	7105	0.96	3.60	0.018	95.4
(D5)	2302	7.54	28.0	0.051	64.4
(D6)	4681	2.68	9.97	0.024	87.3
(D7)	5906	1.53	5.67	0.017	92.8
(D8)	7061	0.87	3.26	0.013	95.9
(D9)	2208	7.59	28.2	0.032	64.2
(D10)	4612	2.60	9.65	0.017	87.7
(D11)	5813	1.45	5.39	0.013	93.2
(D12)	7018	0.77	2.95	0.011	96.3
(D13)	2163	7.49	27.8	0.022	64.7
(D14)	4566	2.48	9.22	0.014	88.3
(D15)	5768	1.34	4.97	0.012	93.7
(D16)	6977	0.69	2.67	0.010	96.6

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