

Parametric Study for Enhancing Ferrocene Vapor Pressure in an ECR Ion Source of KAHIF with Molecular-Flow Simulation

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1. Introduction

The Korea Atomic Energy Research Institute Heavy Ion Irradiation Facility (KAHIF) [1] is actively conducting Fe ion beam irradiation tests, which are crucial for nuclear fusion material development. However, a significant operational challenge has been observed: the ion beam current tends to decrease over time during long-duration experiments. This phenomenon effectively lowers the average DPA (displacement per atom) generation rate per hour, consequently extending the required experiment time and decreasing experimental efficiency. To mitigate this issue and enhance experimental throughput, it is essential to increase the ferrocene partial pressure within the Electron Cyclotron Resonance (ECR) ion source.

Conventional methods for increasing the ferrocene vapor pressure, such as heating the MIVOC (Metal Ions from Volatile Compounds) [2] chamber, are limited in long-term supply due to the potential for ferrocene crystallization at cold spots. Given the constraints in modifying the ECR ion source structure and the existing gas supply tube, this study investigates the feasibility of increasing the ECR ion source ferrocene partial pressure solely by adjusting currently modifiable parameters. This parametric molecular-flow simulation aims to provide design guidelines for optimal and sustained Fe ion beam production.

2. Simulation and Methods

A 3D vacuum model of the KAHIF ECR ion source coupled with a MIVOC system was developed using Molflow+ [3], as shown in Fig. 1. The model consists of the MIVOC chamber, a fixed gas supply tube, the ECR plasma chamber, and the downstream accelerator-side beamline region where pumping is applied. Since the current hardware imposes constraints on modifying the ECR chamber and the gas supply tube, the tube geometry was kept identical in all simulation cases.

Ferrocene was modeled as a neutral molecule with a molecular mass of 186 amu. A uniform outgassing source was assigned to the designated ferrocene-exposed surface inside the MIVOC chamber, and the total outgassing rate Q was scanned from 1×10^{-5} to 1×10^{-2} mbar·L/s in one-decade steps. For comparison with the experimental operation, a baseline case

(MIVOC: $10 \times 10 \times 10$ cm³) was used to identify a representative outgassing condition, and $Q = 1 \times 10^{-4}$ mbar·L/s with a pumping speed of 50 L/s reproduced the measured ECR pressure level.

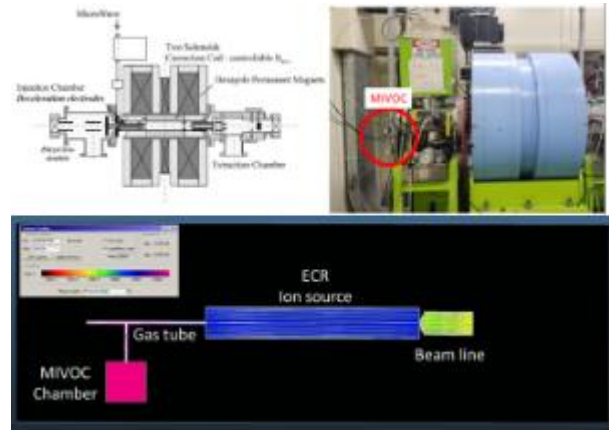


Fig. 1. Molflow+ simulation model of KAHIF ECR Ion source with MIVOC system.

The accelerator-side pumping speed S was scanned from 20 to 100 L/s (step: 20 L/s) while keeping $Q = 1 \times 10^{-4}$ mbar·L/s. In addition, the MIVOC chamber geometry was varied to investigate the effect of the ferrocene-exposed cross-sectional area and the reservoir volume. The main geometry scan fixed the depth D at 10 cm, and scanned Width (W), Height (H) over 10, 20, and 30 cm. One additional case ($10 \times 30 \times 30$ cm³) was included to extend the volume range. The evaluated pressures correspond to the ferrocene partial pressure at steady state, and were recorded at three locations: (i) inside the MIVOC chamber, (ii) inside the ECR ion source chamber, and (iii) in the accelerator-side beamline region.

Table I Scan conditions of MIVOC dimension

Case	W [cm]	D [cm]	H [cm]	Area [cm ²]	Volume [cm ³]
1	10	10	10	100	1000
2		20	10	200	2000
3		30	10	300	3000
4		10	20	100	2000
5		10	30	100	3000
6		30	30	900	9000

3. Results and Discussion

First, the baseline geometry ($10 \times 10 \times 10 \text{ cm}^3$ MIVOC chamber) was used to identify an outgassing condition that reproduces the measured ECR pressure during Fe beam operation. The outgassing rate scan clearly showed that the ECR chamber pressure increases with outgassing rate, and that even under the extremely low effective conductance imposed by the fixed tube, increasing the MIVOC pressure can raise the ECR pressure.

With an outgassing rate of $1 \times 10^{-4} \text{ mbar} \cdot \text{L/s}$ and a baseline pumping speed of 50 L/s , the simulated ECR pressure was found to be comparable to the experimentally observed value of $1 \times 10^{-4} \text{ mbar}$.

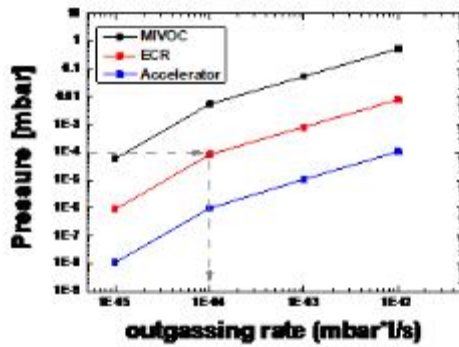


Fig. 2. Outgassing rate scan results for baseline MIVOC geometry ($10 \times 10 \times 10 \text{ cm}^3$).

Using the matched condition, the accelerator-side pumping speed was varied. No meaningful change in the ECR chamber pressure was observed across the tested pumping speeds. This indicates that, for the present configuration, pump capacity is not the limiting factor.

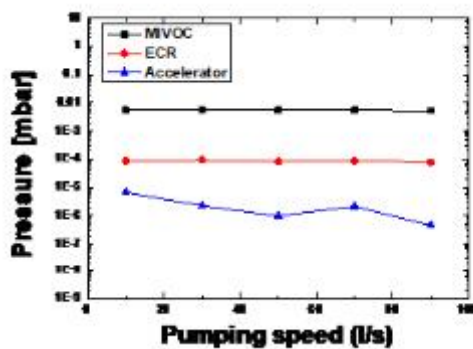


Fig. 3. Pumping speed scan results under matched source condition.

Next, the MIVOC geometry scan was performed to evaluate the effect of (i) ferrocene-exposed area (A) and (ii) chamber volume (V). Because the MIVOC chamber size changes, the absolute pressure levels can differ even at the same outgassing rate. However, for practical operation where the MIVOC pressure is effectively bounded by ferrocene saturated vapor pressure at a

given temperature, the key metric is the pressure ratio between the MIVOC and the ECR chamber.

Across the tested geometries, the pressure ratio ($P_{\text{MIVOC}}/P_{\text{ECR}}$) remained approximately 60–70, and no significant reduction of this ratio was observed. Therefore, within the present system constraints, changing only the MIVOC chamber geometry is not expected to substantially increase the ECR ferrocene pressure if the MIVOC pressure itself is unchanged.

4. Conclusions

A simplified parametric molecular-flow simulation was conducted to investigate feasible approaches to increase ferrocene partial pressure in the KAHIF ECR ion source under the constraint that the gas supply tube geometry cannot be modified.

(1) The ECR pressure increased with ferrocene outgassing rate, confirming that raising MIVOC ferrocene pressure can increase ECR ferrocene pressure even under low-conductance conditions.

(2) Changing accelerator-side pumping speed produced no meaningful improvement, indicating a conductance-limited transport regime.

(3) Varying MIVOC geometry (exposed area and volume) did not significantly change the pressure ratio $P_{\text{MIVOC}} / P_{\text{ECR}}$ ($\approx 60\text{--}70$).

Nevertheless, in real operation, increasing the ferrocene-exposed area may increase the effective evaporation capability without excessive heating, and increasing chamber volume may provide a larger ferrocene inventory and buffering effect, potentially reducing the time-dependent decay rate of Fe beam current during long irradiation runs. These effects will be verified experimentally by fabricating MIVOC chambers with different exposed areas/volumes and measuring the pressure response and beam stability.

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