# Producing a cold, controlled source of radicals

Lok Yiu (Kathy) Wu,[1,2] Omar Mohamed,[1] Andriana Tsikritea[1,2] and Brianna Heazlewood[2]

[1]Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford, OX1 3QZ, UK
[2]Department of Physics, University of Liverpool, Oxford Street, Liverpool, L69 7ZE, UK

## Introduction

Producing a pure, state-selected beam of gas-phase radicals — with a tuneable velocity — in the laboratory is rife with challenges. Yet, it is one of the most important tools we need in our arsenal to prsecisely study ion-radical reactions that are astrochemically and atmospherically relevant.[1] Taking advantage of the paramagnetic behaviour of radicals, we can use external magnetic fields to filter out only the target species (that are travelling at a selected velocity) from a beam containing a mixture of other species.

Conventially, the switching sequence of a Zeeman decelerator is calculated by considering the passage of a hypothetical synchronous particle. A magnetic radical filter (MRF) is put at the end of the decelerator to filter out all unwanted species (including precursor molecules, photofragments and radicals travelling outside the target velocity). The MRF is composed of 4 Halbach arrays and 2 skimming blades, initially set in "standard" positions, determined empirically by trial and error and particle trajectory simulations.

A CMA-ES evolutionary algorithm[2] has been applied to optimise the decelerator switching sequences and the positions of the components of the MRF. The algorithm generates a pure, state-selected for the passage of a beam of H atoms, starting from a source with a mixture of species and passing through a 12-stage Zeeman decelerator and the MRF. The fully optimised parameters result in **significant improvements** in the **intensity** and **purity** of the resulting beam.

## Experimental Set-Up

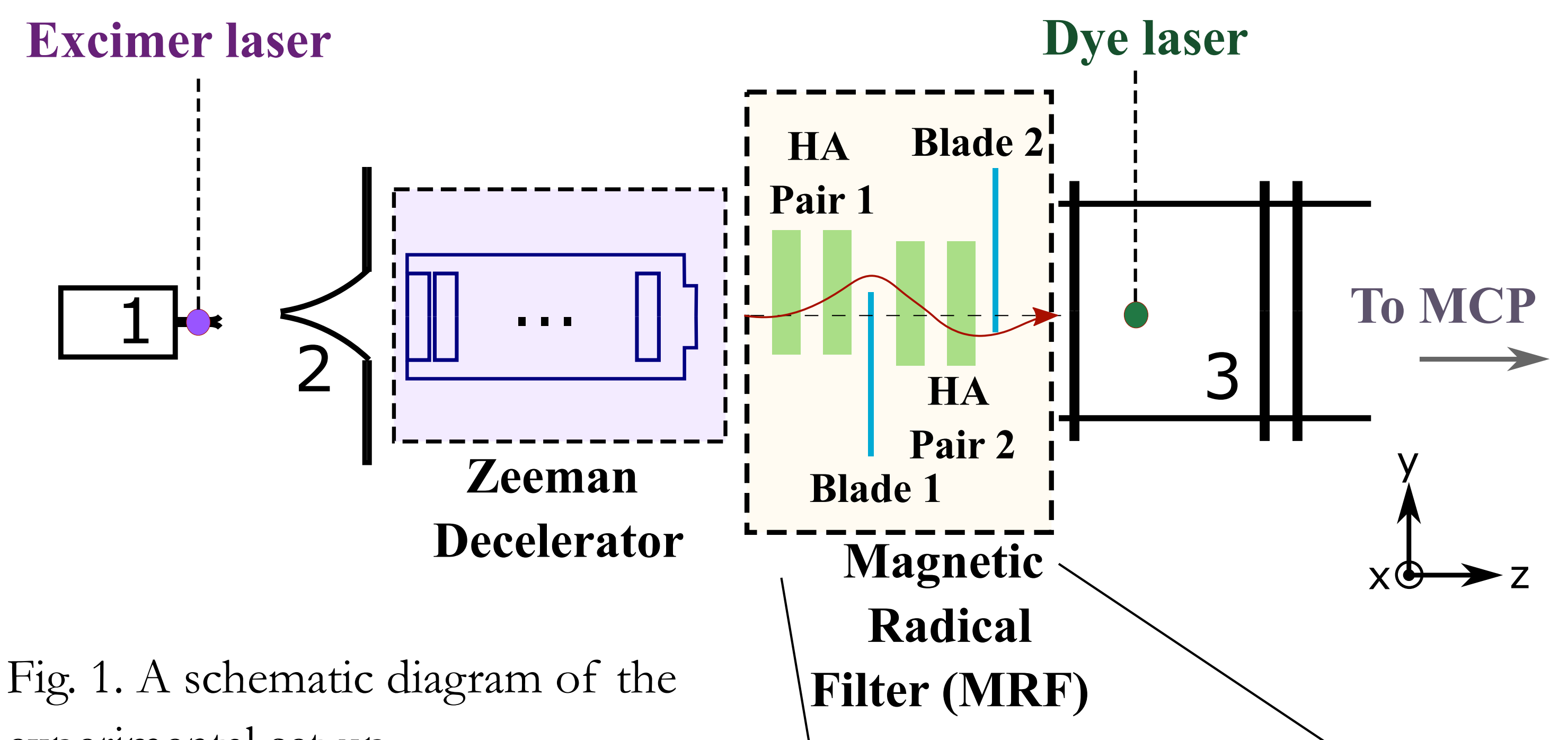
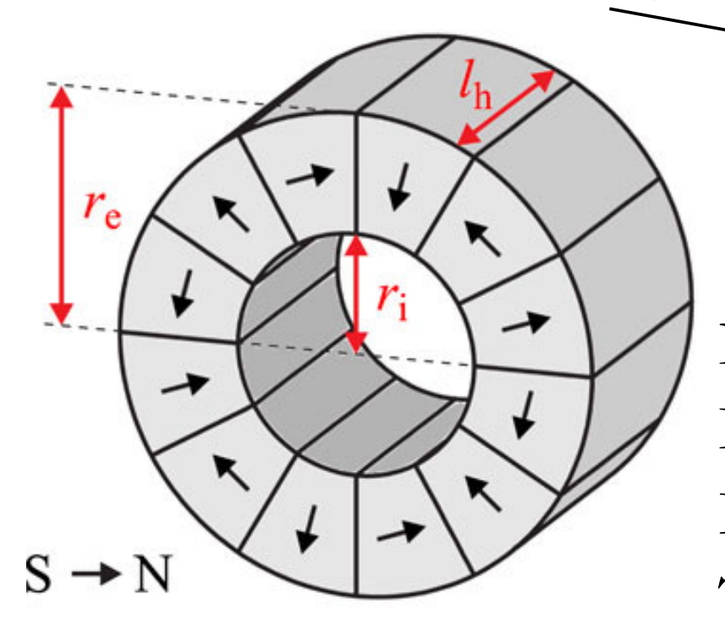


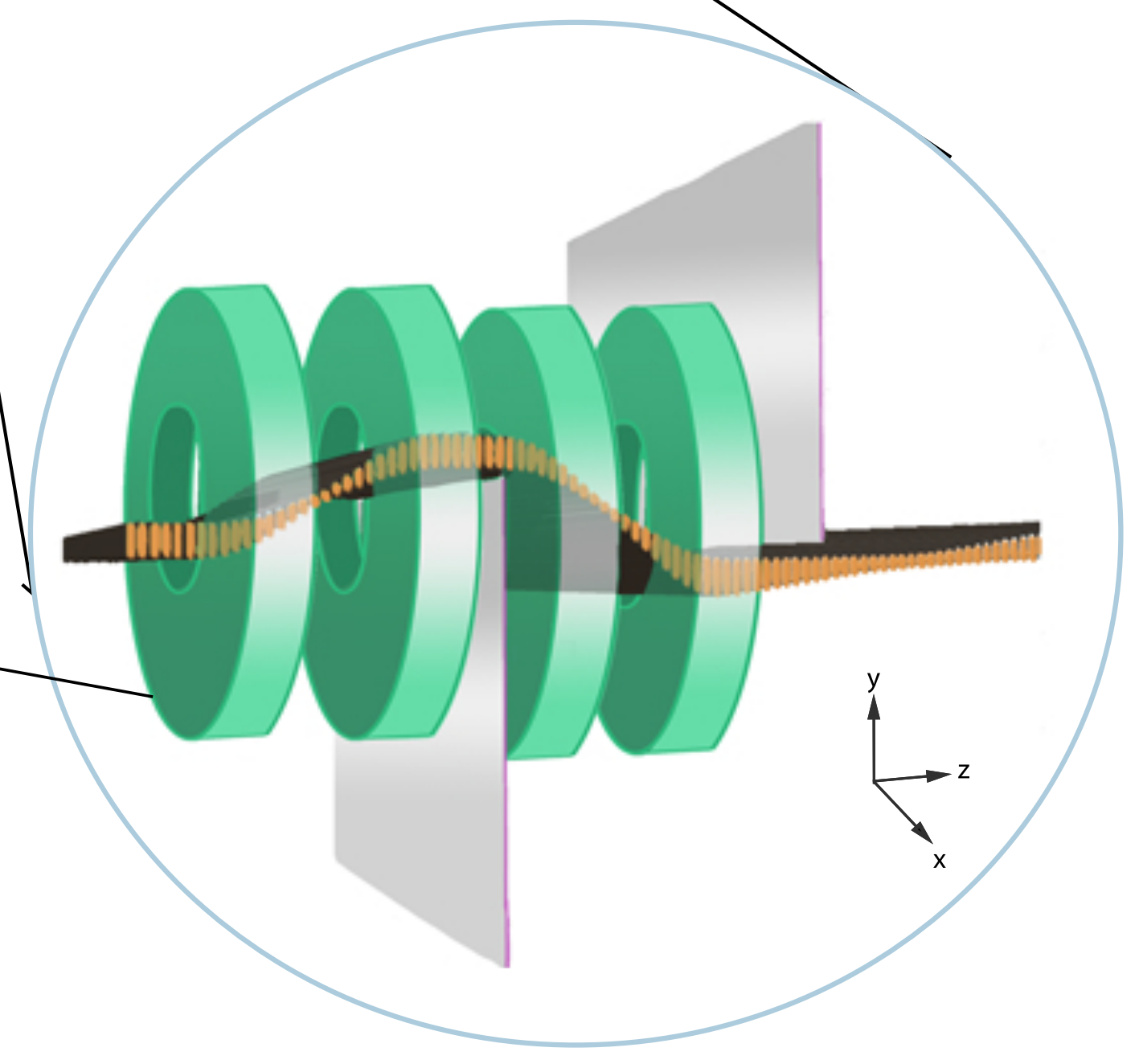
Fig. 1. A schematic diagram of the experimental set-up.

(1) Pulsed Valve.
(2) Skimmer.
(3) Extraction Plates.

**Halbach array**

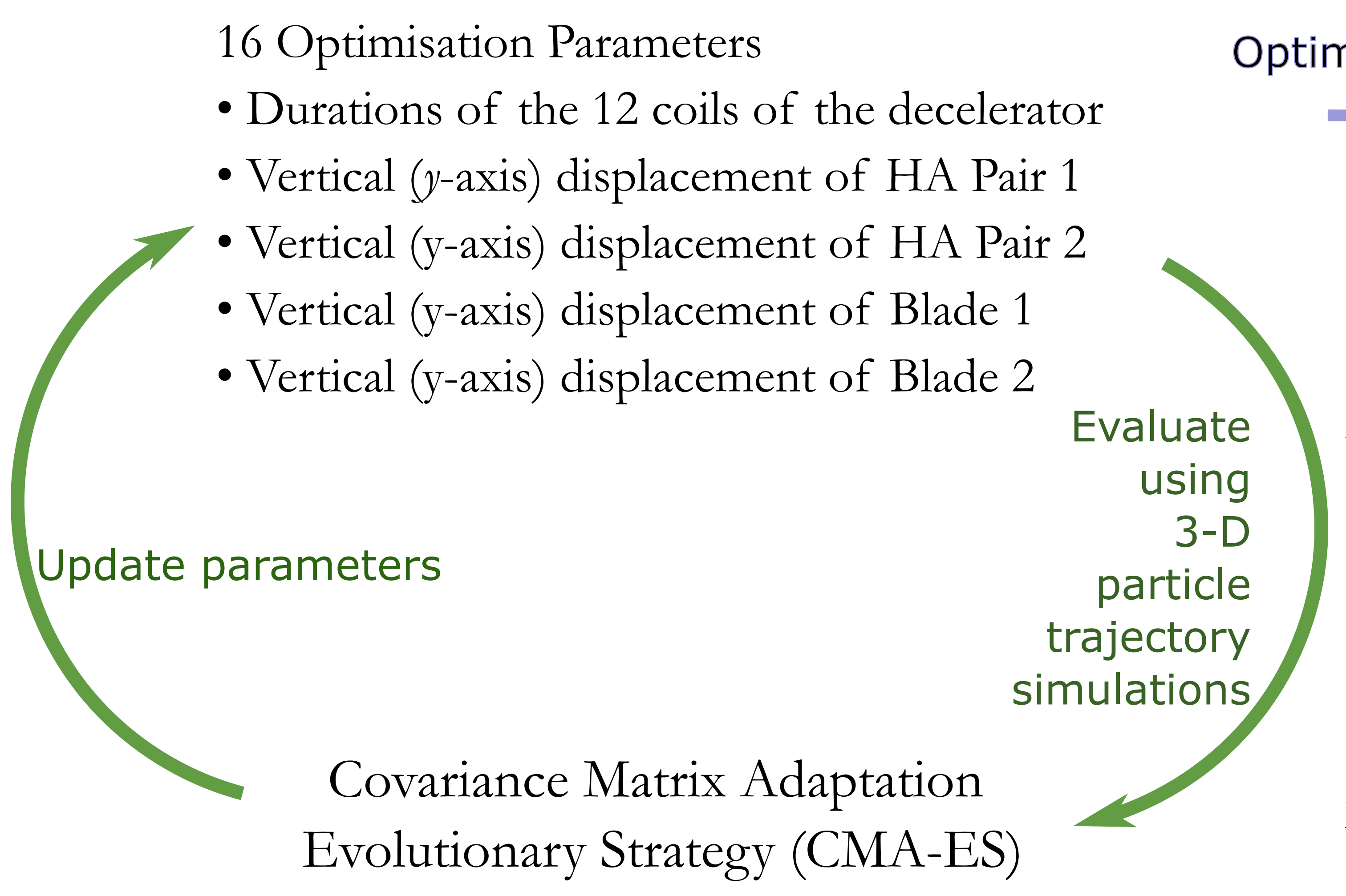


Remanence $B_0 = 1.4$ T
Internal radius $r_i = 3$ mm
External radius $r_e = 7$ mm
Thickness $l_h = 7$mm



*Allows us to target velocities between* **200 and 355 m/s**

## CMA-ES Optimisation



16 Optimisation Parameters
- Durations of the 12 coils of the decelerator
- Vertical ($y$-axis) displacement of HA Pair 1
- Vertical (y-axis) displacement of HA Pair 2
- Vertical (y-axis) displacement of Blade 1
- Vertical (y-axis) displacement of Blade 2

Evaluate using 3-D particle trajectory simulations

Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES)

Update parameters

Optimal parameters are used in experiments

**Findings**

- Compared to previous best[3] methods, the fully optimised parameters yields twice as many target particles
- The resulting beam is also purer — for a target velocity of 300 m/s, the beam has an average velocity of 298.8 ± 4.8 m/s, compared with the previous-best of 304 ± 12.3 m/s
- This is due to greater transverse focusing, leading to a higher density of particles in the acceptance of the MRF

**Targeting particles at 300 ± 10 m/s**

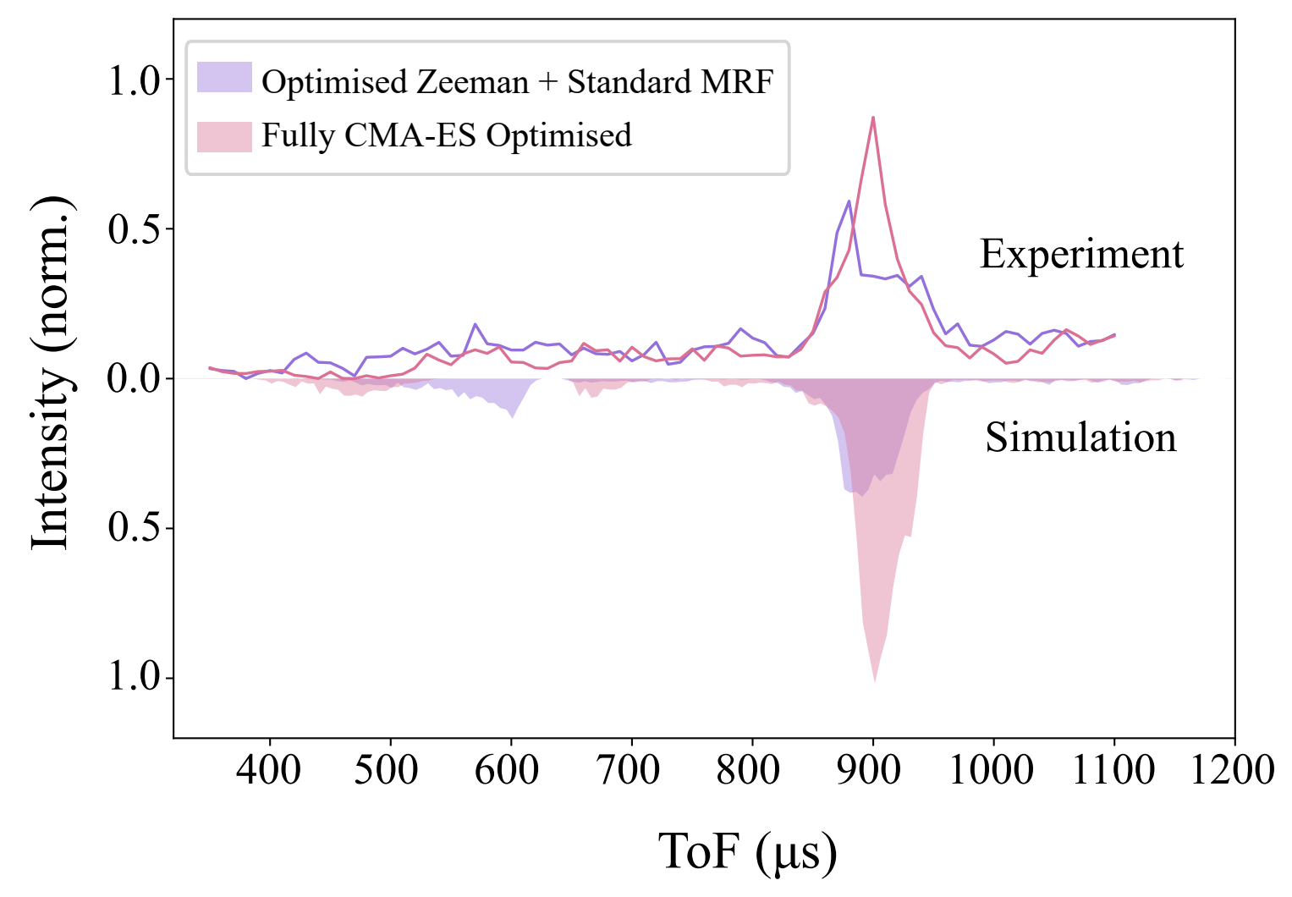


Fig. 2. Time-of-flight (ToF) profiles of the transmitted H atoms

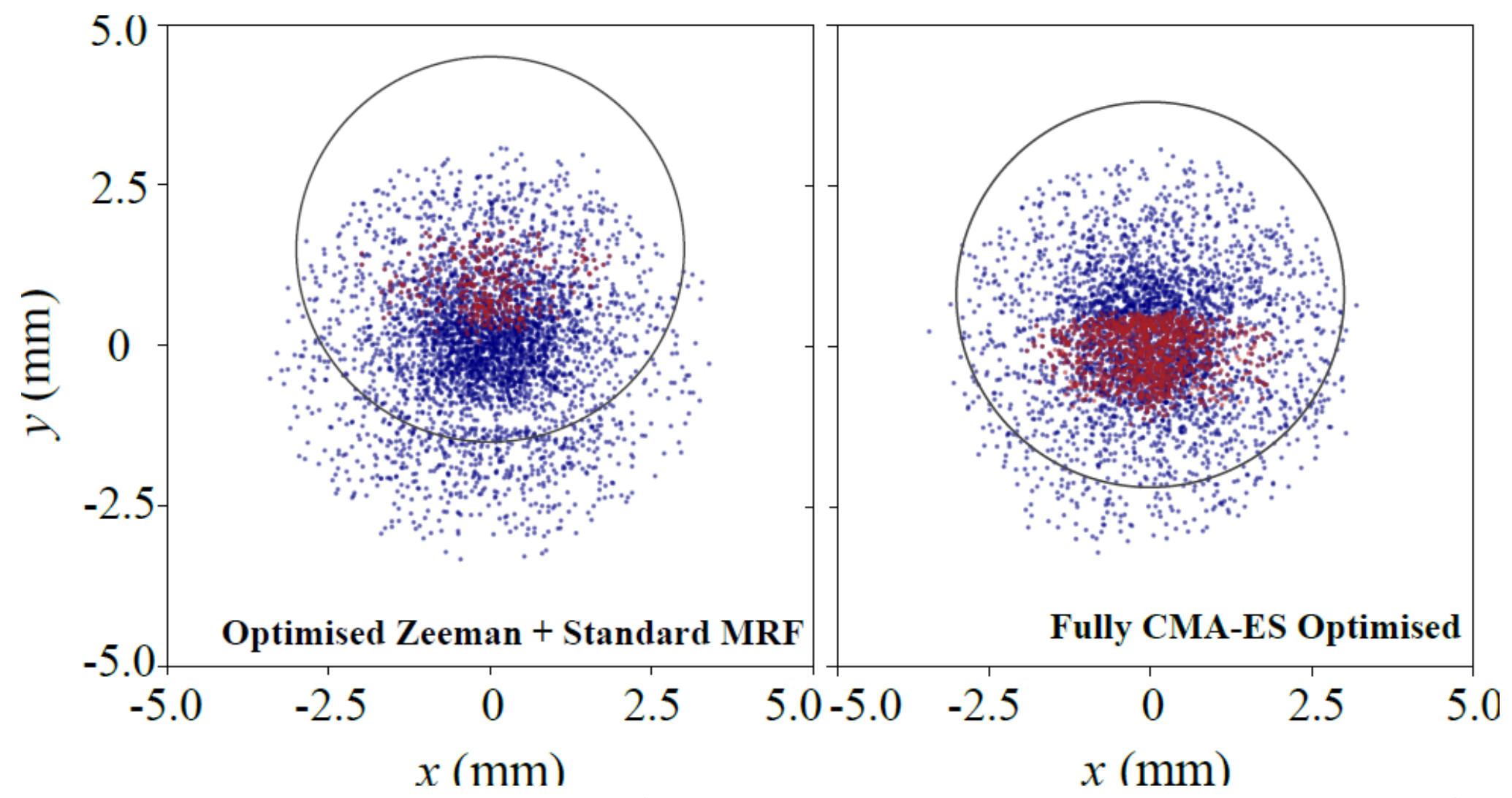


Fig. 3. Scatter plots showing the positions of the target H atoms in the transverse plane at the first HA. Particles in red are those that successfully reach the detection region. Grey circles indicate the inner radius of the first HA.

## Second-generation Magnetic Guide

The second-generation MRF will act as a stand-alone radical filter, and will target O and OH radicals. It will feature an additional focusing element at the start and end of the current MRF design.

This will be interfaced with a liquid surface in collaboration with the McKendrick Group at Heriot-Watt University. This will allow the precise study of O or OH collisions with squalane/squalene liquid surfaces, which will have implications for modelling atmospheric chemistry.

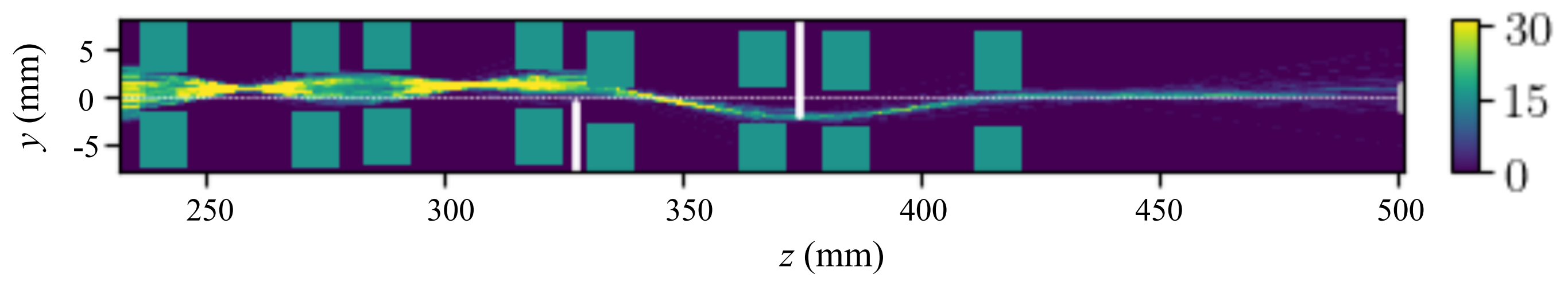


Fig. 4. Preliminary simulation results for OH ($X^2\Pi_{3/2}$), with two additional pairs of Halbach arrays in front and after the current MRF set-up. The positions of the arraysand blades have been determined using CMA-ES optimisation. The green rectangles show the cross-section of the Halbach arrays, while the white lines show the blades. The trajectory of target particles (210 ± 10 m/s) is shown through the MRF.

## References

[1] Heazlewood, B. R.; Softley, T.P. Towards Chemistry at Absolute Zero. *Nat. Rev. Chem.* **2021**, *5* (2), 125-140.
[2] Igel, C; Hansen, N.; Roth, S. Covariance Matrix Adaptation for Multi-Objective Optimization. *Evol. Comput.* **2007**, *15* (1), 1-28.
[3] Toscano, J.; Rennick, C. J.; Softley, T. P.; Heazlewood B.R. A Magnetic Guide to Purify Radical Beams. *J. Chem. Phys.* **2018**, *149* (17), 174201.

## Acknowledgements

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European Research Council
Established by the European Commission

CAMS
Community for Analytical Measurement Science

UKRI
Engineering and Physical Sciences Research Council