Lenses or No Lenses? A Study of Ion Transfer Efficiency at Interfaces in a Lens-free Triple Quadrupole MS

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Introduction

The efficiency of ion transfer between the quad mass analyzers and the Q_2 collision cell in a triple quad is critical for instrument robustness and sensitivity; qualities that make triple quads "work-horses" in quantitative MS today.

Challenging requirements

- Q_2 contains collision gas but there should be no collisions in Q_1 or Q_3, which are in close proximity, in the same vacuum region.
- The ion beam is wide/divergent at the output of each quad but the next quad requires a narrow, collimated beam.

Common implementations today

- Traditional - Lens approach: collision cell around Q_2 with narrow apertures in and out to limit gas flow. Electrostatic lenses used to refocus ions in and out. Common but requires complex tuning, prone to contamination, noding.
- Newer - Lens-free approach (Fig. 5): collision area is defined with seals around and outside of Q_2 ion guide path (US Pat 6576897). RF-only ion guides and not lenses are used to guide ions in and out of Q_2. Can provide high transmission, simple/robust instrument design.

This computational work studies the ion transfer efficiency and fundamental limitations of the two approaches above.

Configuration	Q1	Q1 post-filter	L1	L2	L3	Q2	L1	L2	L3	Q3 pre-filter	Q3
Q1-Q2	-5	-5				-5					
Q2-Q3						-5				-5	-5
Q1-LLL-Q2	-5	-8	-200	-10	-200	-5					
Q2-LLL-Q3						-5	-100	-10	-75	-20	-5

Table 1. Tuned voltages for quad axes and lenses at m/z 264.

Methods

Quad interface models (Fig. 1)

- Lens-free (Q_1Q_2 and Q_2Q_3), Fig. 1a. Gas cell boundaries are marked with dashed lines. Ion transfer is achieved through close proximity RF-only ion guides: Q_1 post-filters, Q_2 RF-only input and output sections and Q_3 pre-filters.
- Three-lenses (Q_1LLLQ_2 and Q_2LLLQ_3), Fig. 1b. Gas is contained in Q_2 with one narrow aperture and 2 other ion lenses at each end for refocusing the ion beam. Q_1 post-filters and Q_3 pre-filters.

Ion trajectory simulations are done using SIMION 8 (SIS Inc., Ringoes, NJ 08551; www.simion.com) and LUA programming.

Simulation Details

Geometry (Fig. 1): Round rod quads r_0 4 mm and length 40 mm; pre-post filter length 12.5 mm; square-rod Q2 r_0 3 mm, sides 4.5 mm, length 40 mm. 1.5 mm per grid point. Axial distance between all elements 1 mm. For Q_1LLLQ_2, lens 1 ID 6 mm, length 4 mm, lens 2 ID 6 and 4 mm, length 15 and 1 mm, lens 3 ID 2 mm, length 2 mm. For Q_2LLLQ_3, lens 1 ID 2 mm, length 2 mm, lens 2 ID 5 and 3 mm, length 9 and 1 mm, lens 3 ID 3 mm, length 3 mm.

Voltages: RF frequency 1 MHz, quad RF voltages 306 V at m/z 264, DC voltages adjusted for unit mass separation; q-values pre/post filter 0.5, q-value Q_2 0.5. Tuning voltages without collisions are in Table 1, with collisions Q2 axis voltage is added to all following elements.

Ion beam: Circle distribution 1 mm diameter, ion energy 5 eV. Trajectories: 96 ions, 8 RF phases per simulation point. Ion m/z 264 or as described in the text.

Collisions: Elastic, hard sphere model, collision gas Ar (40 Da), pressure 0.266 Pa. Collision cross section 220 Å². Collisions are assumed to be present outside the collision cell a distance equal to the diameter of collision cell hole.

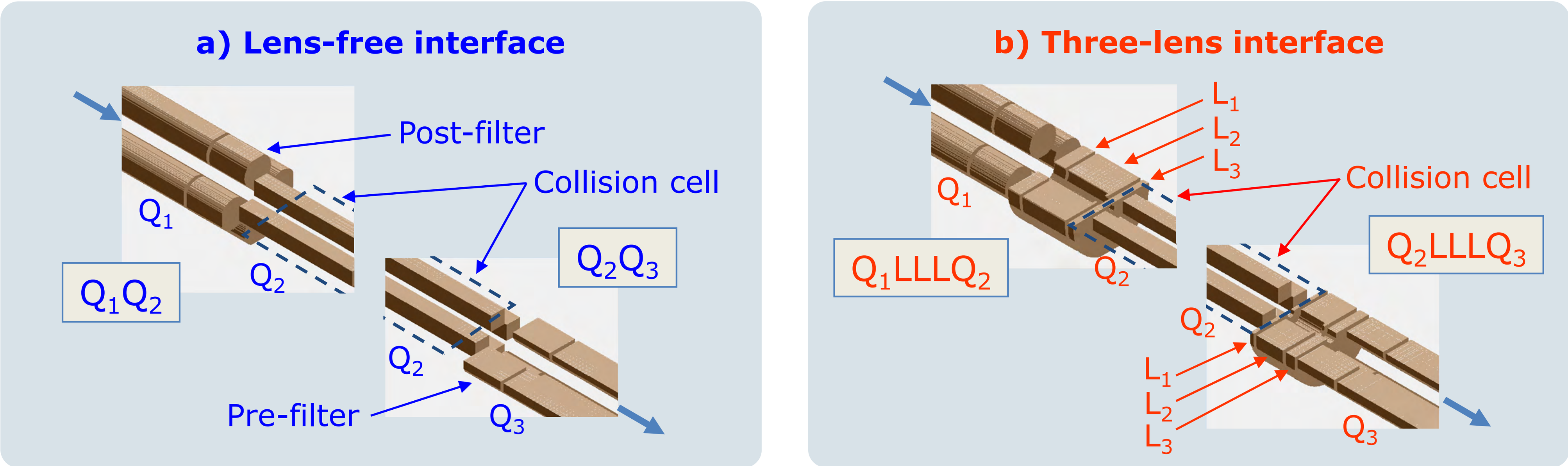

Fig. 1 Geometry details of the quad-interface models studied here.

Results

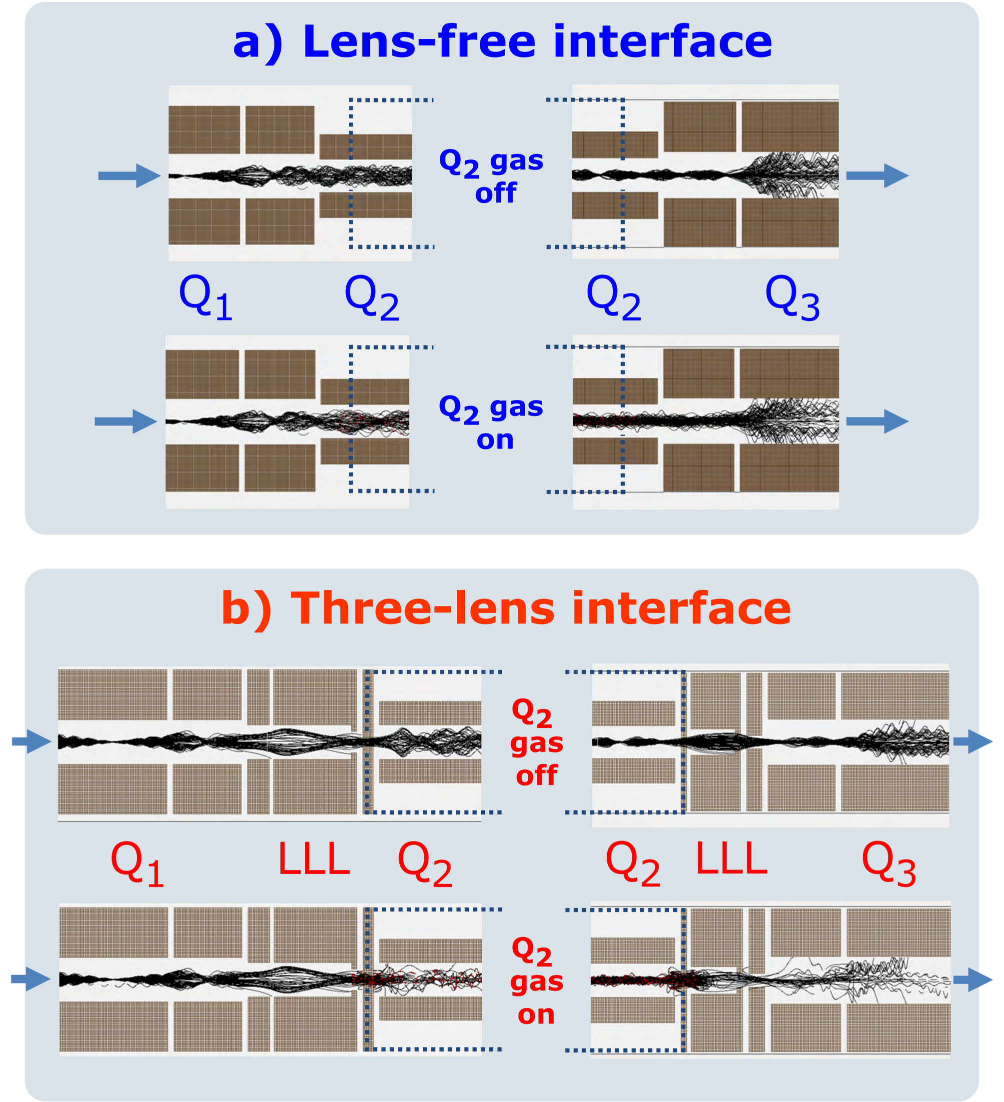

Fig. 2 Details of ion trajectories in and out of Q_2 for the lens-free (a) and three-lens (b) quad interfaces with and without gas in Q_2.

Ion trajectory analysis. Lens-free quad interface (Fig. 2a)

- Smooth transfer between RF-only quad sections.
- No loses due to collisions when Q_2 gas is on. Collisions occur within RF-only guides, they help collimate the ion beam and improve transmission efficiency.
- Most ion loses occur in Q_3, due to limited mass filter acceptance.
- No significant electrostatic focusing can be achieved with the pre-post filter ion guides.

Three-lens quad interface (Fig. 2b)

- Efficient ion focusing and transfer when Q_2 gas is off and no collisions occur.
- Significant loses when collision gas is on. Most ion loses occur within the electrostatic lenses, especially in the aperture region.
- Lenses cannot efficiently focus ions in a collision environment.

Ion transmission analysis (Fig. 3)

Voltages in both systems are "tuned" vs. mass for maximum efficiency in absence of collisions. When collision are on, voltages following Q_2 are adjusted to account for ion energy loss.

- The ion transfer out of Q_2 is less efficient than into Q_2 due to the smaller acceptance of analyzing quad Q_3 compared to the RF-only quad Q_2 (see Fig. 3, $Q_2…Q_3$ vs. $Q_1…Q_2$).
- The lens-free transmission is rather un-affected by collision pressure, energy or mass, except at low masses < m/z 200.
- The 3-lens transmission is significantly affected by collision pressure, energy, and mass.
- The 3-lens transmission improves with collision energy due to reduced scattering loses.

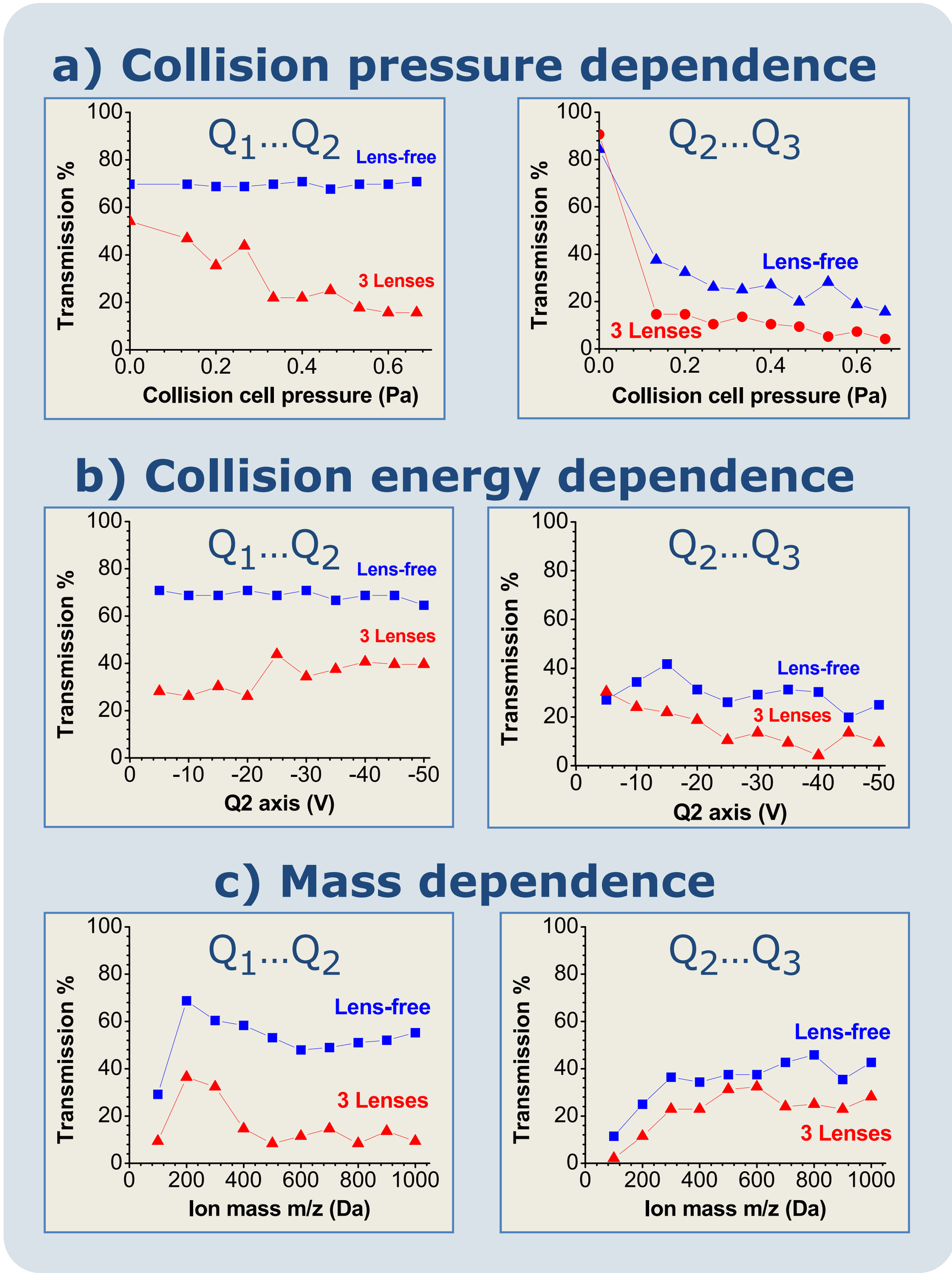

Fig. 3 Transmission efficiency in and out of Q_2 for the lens-free and the 3-lens interfaces as a function of Q_2 pressure (collision energy 25eV and m/z 264), collision energy (pressure 0.266Pa and m/z 264) and mass (collision energy 25eV and pressure 0.266Pa).

Q3 low res.

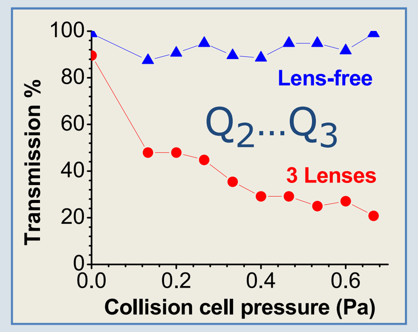

Fig. 4 Transmission efficiency Q2…Q3 when Q3 is set to lower resolution.

- As collision pressure increases, the lens-free interface is significantly more efficient than the 3-lens interface (Fig. 3a).
- When Q_3 acceptance is increased by reducing Q_3 resolution, the lens-free interface provides mostly 100% efficiency but the efficiency of the 3-lens interface is still limited due to collision loses (Fig. 4).

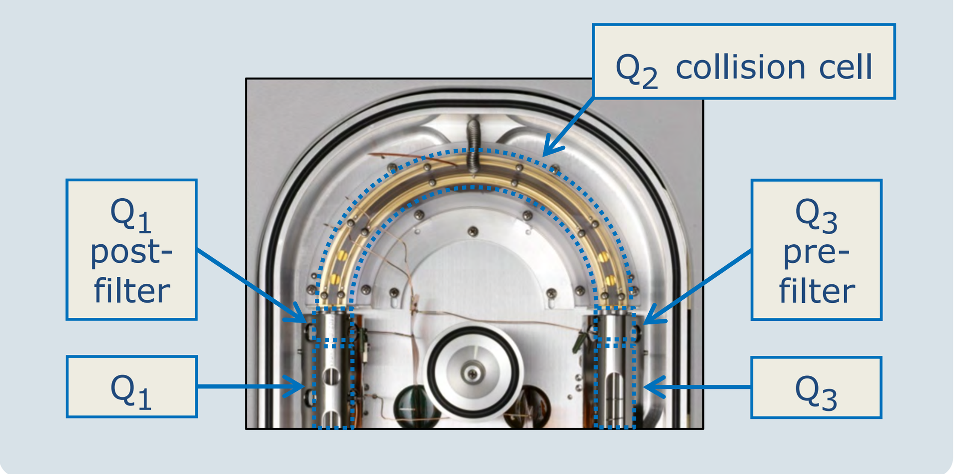

Fig. 5 An example - the lens-free QQ_2 and Q_2Q coupling in the Bruker 320 triple-quad.

Conclusions

- Gas collisions may increase the efficiency of a lens-free, RF-only interface between a quad and collision cell but they significantly reduce the efficiency of lens-based interfaces.
- Collision pressure, energy, and mass have little influence to the ion transfer efficiency of a lens-free interface while they significantly change the efficiency of lens-based interfaces
- Overall, a lens-free, RF-only interface is not just simpler and more robust than a lens-based interface but it also provides significantly higher efficiency.

Triple Quad MS