ION TRANSPORT VIA A TRAVELLING WAVE IN A CYLINDRICAL GUIDE

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OVERVIEW

Theoretical analysis was done on the motion of ions in a cylindrical ion guide, propelled by a confining travelling-wave electric field. The results were then verified by comparing them against numerical simulations. It was found that:

- Ion motion separates into two regimes: a slowly propagating 'helical' motion and a de-focusing 'depletion' region.
- Ions in the 'helical'-motion regime travel at a radial position -dependent mean drift speed, which is slower than the confining wave.
- Ions in the 'depletion' region will be directed towards the guide edge.

WHY TRAVELLING WAVES?

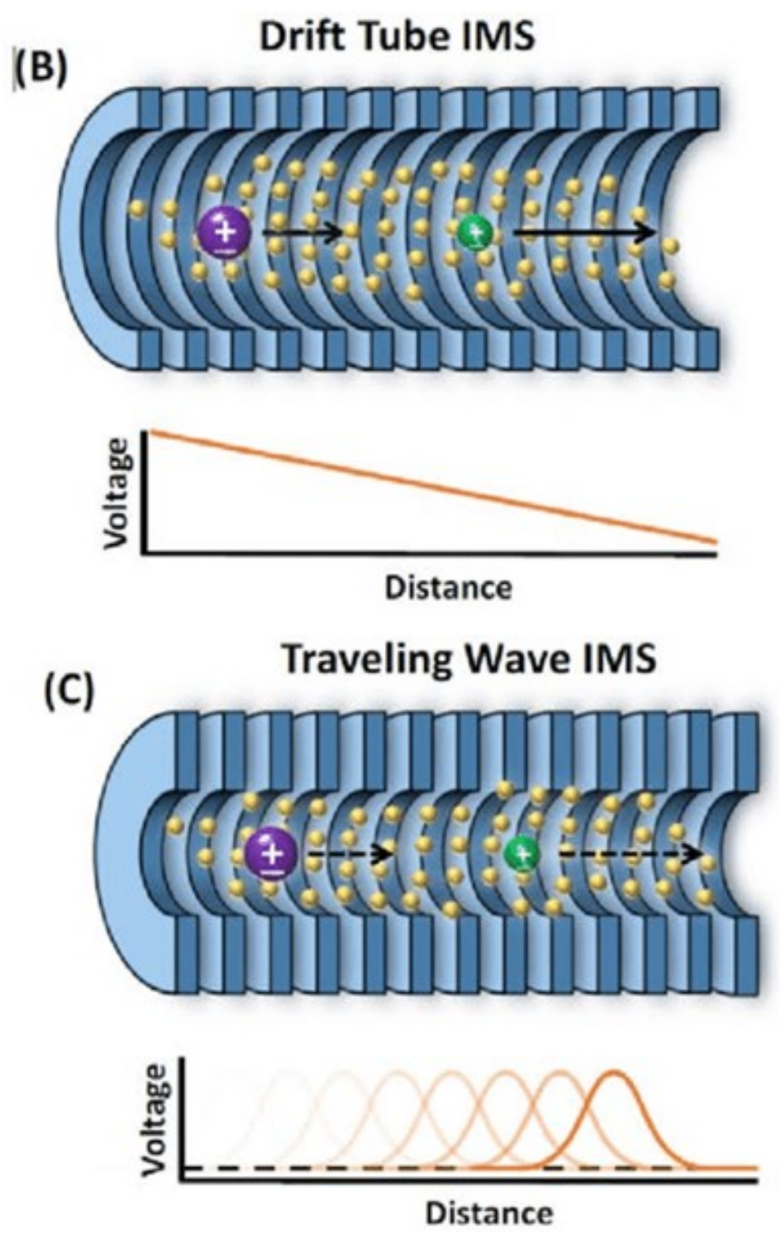

Figure 1. Difference between DTIMS and TWIMS: sustaining a constant gradient reaching high voltages vs constant amplitude at lower voltages [1].

METHODS

The setup

- **Monochromatic** travelling-wave electric field
- **No** radio-frequency (RF) standing wave

Theoretical analysis

$$\underbrace{\gamma\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}}_{\text{drag force}} = \underbrace{q\mathbf{E}(x,y,kz-\omega t)}_{\text{electrostatic force}} + \underbrace{\sqrt{2k_BT\gamma}\boldsymbol{\xi}(t)}_{\text{Brownian noise}}$$

- Axial and radial components of Newton's 2nd law
- Axial—mean drift speed
- Radial—perturbative motion
- Inertia small—neglected

Numerical solution

- Euler's method (MATLAB)

Parameter	Symbol	Value	Units
mass	m	454	Da
charge	q	+1	e
drag	γ	1.01×10^{-17}	kg/s
pressure	p	500	Pa
temperature	T	300	K
wavelength	$\lambda = \frac{2\pi}{k}$	8.64	mm
wave speed	$c = \frac{\omega}{k}$	300	m/s
wave amplitude	V_1	50	V
guide radius	r_0	7.5	mm
timestep	-	100	ns

Table 1. Parameters used in .the simulations.

PRELIMINARY RESULTS

Figure 2(a) shows the general setup of the problem.

Key characteristics of trajectories:

- 'Helical'/'Spiral' motion
- De-focusing behaviour
- Noise-dominated near centre

We seek to explain these properties.

'Helical'

- Mean drift speed (monochromatic waves)

$$\bar{v}(r) = c\left(1 - \sqrt{1 - \left(\frac{qkV_1}{\gamma c}\frac{I_0(kr)}{I_0(kr_0)}\right)^2}\right)$$

- 'Defocusing' beyond certain radial position—'surfing' limit, where ions 'surf' at wave-speed and 'depletion' region, where ions directed towards guide walls
- Drift and 'spiral' effects small near centre of guide—noise dominates.

ANALYSIS

De-focusing

- Ions entering the 'depletion' region eventually hit guide walls.
- Need for RF focusing waves to confine ions.
- If walls are permeable, ions would approach an asymptote in the wave frame.

Radial extent of spirals (monochromatic waves)

$$\Delta r = \frac{2qV_1}{\gamma(1-\bar{v}(r)/c)}\frac{I_1(kr)}{I_0(kr_0)}$$

- Contributes towards the 'depletion' region.

Summary

- Mean drift speed increases with radial position regardless of wave-form
- Spiral sizes also increase with radial position
- These are **geometrical effects** unseen in one-dimensional analyses [2].
- 'Depletion' region generally exist, limiting transport efficiency.

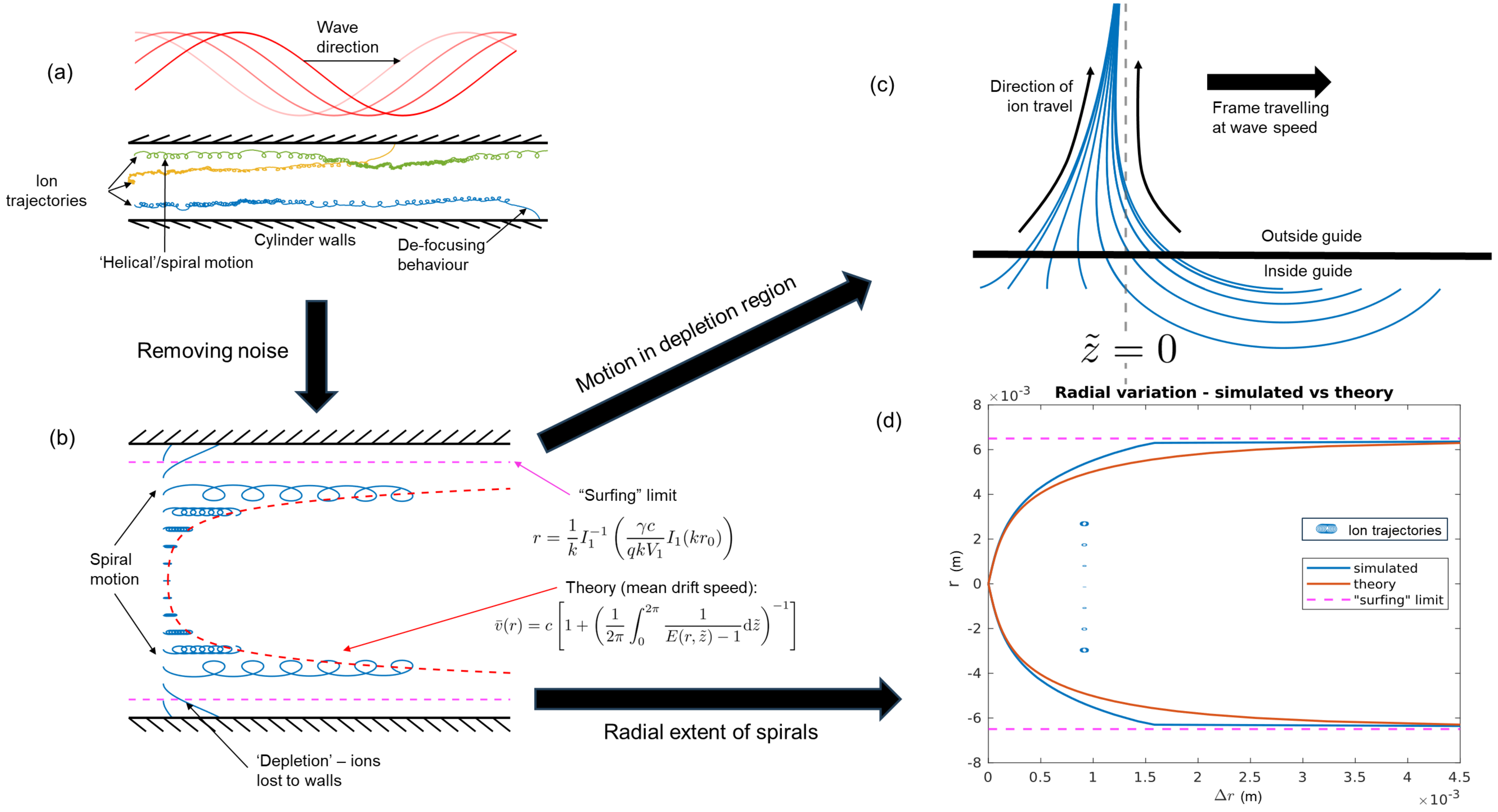

Figure 2. (a) Preliminary simulation showing general ion behaviour with noise; (b) removing noise shows 'spiral' and de-focusing behaviour varying with radial positions; (c) motion of ions in the de-focusing regime/'depletion' region; (d) agreement between theory and simulations for radial extent of 'spirals' varying with radial position

CONCLUSIONS

- Overdamped analysis of ion motion in cylindrical confining travelling wave predicts key characteristics observed in noisy motion—'helical' and 'depletion' regimes.
- Mean drift speed of ions in the 'helical' regime are dependent on radial positions—slower near the centre of the guide and faster further away.
- Ions will be lost once they enter the 'depletion' region, resulting in reduced transport efficiency.
- Radial extent of the 'helical' motion is also position-dependent, which is smaller at the centre of the guide and larger near the edges.
- Theoretical predictions of the mean drift speed and the radial extent of the 'helical' motion agree well with numerical simulations.
- Further work to be done on inertial corrections, many-body interactions, many-wave interactions and advection-diffusion approximation to the particulate problem.

ACKNOWLEDGEMENTS

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References

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