Improving the worthiness of the Elder problem as a benchmark for buoyancy driven convection models

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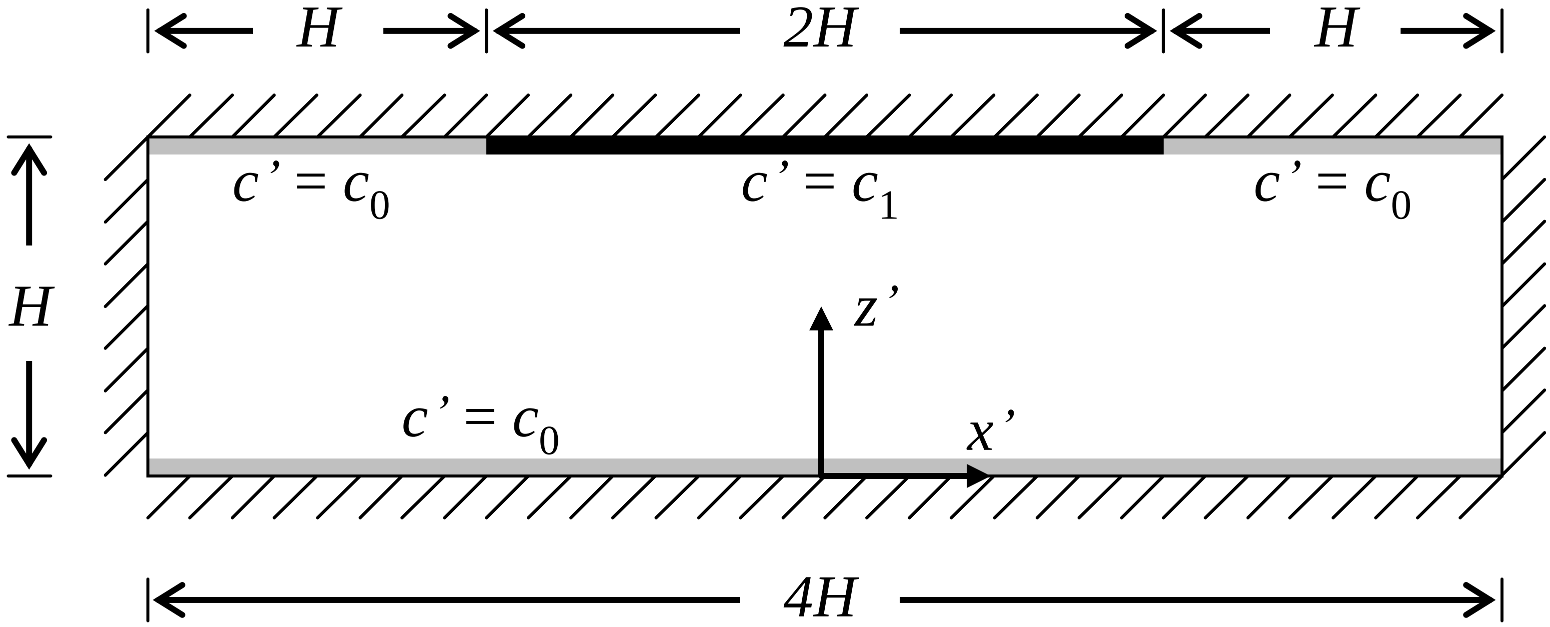
Abstract

An important trapping mechanism associated with the geosequestration of CO_2 is that of dissolution into the formation water. Although supercritical CO_2 is significantly less dense than water, experimental data reported in the literature show that the density of an aqueous solution of CO_2 could be slightly greater. Under normal situations, the transfer of gas to solution is largely controlled by the relatively slow process of molecular diffusion. However, the presence of variable densities can trigger off gravity instabilities leading to much larger-scale convection processes. Such processes can potentially enhance rates of dissolution by an order of magnitude. Consequently there is a need for future performance assessment models to incorporate buoyancy driven convection (BDC).

A major issue associated with BDC models is that of grid convergence when benchmarking to the Elder problem. The Elder problem originates from a heat convection experiment whereby a rectangular Hele-Shaw cell was heated over the central half of its base. A quarter of the way through the experiment, Elder (1967) observed six plumes, with four narrow plumes in the center and two larger plumes at the edges. As the experiment progressed, only four plumes remained. The issue is that depending on the grid resolution used when seeking to model this problem, modelers have found that different schemes yield steady states with either one, two or three plumes. The aim of this paper is to clarify and circumvent the issue of multiple steady state solutions in the Elder problem using a pseudospectral method.

Schematic diagram of the problem



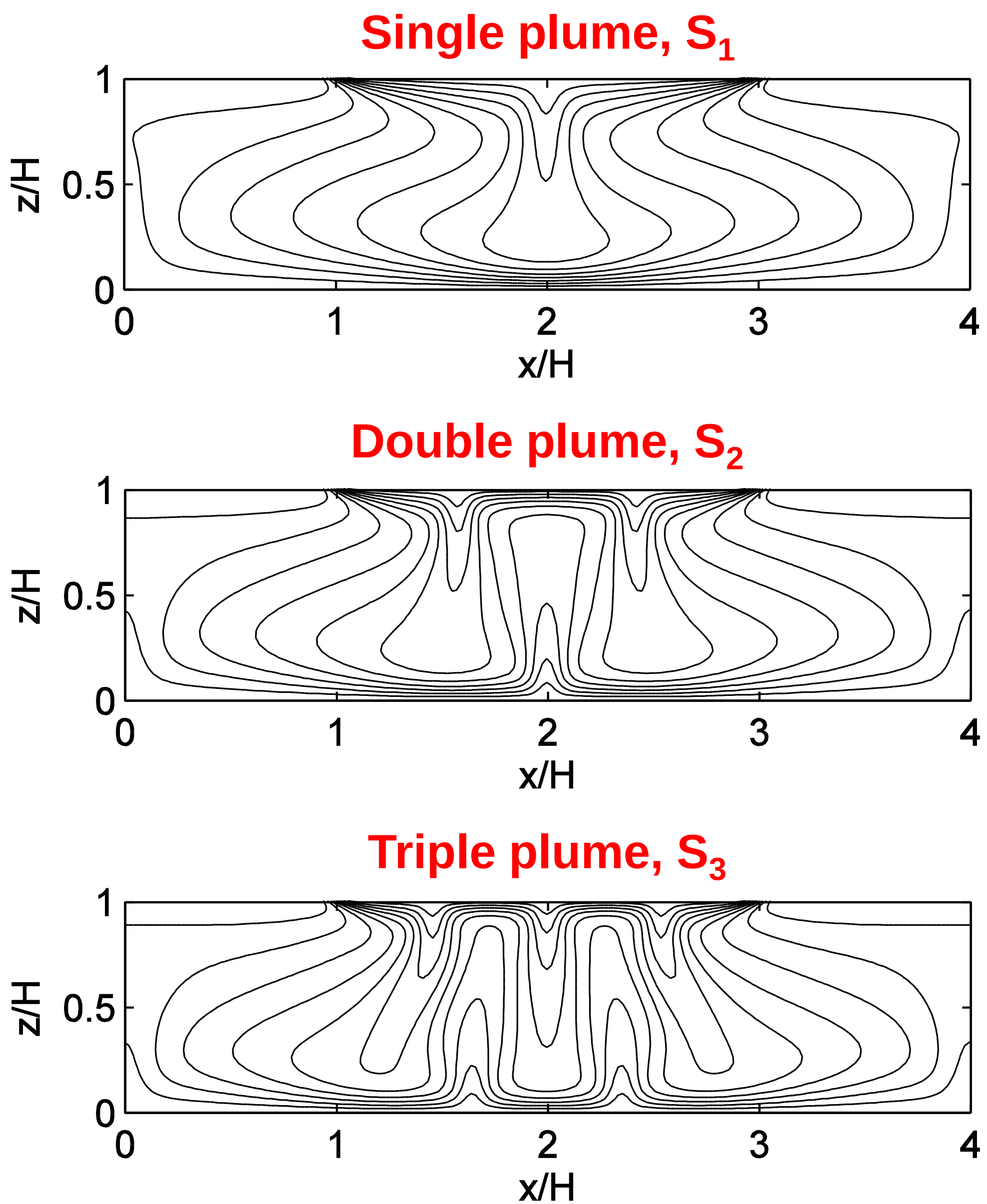
Elder's experiment is characterized by a Rayleigh number, $\mathrm{Ra} = \dfrac{\alpha \rho_0 k g (c_1 - c_0) H}{\mu D_E} = 400$

$\alpha = \rho_0^{-1} dc'/d\rho$ [ML^{-3}]	$(c_1 - c_0)$ [ML^{-3}] is the concentration difference
ρ_0 [ML^{-3}] is the desnsity when $c' = c_0$	H [L] is the domain thickness
k [L^2] is permeability	μ [ML^{-1}T^{-1}] is the dynamic viscosity
g [LT^{-2}] is gravitational acceleration	D_E [L^{2}T^{-1}] is the effective diffusion coefficient

The multiple steady states

Depending on the numerical model and grid-resolution, the stable steady states S_1, S_2, and S_3 are observed.

Do these ambiguities render numerical predictions useless?



A pseudospectral code for simulating buoyancy driven flow

Governing equations:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \frac{\partial c}{\partial x}$$

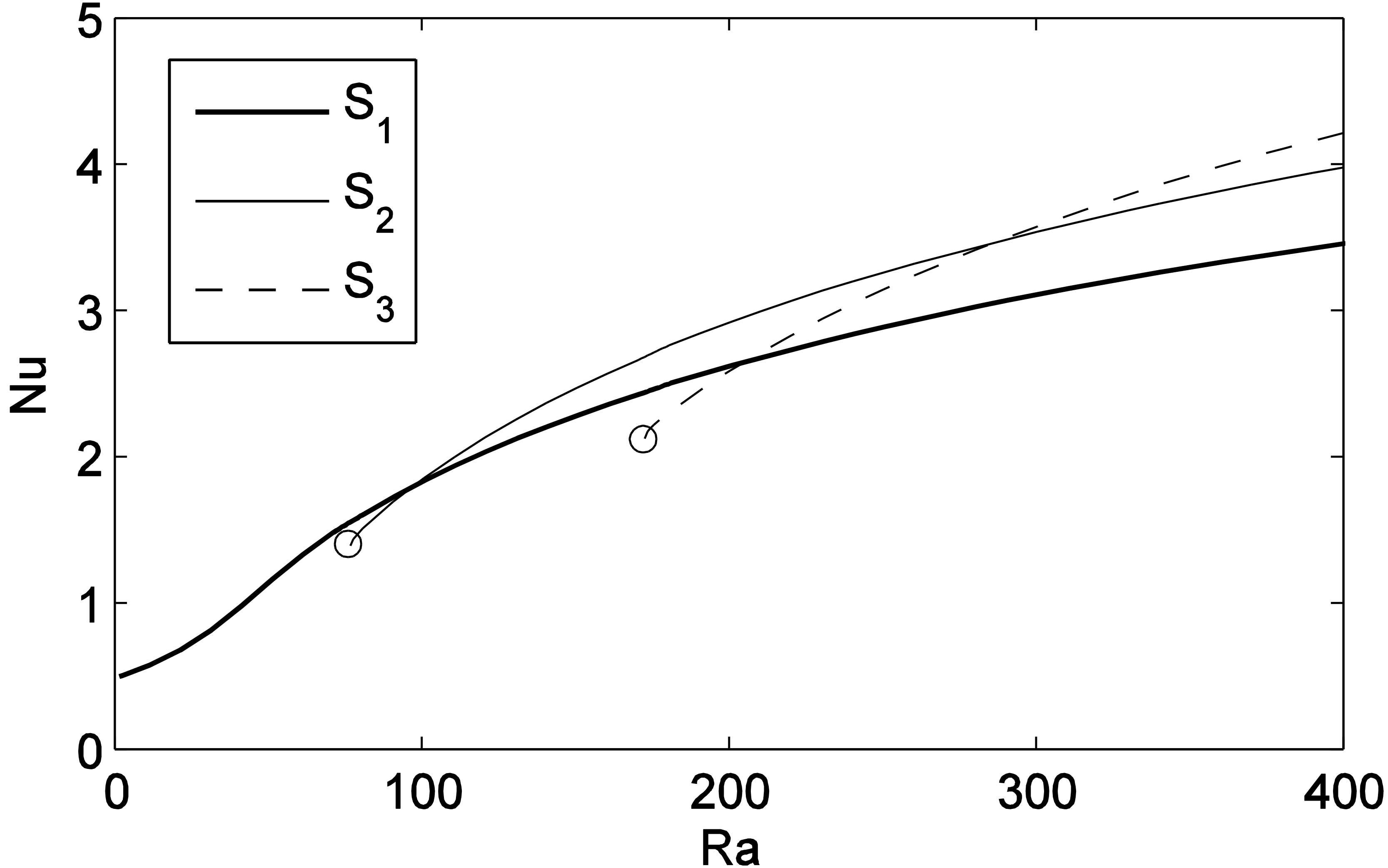
$$\frac{\partial c}{\partial t} + \mathrm{Ra}\left(\frac{\partial \psi}{\partial z}\frac{\partial c}{\partial x} - \frac{\partial \psi}{\partial x}\frac{\partial c}{\partial z} \right) = \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial z^2}$$

where ψ is the streamfunction and c is the concentration.

These equations are solved with a pseudospectral method which employs sine-and cosine-series in the horizontal (x) direction and Chebyshev polynomials in the vertical (z) direction.

The use of a pseudospectral method avoids all truncation error associated with differentiation.

Bifurcation diagram



Bifurcation diagram - observations

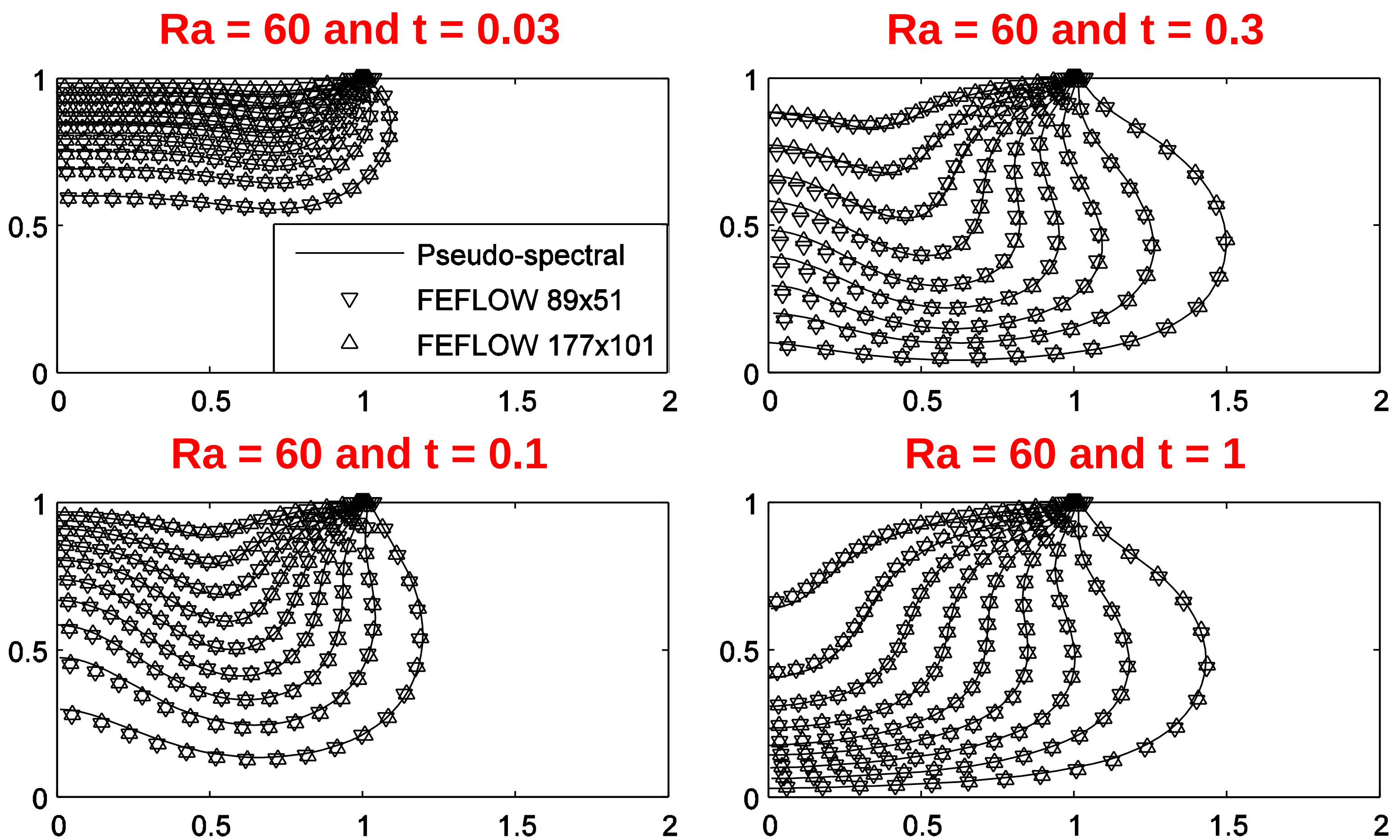
- At $\mathrm{Ra} = 400$ there are three stable steady state solutions;
- The higher states S_2 and S_3 come into existence via a fold-bifurcation (Johannsen, 2003);
- Below $\mathrm{Ra} = 76$, there is only one stable steady state.

Hence, the ambiguities are physical rather than numerical; at $\mathrm{Ra} = 400$, three stable steady states co-exist.

If Ra is lowered to 60, there will be only one stable steady state.

We call this the Low Rayleigh Number Elder Problem.

Low Rayleigh Number Elder Problem (Ra = 60)



A comparison of the pseudospectral method with the commercial groundwater-flow simulation software FEFLOW shows excellent agreement, regardless of the initial conditions employed.

Conclusions

- The aim of this paper is to clarify and circumvent the issue of multiple steady state solutions in the Elder problem.
- A pseudospectral method was used to produce a bifurcation diagram for $0 < \mathrm{Ra} < 400$ which is free of spatial discretization error.
- The results confirm that the multiple steady states are indeed an intrinsic characteristic of the Elder problem.
- The existence of multiple steady states makes the original $\mathrm{Ra} = 400$ Elder problem unsuitable for benchmarking numerical models.
- To avoid the multiple steady states, we propose a benchmark at $\mathrm{Ra} = 60$.
- Look out for:

M. van Reeuwijk, S. A. Mathias, C. T. Simmons, J. D. Ward (2009) Insights from a pseudospectral approach to the Elder problem. *Water Resour. Res.*