Stanford Public Release Electrophoretic Separation Solver (SPRESSO)

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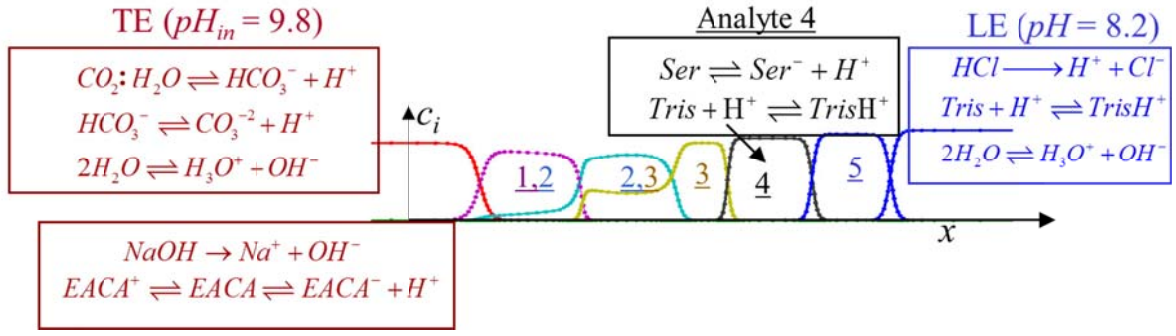
At Stanford Microfluidics Laboratory, we have developed a novel and unique tool for simulations of a wide range of electrokinetic (including electrophoresis) phenomena. We have named this tool SPRESSO and it is available for free at http://microfluidics.stanford.edu/spresso. SPRESSO is an open source simulation tool which uses compact schemes along with adaptive grid algorithm for fast and high resolution simulations of nonlinear processes in electrokinetics. We wrote the source code of this tool in MATLAB in order to facilitate user development, modification, and understanding of our tool. We further summarize its capabilities below. Our development of this tool has been published in four journal papers listed below.[1-4] These publications contain the basic physics, formulations, numerical schemes, speed tests, example simulations, verification and experimental validation of SPRESSO. The tool has also been featured in several review articles[5,6] and magazine articles,[7-10] including Science Magazine News[7] and PhysOrg.[9]

We have created an extensive website (http://microfluidics.stanford.edu/spresso) to describe and openly distribute SPRESSO. This includes three tutorial videos with step by step instructions and tips on running the tool, and a series of example input files and example problems for simulating zone electrophoresis and isotachophoresis. Our tool has been downloaded a total of 270 times since September 2008, with 180 unique downloads in the first year of its release. We are constantly working on enhancing the features of SPRESSO and we have actively provided support to its users, which include, for example, researchers at the Lawrence Livermore National Laboratory, Department of Clinical Pharmacology at University of Bern (Switzerland) and the School of Chemistry at University of Tasmania (Australia).



Example SPRESSO simulation of isotachophoresis (ITP). The plot shows a snapshot of unsteady concentration profiles in anionic ITP. The points along the curves are grid points in this adaptive grid simulation. This high electric field, ~13 species simulation with equilibrium reaction chemistry was completed in less than about 3 minutes. The text boxes highlight several relevant equilibrium equations as examples, including equations modeling the effect of atmospheric carbon dioxide on bicarbonate ion generation. TE and LE are respectively trailing and leading electrolytes.

Capabilities and features of SPRESSO

- Multispecies solver for problems of coupled advection, diffusion, and electromigration.[1-3]
- Chemical equilibrium for general weak electrolytes including ampholytes.[11]

- One-dimensional area-averaged formulation which captures Taylor-Aris type dispersion due to secondary flows.[4]
- Non-uniform electroosmotic flow simulation and internal pressure generation.[4]
- Compact 6th order spatial discretization scheme[1,2] for higher resolution using lesser grid points.
- Adaptive grid refinement for dynamically concentrating grid points at regions of high gradients.[1,2,12]
- Adaptive time step algorithm[1,2] for optimal operation across different electrokinetic problems.
- Moving frame of reference with non-reflective boundary conditions[1,2] for smaller computational domain and faster simulations.
- Detailed model for dependence of mobility and dissociation constants of chemical species on ionic strength.[3,13]
- Built-in database of over 300 chemical species including common buffer species.[14-16]
- Under development: Variable cross-section model[17] and unconditionally stable SLIP (Symmetric Limited Positive) numerical scheme for enhanced capability, faster simulations and robust performance.

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Acknowledgements

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