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# Theory and Simulation of Fick's Historical Verification of the 2nd Law

M. E. Glicksman[1], R. DiDomizio[2], A. Lupulescu[1]
[1]Materials Science and Engineering Department
Rensselaer Polytechnic Institute, Troy, NY, 12180, USA
[2]GE Global Research Center
Niskayuna, NY, 12309, USA

## 1. Introduction

The initial verification of Adolf Fick's second law was provided by his famous salt experiments. Fick placed a layer of sodium chloride crystals at the bottom of two differently shaped funnels connected to large reservoirs of fresh water. As the experiment progressed and salt molecules diffused up and out of the funnel, the reservoirs were refreshed steadily with pure water to establish eventually a steady-state concentration gradient. His measurements, conducted via densitometry, of the NaCl concentration profile showed that a right-circular cylindrical funnel yields a linear variation of density versus distance down the funnel, whereas a conical funnel yielded a non-linear (concave downward) plot of density versus distance. These experimental results matched his theoretical calculations, proving the validity of Fick's now famous "second law."

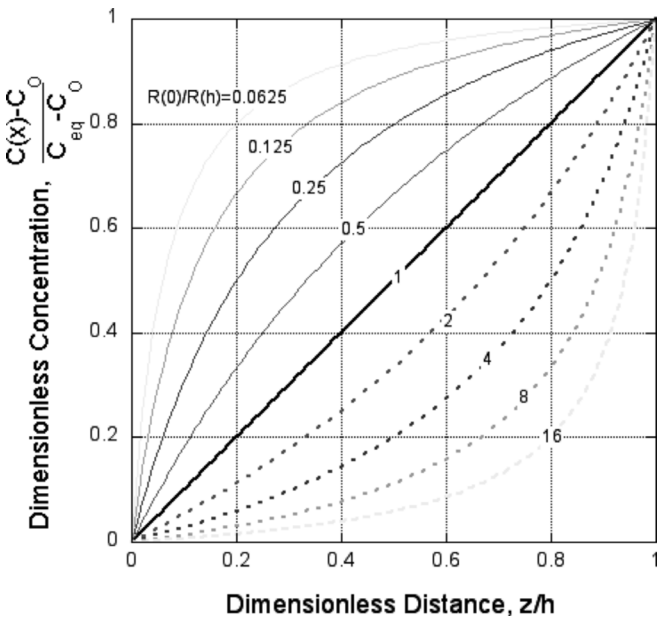


Fig. 1 Dimensionless steady–state concentration versus depth, *z*.

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## 2. Results

Exact steady-state solutions to Fick's linearized differential equations of diffusion are easily found. The theoretical predictions provide time-independent concentration fields, $C(z)$, that vary nonlinearly with $z$, excepting the case of a uniform cylindrical funnel. A computer model based on a Monte Carlo random walk algorithm was developed and run on the Matlab® platform to simulate the molecular diffusion process, and to verify the theoretical solution using modern methods. To permit the simulations to be conducted efficiently in two spatial dimensions, the shape of the funnel was modified from one used by Fick with a varying circular cross section, to one with a varying rectangular cross section of constant thickness. Simulations were run for various geometries by varying the maximum and minimum dimensions of the diffusion path.

## 3. Conclusion

The results produced by the Monte Carlo simulation compare well with solutions to Fick's laws, provided that sufficient realizations are employed and that the random walkers are permitted to travel the full length of the funnels.