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Boltzmann's transformation for hydrogen diffusion in a system with traps

Boltzmann's transformation [1,2] is a substitution that under certain boundary conditions reduces diffusion equation in one dimension from partial to ordinary differential equation that depends on a single variable $u=x/\sqrt{2Dt}$, where x is the coordinate, D the diffusion coefficient, and t the time. After that, numerical integration is possible that is faster and more precise than for the initial partial differential equation. We show that Boltzmann's transformation can be also applied to a McNabb-Foster equation describing hydrogen diffusion in a metal containing traps. In the case of a single trap, further simplification to a particularly simple parameterless differential equation is possible. We further show that this transformation is applicable in the case of two and more traps, although the equation becomes rather complicated. The transformation works also for cylindrical and spherical geometries and for the traps that can be occupied by more than one hydrogen atom. The results obtained are compared with numerical results obtained using the FESTIM software [3].

1. L. Boltzmann, Annual Review of Physical Chemistry 53, 959 (1894).
2. J. Crank, The Mathematics of Diffusion. Clarendon Press, Oxford (1975), p. 105.
3. R. Delaporte-Maturin et al., Int. J. Hydrogen Energy 63, 786 (2024).

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