

Noble gases isotopic and elemental fractionation by diffusion in oil and gas under reservoir conditions: A molecular dynamics perspective

HAI HOANG¹, ROMAIN VERMOREL¹, GUILLAUME GALLIERO^{1*}, MAGALI PUJOL²

¹LFCR– IPRA, UMR5150 TOTAL-CNRS, Univ. Pau & Pays Adour, BP1155, 64013 PAU Cedex, France

(hhoang052@gmail.com, romain.vermorel@univ-pau.fr,

*correspondence : guillaume.galliero@univ-pau.fr)

²TOTAL EP, CSTJF, Avenue Larribau, 64000 Pau, France
(magali.pujol@total.com)

Noble gases are widely used as natural tracers to characterize migration and origin of fluids in geological environments. As they are chemically inert, they are only fractionated by physical phenomena. Molecular diffusion is one of these phenomena. To quantify such a fractionation, the “square root relationship”, i.e. a fractionation proportional to the reciprocal of the square root of the atomic masses, is mostly used [1]. However, such an approximation derived from kinetic gas theory should be valid only for isotopes in cosmic environments or in the limit of ultra-tight porous medium, i.e. in the free-molecule diffusion regime [2]. Thus, the applicability of this relationship is questionable when dealing with noble gases and their isotopes in geofluids [3, 4] such as those in petroleum reservoirs.

To address this point we performed extensive classical molecular dynamics computations of diffusion coefficients of some noble gases (Ne, Ar, Kr, Xe) and their isotopes in various hydrocarbons fluids (gas and oil) under reservoir conditions. Molecular simulation results showed that the “square root relationship” is inadequate and tends to overestimate the isotopic fractionation in all cases consistently with what is obtained in water [4]. Interestingly, it was found that it is possible to generalize a relationship based on the gas mutual diffusion formulation [2] to describe all results. Concerning elemental fractionation by molecular diffusion, rather surprisingly simulations showed that the “square root relationship” correlates well the results for a large class of fluids and thermodynamic conditions.

[1] Ozima & Podosek (2002) *Noble Gas Geochemistry*, Cambridge University Press. [2] Marty (1984) *Geochem. J.* **18** 157-162. [3] Tyroller et al. (2014) *GCA* **136** 60-66. [4] Bourg & Sposito (2008) *GCA* **72**, 2237-2247.