

Revisiting Noble Gas behaviour in Natural Energy Resources from a Molecular Simulation perspective

GUILLAUME GALLIERO^{1*}, HAI HOANG², ROMAIN VERMOREL¹, MAGALI PUJOL³

¹ LFCR, UMR 5150 TOTAL-CNRS-Univ. Pau & Pays Adour, E2S, BP 1155, 64013 Pau Cedex, France (romain.vermorel@univ-pau.fr, *correspondence : guillaume.galliero@univ-pau.fr).

² IFAS, Duy Tan University, 10C Tran Nhat Duat Street, District 1, Ho Chi Minh City 70000, Viet Nam.

³ TOTAL EP, CSTJF, Avenue Larribau, 64000 Pau, France (magali.pujol@total.com).

Noble gases are widely used as natural tracers to characterize storage, migration and origin of fluids in geological environments [1]. As they are chemically inert, they are only fractionated by physical phenomena, such as phase partitioning, mass diffusion or thermodiffusion. However, the quantification, and the modeling, of the related physical parameters (Henry's constant, diffusion coefficient, thermal diffusion factor) is not an easy task especially when dealing with petroleum systems [2].

To address the quantification and the modeling of noble gas fractionation in natural energy resources, molecular simulation is an appealing option as this numerical tool provides complementary information to experiments. Thus, during the talk we will show how molecular simulations can be used to provide quasi experimental data on noble gas phase partitioning, mass diffusion and thermodiffusion in model petroleum fluids helping to revisit the existing modeling of such systems [3].

[1] Ozima & Podosek (2002) *Noble Gas Geochemistry*, Cambridge University Press. [2] Ballentine et al. (2002), *Rev. Min. Geoch.* **47** 539-614. [3] Hoang et al. (2019) *Eur. J. Phys. E* accepted.