Moisture slows down propane diffusing through rocky pores

Natural gases emanate from the ground passing through tiny pores and fractures in silica rich rocks. These tiny pores alter the behavior of the gases passing through them. To understand the fundamental processes involved in gas migration through these pores and to aid better recovery of these gases from the earth, it is essential to understand the behavior of gases inside model pores. For this reason, several studies have been carried out to understand the behavior of methane, ethane and propane in engineered silica pores. In natural environment however, the pores are often laden with moisture and so it is important to understand the effects this moisture might have on the migration of gases through the pores. One way of investigating gas motion through porous materials is using neutron scattering experiments. In such experiments, a beam of neutrons with a known energy is bombarded on a material to be studied.

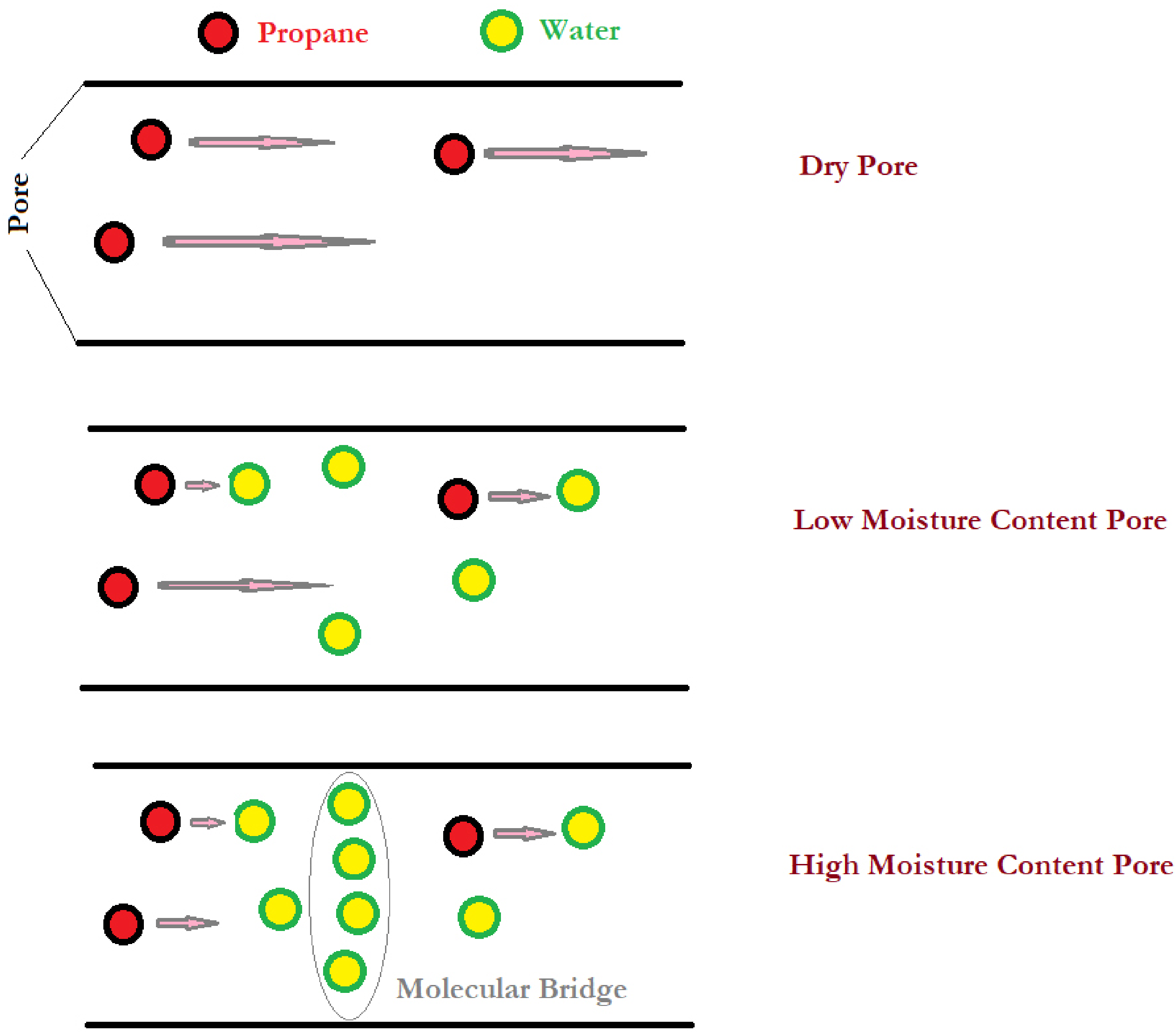

Fig. 1. Slowing down of propane motion through silica pores by water. In absence of water, propane (red discs) molecules are able to move through the silica pores unhindered (top panel). When some water molecules (yellow discs) are introduced in the pore, they tend to slow down propane (middle panel). At very high contents of water, some water molecules form a bridge across the pore, thereby blocking propane motion (bottom panel).

The neutrons get scattered by the molecules in the material and in the process change their direction and speed. The scattered neutrons are detected and the change in their speed and direction is also recorded. These changes encode information, respectively, on the motion and structural arrangements of the molecules in the material being studied. In a recent experiment, we used quasielastic neutron scattering (QENS – a type of neutron scattering specifically suited to study diffusive motion) to study the effect of moisture on the diffusive motion of propane inside 1.5 nm wide pores of silica material. These experiments revealed that presence of moisture slows down the diffusive motion of propane through silica pores. To understand the molecular origin of this finding we carried out computer experiments using molecular dynamics simulations. In these experiments models of the real system are made and Newton's equations of motion for the system are solved numerically. These calculations provide trajectories of each molecule constituting the system in time. These molecular trajectories are akin to molecular movies in which behavior of molecules over a period lasting several nanoseconds can be seen. The results from the computer experiments confirmed the experimental findings. Further, it was found that the slowing down effect of moisture on propane motion becomes stronger at higher contents of moisture. At very high contents of moisture, motion as well as the structural arrangement of propane molecules inside the pores are severely affected. Further, the computer experiments show that the slowing down of propane in moist pores is due to the water molecules making bridges across the pore that block the motion of propane molecules (see illustration). Our experiments in the lab and with computers thus explain the effect moisture has on the motion of propane through silica pores. These findings have important implications for gas extraction and recovery from sub terrestrial environment.

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Effects of water on the stochastic motions of propane confined in MCM-41-S pores.
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