

# Deep Earth Water Model for Predicting the Formation of Immiscible Hydrocarbons in Subduction Zones

JINGYI HUANG<sup>1</sup>, DIMITRI A. SVERJENSKY<sup>1</sup>, ISABELLE DANIEL<sup>2</sup> AND ALBERTO VITALE BROVARONE<sup>3,4,5</sup>

<sup>1</sup>Johns Hopkins University

<sup>2</sup>Laboratoire de géologie de Lyon UMR 5276, Université Lyon1  
- Ens de Lyon - CNRS

<sup>3</sup>Università di Bologna

<sup>4</sup>Institute of Geosciences and Earth Resources, National  
Research Council of Italy

<sup>5</sup>IMPMC, Sorbonne Université - Muséum National d'Histoire  
Naturelle - UMR CNRS 7590 - IRD

Presenting Author: [jyhuang@jhu.edu](mailto:jyhuang@jhu.edu)

Fluids generated from subducted slabs are important for the carbon cycle in the deep crust and upper mantle. In these fluids, both inorganic and organic carbon are important. To date, natural CH<sub>4</sub>-H<sub>2</sub> fluid inclusions in the ophicarbonates in metamorphosed ultramafic rocks have demonstrated the existence of hydrocarbon fluids at upper mantle conditions [1]. Experimental studies of the disproportionation reaction of 0.5 M Ca-acetate solution at 300 °C and 1.6 – 4.6 GPa have documented the formation of immiscible hydrocarbon fluid containing methane, ethane, propane, and isobutane coexisting with aqueous HCO<sub>3</sub><sup>-</sup> and CO<sub>3</sub><sup>2-</sup>, and aragonite or calcite minerals [2].

To investigate the conditions under which immiscible hydrocarbon fluids form, we set up a chemical mass transfer model using equilibrium constants from the Deep Earth Water model to simulate the reactions in the experiments and in nature. We calculated the standard Gibbs free energies of fluid methane, ethane, propane, and isobutane at 300 – 650 °C and 1.5 – 4.5 GPa. The fluid hydrocarbons were treated as a fluid solution so they could form a separate phase immiscible with aqueous C-species coexisting with minerals. In the model, reaction progress caused changes of pH, logfO<sub>2</sub>, and aqueous species, and the formation of hydrocarbon fluids and aragonite. Hydrocarbon fluids were more stable at high pressures. In contrast, aragonite was stable at 1.5 GPa but undersaturated at 4.5 GPa. Both results are consistent with experiments. Methane was the most abundant hydrocarbon species in all the models, whose mole fraction slightly decreased with pressure. However, isobutane was significant in some experiments, suggesting that experiments might not have reached equilibrium when the Raman spectroscopy ratios of acetate/HCO<sub>3</sub><sup>-</sup> reached steady state. Oxygen fugacity decreased with increasing temperature and pressure relative to the QFM buffer. We then applied our fluids to react with metamorphic mineral assemblages to simulate the stability of hydrocarbons in pelitic, mafic and ultramafic environments. Our models indicate possible conditions for the formation of immiscible, abiotic hydrocarbon fluids in subduction zones.