Soil vapour characterization and intrusion to indoor air: a reactive transport modelling approach

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Introduction

Vapour intrusion to indoor air often represents a significant exposure pathway for risk assessment at sites contaminated by volatile petroleum hydrocarbons. While the importance of biodegradation processes on the fate and transport of petroleum hydrocarbon vapours is well established [1; and references therein], fewer studies have investigated site specific factors such as source concentration and location with respect to the building, pressure conditions, and soil properties, all of which have been shown to impact the potential for vapour intrusion [e.g., 2-4]. In this numerical modelling study, site specific factors are evaluated using the multi-component reactive transport code MIN3P-DUSTY [5-6]. The model includes the key processes of hydrocarbon volatilization, gas- and aqueous-phase diffusion, gas-phase advection, aerobic biodegradation (using dual-Monod kinetics formulation) and sorption in a domain comprising the subsurface and the building foundation. Benzene and iso-octane are used as surrogates of the aromatic and aliphatic compounds of the gasoline vapours. Initially, a sub-model for transport through concrete and within foundations cracks was developed and benchmarked against an analytical solution. The model was calibrated based on a high quality data set for an unoccupied research house located above a petroleum hydrocarbon plume (located in North Battleford, Saskatchewan, Canada), and then used to predict the hydrocarbon vapour distribution for a range of observed and hypothetical conditions.

Results & Conclusion

For the observed site conditions, the calibrated model indicates soil vapour transport is dominated by diffusion and aerobic biodegradation, and that building pressures and soil gas advection have little influence on soil vapour concentrations. Comparison of wetter (spring) and drier (winter) conditions indicate that the vadose zone oxygen concentrations above the contamination source area are lower for wetter spring conditions because of the reduced diffusion through relatively wet surface soils. For most scenarios simulated, there is rapid attenuation of benzene within approximately 1 m of the source; however, less attenuation of iso-octane is predicted, consistent with site data. For a shallow NAPL scenario, a concrete foundation slab resulted in an oxygen shadow and increase in benzene and iso-octance concentrations below the building.

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Clumped isotope Vs. fluid inclusion thermometry in crystals from Oman.

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Clumped isotopes are a new exciting tool in the domain of paleothermometry. The “clumped isotopes carbonate paleothermometer” has been tested and used as a new temperature proxy for paleoclimate studies during the last few years. Indeed, clumped isotopes (Δ47) appear to be a great proxy since they are based on the degree of association of ^{13}C and ^{18}O into the carbonate ions, a function of thermodynamics. Therefore, measuring Δ47 allows the determination of the formation temperature of the carbonate material independent of the isotopic composition of the precipitating fluid. Furthermore, unlike other proxies, Δ47 seems insensitive to potential ‘vital effects’.

However, there is still a lot to unravel in this field of geochemistry, and some improvement and development are necessary. Some processes, such as kinetic fractionation, need to be identified and better understood in order to apply this proxy in the most precise way possible. Studies need to include comparisons between clumped isotopes and other temperature proxies.

Here we intend to compare data from both fluid inclusions microthermometry and clumped isotopes measurements carried out on the same material. Our focus has been placed on calcite crystals sampled in the carbonate carapace of a salt dome at Jebel Madar, Oman, where preliminary data suggest a low temperature precipitation.

As carbonates are very reactive minerals, diagenesis and metamorphism could re-order the isotope clumping configuration in the carbonate and the measurements would reflect the equilibrium temperature of recrystallisation. Hence, careful consideration needs to be given to sampling strategies. Calcite crystals were sampled in fractures showing multiple pulses of opening, and the crystals themselves show evidence for growth zoning and fracture healing. We focus our study on deciphering and understanding the processes and effects of diagenesis on the reliability of the carbonate clumped isotope paleothermometer.

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