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A Promising Portable Tool for the Continuous, Online, and Field Monitoring of Pressured Processes

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s exemplified by the recent massive gas leak at Porter Ranch California, hydraulic fracking¹ or other human activities,² their impacts on our groundwater and other deep water reservoirs (brines) could be significant and should be monitored on a continuous basis. But, unfortunately, this is not always the case for all pollutants, especially when field operations and high pressure measurements are required. Hence, in the largest sample pool and most cited study on the pollution associated with hydraulic fracking,¹ water analyses were performed in the laboratory by mass spectrometry on samples taken in a oneoff manner at water wells. Therefore, being able to monitor, in real time (online), and over a long time period, the composition of ground waters is yet a challenge which, once solved, has the potential to lead to significant societal impact. Therefore, it is a very promising solution that is being brought to the scientific community in the article of the Mizaikoff group.³

Indeed, this month, the Mizaikoff group reports their studies of CO_2 and CH_4 concentration measurements when dissolved under harsh conditions (high pressure in simulated deep saline aquifers). This is done using a portable infrared spectrometer equipped with a specifically designed attenuated total reflection (ATR) cell (Figure 1), enabling



Figure 1. Schematic of the ATR pressure cell (red line represents the IR beam). Figure reproduced with permission from ref 3. Copyright 2016 American Chemical Society.

reproducible measurements to be performed in such conditions as can be found underground (especially high pressures, up to 14 MPa). It is shown that stable, linear and reproducible calibration curves can be obtained enabling the We need better, faster, and *in situ* tools, like that of Mizaikoff et al., to track ground water quality (*ACS Sensors*).



As we continue to manipulate our groundwater reserves through drilling, fracking, and other activities, it becomes ever more important to be able to monitor these reserves in real time.

calibration of the sensor and therefore the measurement of $\rm CO_2$ and $\rm CH_4$ concentrations in simulated downhole conditions.

This study is paramount to enable the understanding, modeling, and eventual usage of such aquifers for the deployment of CO_2 and CH_4 sequestration strategies. The compact FTIR that has been developed to do so can

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be fitted to most downhole pressure lines and therefore is suitable for permanent and online/in-line monitoring (note that it also measures temperature and pressure, which are key for real life measurements and calibrations). But beyond sequestration, measuring concentrations of molecules in the reservoir's conditions will enable a much better understanding of their chemistries.

What is clear from the data presented is that this approach could be used for many other purposes and chemical mixtures, since fairly large functioning windows exist in the IR spectra of the ATR cell (Figure 2), including other



Figure 2. Typical FT-IR-ATR spectrum obtained showing simultaneous detection of CO_2 and CH_4 as well as the wide available wavenumber range available for more complex mixtures studies. Figure provided by T. Schaedle and B. Mizaikoff.

alkanes, ammonia, nitrates, and other chemicals of interest. Ammonia is especially important as its impact on the environment is too seldom studied currently due to the lack of adequate ammonia sensors.^{4,5}

For all these reasons, we suspect that, if such a cell could quickly be made available to the research community, it would become a standard for online, in field, studies in the harsh conditions of ground waters. We therefore look forward to future reports from this group using this device on more complex mixtures, including ammonia and other alkanes, not to mention the study of carbonate's chemistry in real such environments and their reaction kinetics.⁶ Such kinetics will indeed play a key role in enabling or disabling industrial CO₂ sequestration, just as it did to enable multicellular life thanks to the carbonic anhydrase enzyme.^{7,8} The influence of the temperature on the calibration's stability will also have to be studied.

Finally, it would be interesting to benchmark the ATR cell developed here with the remote analytical capability made possible with chalcogenide or silver halide IR fibers used in evanescent wave spectroscopy.^{9,10}

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