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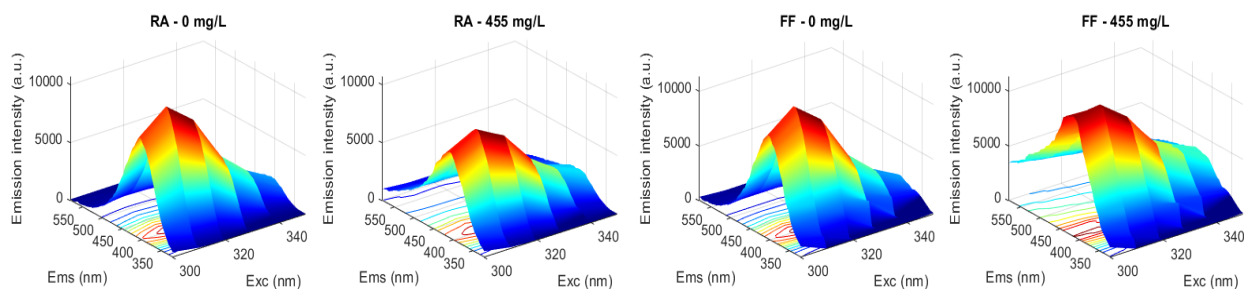
# Assessing information on both dissolved and dispersed species in oil-in-water dispersions by 3D fluorescence spectroscopy and chemometrics

Isabelle M. A. Viegas<sup>\*†1</sup>, Simon I. Andersen<sup>1</sup>, and Åsmund Rinnan<sup>2</sup>

<sup>1</sup>Danish Offshore Technology Centre, Technical University of Denmark, Elektrovej 375, 2800, Kgs. Lyngby, Denmark

<sup>2</sup>Department of Food Science, University of Copenhagen, Rolighedsvej 26, 1958, Frederiksberg C, Denmark

Produced water (PW) consists of non-polar oil droplets dispersed in a water phase rich with aromatic components. Although PW is submitted to de-oiling processes before discharge to the sea, such processes only remove dispersed oil, and a considerable concentration of aromatics and other toxic dissolved components remain in the water thereafter considered appropriate for discharge. In this context, fluorescence spectroscopy is a promising technique for the quantification of crude oil in water because, in addition to being fast, low-cost, and simple, it detects both dissolved and dispersed species, when properly explored. Since crude oil is a complex matrix, a single emission spectrum per sample usually is not sufficient to provide information on dissolved and dispersed species. Therefore, we propose the use of 3D fluorescence landscapes treated with appropriate chemometric tools to overcome inner-filter effects and to unmix the signal from dissolved and dispersed oil components. The first set of samples consisted of oil-in-water emulsions with dispersed oil concentrations ranging from 0 to 1250 mg L<sup>-1</sup>, prepared in a water phase with a constant, saturated concentration of dissolved oil compounds. The second set of samples was composed of a dilution series of oil-in-water emulsions with stable droplets and, therefore, a nearly constant concentration of oil inside the droplets. The 3D fluorescence landscapes of all samples were measured with excitation from 300 to 350 nm and emission from 320 to 580 nm, by both front-face (FF) and right-angle (RA) cuvette geometries. Some of the landscapes are depicted in **Figure 1**. Increasing the concentration of dispersed oil caused redshift and decreased the emission intensities in RA and led to increases in emission intensities in FF, which is due to different optical path lengths for the two cuvette geometries. In RA the excitation beam hits more fluorophores along the optical path and therefore is more affected by inner-filter effects than FF for higher oil concentrations. The excitation-emission matrices (EEM) were preprocessed to remove the 1<sup>st</sup>-order Rayleigh scattering and decomposed into two or three pure components (factors) by trilinear factorization. The saturated water phase (initially not containing dispersed oil, i.e., “0 mg L<sup>-1</sup>”) had high scores for some factors that responded to the additions of oil decreasing the RA signal and were nearly constant by FF. Therefore, such factors were associated with the dissolved oil in the water phase. On the other hand, another factor had increasing scores as the dispersed oil concentration increased, which might be directly related to the dispersed phase. We could conclude that the signals from dissolved and dispersed oil are different for different cuvette irradiation geometries and are related to the distribution of the fluorophores inside the droplets and in the water phase, and they can be differentiated by factorized 3D fluorescence data.



**Figure 1.** 3D fluorescence spectra of oil-in-water dispersions saturated with dissolved oil and 0 (A and C) and 455 mg L<sup>-1</sup> (B and D) of dispersed oil.

\*Speaker

†Corresponding author: iviegas@dtu.dk