



Quantitative Survey and Structural Classification of Fracking Chemicals Reported in Unconventional Gas Exploitation

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Few technologies are being discussed in such controversial terms as hydraulic fracturing (“fracking”) in the recovery of unconventional gas. Particular concern regards the chemicals that may return to the surface as a result of hydraulic fracturing. These are either “fracking chemicals” – chemicals that are injected together with the fracking fluid to optimize the fracturing performance or geogenic substances which may turn up during gas production, in the so-called produced water originating from the target formation. Knowledge about them is warranted for several reasons.

(1) Monitoring. Air emissions are reported to arise from well drilling, the gas itself or condensate tanks. In addition, potential spills and accidents bear the danger of surface and shallow groundwater contaminations. Monitoring strategies are therefore warranted to screen for “indicator” substances of potential impacts. (2) Chemical Analysis. To meet these analytical demands, target substances must be defined so that adequate sampling approaches and analytical methods can be developed. (3) Transformation in the Subsurface. Identification and classification of fracking chemicals (aromatics vs. alcohols vs. acids, esters, etc.) is further important to assess the possibility of subsurface reactions which may potentially generate new, as yet unidentified transformation products. (4) Wastewater Treatment. For the same reason chemical knowledge is important for optimized wastewater treatment strategies. (5) Human and Ecosystem Health. Knowledge of the most frequent fracking chemicals is further essential for risk assessment (environmental behavior, toxicity) (6) Public Discussions. Finally, an overview of reported fracking chemicals can provide unbiased scientific into current public debates and enable critical reviews of Green Chemistry approaches.

Presently, however, such information is not readily available. We aim to close this knowledge gap by providing a quantitative overview of chemical additives reported for use in hydraulic fracturing. For the years 2005-2009 it is based on the Waxman report, and for the years 2011-2013 it relies on the database FracFocus, where it makes use of the data extracted and provided by the website “SkyTruth”. For the first time, we list fracking chemicals according to their chemical structure and functional groups, because these properties are important as a starting point for (i) the design of analytical methods, (ii) to assess environmental fate and (iii) to understand why a given chemical is used at a certain stage of the fracturing process and what possible alternatives exist.