11th World Conference on
Chemistry and Chemical Engineering
May 21-22, 2026 | Vienna, Austria

https://doi.org/10.62422/978-93-47569-00-5-008

Real-time dynamic analysis of liquid matrices with online measurements: Determination of initial headspace concentration and gas-liquid equilibrium

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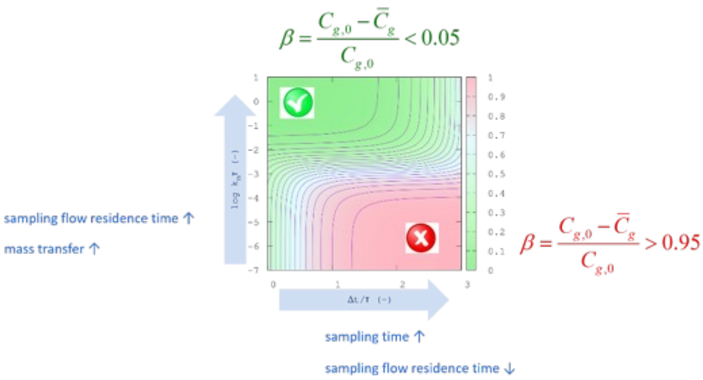
Dynamic headspace sampling is a crucial technique for analyzing consumer products, studying biological samples, and conducting environmental water tests. Specifically, initial headspace concentrations are vital in forensic investigations and in calculating Henry coefficients. In the latter context, ‘initial’ refers to equilibrium with the liquid phase, where deviations are undesirable. However, during dynamic measurements, achieving true equilibrium is often challenging, leading to potential inaccuracies if only the initial concentration is considered.

This work examines how experimental parameters – such as sampling time, flow rate, headspace volume, liquid volume, and Henry coefficient – affect the measured average concentrations. A corresponding analytical expression, as a function of these variables, is introduced to quantify the deviation of the initial headspace concentration. A measurement accuracy criterion (error below 5%) is also provided. The model is a bi-exponential function that consolidates various existing models for recovery in dynamic sampling into a unified expression (Heynderickx, 2019).

Additionally, the developed model can be applied to determine Henry coefficients for gas compounds in non-ideal solutions through parameter estimation, allowing the effects of real liquid phase conditions to be inferred from gas phase measurements.

Graphical Abstract



Reference

Heynderickx, P. M. (2019) Dynamic headspace analysis using online measurements: modeling of average and initial concentration. Talanta, 198, 573-584. https://doi.org/10.1016/j.talanta.2019.02.038

Biography:

Philippe M. Heynderickx is professor at Ghent University Global Campus (GUGC), South Korea, where he works on catalyst characterization for indoor air cleaning purposes (gas phase pollution mitigation) and in-depth modeling of photocatalysis as pollution remediation technique for air and aqueous phase systems. He is also active in the field of hydrothermal carbonization for upgrading waste (from marine origin, but also food waste and waste plastic) into hydrochar (adsorbent material) and activated carbon (adsorbent, catalyst carrier material…). Recently, he is involved in waste plastic upgrading via hydrothermal carbonization. In addition, he works on fundamental understanding of process phenomena by combining aspects from chemistry, engineering and mathematics. He is (co-)author of +100 publications in high-impact journals (average IF = 8.0). He received the Young Scientist Award on the 14th International Congress on Catalysis (ICC) in Seoul, Korea (2008).