Atmospheric
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Techniques

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Discussions

Interactive comment on "Separation and detection of aqueous atmospheric aerosol mimics using supercritical fluid chromatography–mass spectrometry" by D. N. Grace et al.

Anonymous Referee #1

Received and published: 14 March 2019

- GENERAL REMARKS The authors present a supercritical fluid chromatography–mass spectrometry method for separation and detection of aqueous atmospheric aerosol mimics. In this study SFC-MS was used to study methylglyoxal and ammonium sulphate creation mixture as mimics of reaction mixtures in atmospheric droplets. ESI and APCI ionisation modes were used for the detection of various species present in the reaction mixture. five different columns were screened to optimise separation and fourteen reaction products, detected for the first time, were reported. The study address challenges like separation of compounds with different polarities and reduction of analysis time. Identification of unknown fragments/compounds can be a strength of the work presented here. The study is relevant for the scientific community however

the study design is not comprehensive and several important aspects of experimental work are not completely described. I give some suggestions hereinafter.

- MAJOR COMMENTS - Aerosols are a mixture of solid particles and liquid droplets suspended in gases (air). The terms use of terms e.g. aqueous molecules, aqueous atmospheric systems and atmospheric droplets should be explained and the terminology should be consistent throughout the text to assist readers. - Introduction needs to be revised, ideally introduction should address 1) gaps in knowledge, 2) specific research question(s), 3) approach used to answer the research question(s) and 4) comparison with already available knowledge. In the current state, large part of introduction focuses on the theory of SFC which better fits in an SFC (P2, L28-35 and P3, L1-6 needs to be revised and should focus more on the analytes in question). - Authors compare SFC with LC and GC. With the development of UHPLC, analysis time has significantly reduced. Describing the benefits of SFC should not be stop having a nice comparison with available UHPLC methods. - In modern SFC, there is a huge range of packed columns available today. The authors should motivate why BEH (three types), HILIC and C18 columns were used for the screening for suitable stationary phase. - Section 2.3.2, L9 (optimal mobile phase conditions varied slightly with the identity of the column........). Why different mobile phase conditions were used to compared column efficiencies? For any comparison all the variables must be same except the one subject to comparison. Secondly what were the varied mobile phase compositions used for comparison? Why not to make use of supplementary information and add a figure/table to describe the actual experimental conditions? - Section 3.2.2, L6-7: include chromatograms in supplementary information - Section 3.3, L30-34: include mass spectra in supplementary information - ESI and APCI methods were not optimised for higher signal of the analyte, therefore, it is inappropriate to claim that APCI is not a better method based on the results. However, more information can be included from literature to motivate if APCI is a suitable ionisation source for polar compounds.

- MINOR COMMENTS - Suitable keywords should be included with abstract - P2, L3-4:

include a reference - Section 2.2, L10: "the mixture was allowed to react for at least a month......"; an accurate time must be included - P4, L22: add "that" between "to ensure" and "the mobile phase" - P6, L25: "......polar molecular interactions between analytes may be driving the solution through the column", a reference must be added to support the assumption - P7, L5: "........although all temperatures and modified conditions discussed below were tested on each column with similar results"; it is insufficient to state "similar results" when there is a possibility to include chromatograms in supplementary information and generate a more quality discussion - P7, L16: Its better to discuss the strengths/weaknesses of certain mobile phase in relation to properties of analytes rather then SFC itself. - P9, L8-15: the text should be revised considering both mobile phase density and kinetic effects should be considered in relation to retention times - The language needs revision in terms of use of article "the"