

Interactive comment on “An ion-neutral model to investigate chemical ionization mass spectrometry analysis of atmospheric molecules – application to a mixed reagent ion system for hydroperoxides and organic acids” by Brian G. Heikes et al.

Anonymous Referee #2

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This paper aims to develop and test a model of ion-neutral chemistry occurring in a reduced pressure chemical ionization flow reactor whereby ions are generated using a mixture of N₂, O₂, and CH₃I to produce O₂⁻ and I⁻ simultaneously.

The model focuses mostly on reactions stemming from clusters of the main reagent ions with water, and the implications for detection of formic acid, acetic acid, H₂O₂, and CH₃OOH product ions.

The paper is well written, and the methodology largely sound, if a bit incomplete (see

C1

below). I don't have any scientific or technical concerns that would prevent this paper from being published. The paper can be accepted as is, but the authors may wish to address a few minor comments listed below.

1) The authors have done a commendable job trying to develop a mechanistic understanding of the ion chemistry occurring in their chemical ionization region. The ion chemistry chosen seems rather complicated, but it seems the broad trends can be rationalized. One aspect I didn't see directly addressed was proton abstraction from weak acids by O₂⁻. Could this be more explicitly stated as to whether e.g. acetate ions or other carboxylate ions are produced, and if so what would be the resulting secondary ion chemistry in the flow reactor. Would that produce other possible interfering ions?

2) It is not clear how O₃⁻ and CO₃⁻ ions are generated.

3) The role of O₃ was not well developed in that I couldn't follow why it was tested aside from possibly causing an interfering ion in the O₂⁻ chemistry. What about I⁻ chemistry?

4) There are some rate constants given without units.

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C2