

# ***Interactive comment on “Modeling the dynamic behavior of a droplet evaporation device for the delivery of isotopically calibrated low-humidity water vapor” by Erik Kerstel***

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The Author reports on an important aspect of instrumental analysis namely calibration, in that the reliability of all analytical data is only as good as the standard it's compared against. A vapour calibration device for isotope analysis and the associated mathematical model are presented by the Author. To generalise, although the positive aspects of the calibration device and model are dealt with, it would be beneficial if the Author further addresses some of the system's limitations. For example, what tolerance or accuracy does the device operate under? Can the Author quote a reliability of plus or minus X%? How applicable is the calibration in the low temperature Arctic conditions

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reported, when the model employs diffusional data derived at 35oC? What part of the calibration curve does the device operate under, is it similar to real-world conditions? If manufactured commercially, would variance in reproducibility and accuracy between manufactured devices be a problem? Would such devices need to be re-calibrated and how often? The Author may also like to consider the following. . .

- Line 1: Consider using the term “water vapour” rather than “water concentration”.
- Line 2: “isotope ratios”. . . What isotope ratios are being discussed, oxygen, hydrogen. . . not actually mentioned until line 91.
- Line 3: “nL-droplet” . . . Define the term nL, is it nano-litre?
- Line 8: Consider replacing “We” with. . . “it can be shown”. Also, there’s a tendency for the Author to use the plural “We” throughout the whole narrative, rather than the singular.
- Line 23: Consider revising the English, remove. . . “we provide” and replace with “a theoretical quantitative model is presented”.
- Line 24: Title spelling - also see main title spelling: Modelling has two l’s, and consider removing “syringe water” and replacing with. . . “Modelling the syringe water isotope delivery module”
- Line 25: Consider re-wording the statement and check spelling of behaviour, for example. . . “The dynamic behaviour of the water concentration (humidity) and isotope ratios of a low humidity-level generator (LHLG), such as described in the companion paper by Leroy-Dos Santos et al. (2020), are modelled here.”
- Line 34: “standard water” is an ill-defined term, does the Author mean calibration standard?
- Line 38 and 219 to 220: Can the Author put forward a mechanism that drives the isotope fractionation? Is it diffusional in nature, and would surface molecular diffusion play any part in this mechanism i.e. where  $Nu$  and  $Sh$  approaches a value of 2.
- Lines 35 to 40: How does the Author know the isotope composition at any one time during the instrument’s start-up, steady-state equilibrium, and variations in steady-state operation e.g. due to changes in droplet size. How was this analysed? What is the frequency or need for isotope re-calibration?
- Line 43: Does the needle tip have a bevelled tip as most Hamilton syringes do, as this would affect the shape, mass and consequently the transport properties of the suspended droplet. Was the needle tip profile engineered in any way?
- Line 60 and 70: To what

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extent has the Author considered the model's response in terms of heat and mass transfer, to the following. . .

- o Changes in droplet temperature.
- o Molecular diffusion, convection, and conduction via the needle to and from the droplet.
- o Surface tension and surface energy. . . at 0.1mm in diameter these energies must be high.
- o Is there any isotopic absorption-desorption equilibrium at the evaporation chamber wall?
- o Are there any static effects that need to be considered?
- o The droplets are hemispherical in geometry; would a spherical droplet experience enhanced heat and mass transfer due to droplet instability such as oscillations or distortions in the chamber airflow?
- o What type of water did the Author use. . . distilled, degassed, isotope enriched?
- o How is the evaporation chamber temperature is maintained? What are the tolerances?

â€” Line 124: The following statement raises questions about the reliability of the data produced by the instrument. . . “a home-built, low-humidity water isotope spectrometer”

â€” Line 136: Similarly, the following statement raises questions of reliability in the calibration process e.g. do these standards deteriorate with time? . . . “The standard waters used were left-over working standards”

â€” Line 160 and 167: Table 2, data evaluated at 35oC. Is it valid for the Author to use this data? What is the modelling temperature and operational temperature of the device?

â€” Line 186: The Author uses the term "useless results". . . if used to validate data, whether in a positive or negative sense, the data can hardly be described as useless!

Please also note the supplement to this comment:

<https://amt.copernicus.org/preprints/amt-2020-428/amt-2020-428-RC1-supplement.pdf>

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Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2020-428, 2020.

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