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*Supplement of*

## **Performance of a new coaxial ion–molecule reaction region for low-pressure chemical ionization mass spectrometry with reduced instrument wall interactions**

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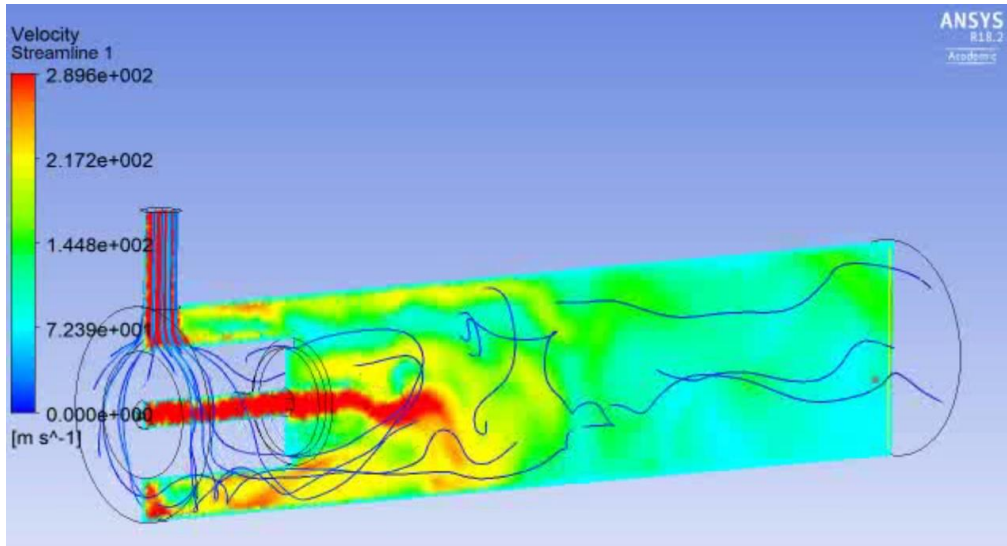
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1 Table S1. The hydroxynitrate (HN), dihydroxynitrate (DHN), and dihydroxycarbonyl (DHC) oxidation  
 2 products sampled in this study. This table is reproduced with permission from the Supplemental  
 3 Information in Liu et al., (2019).

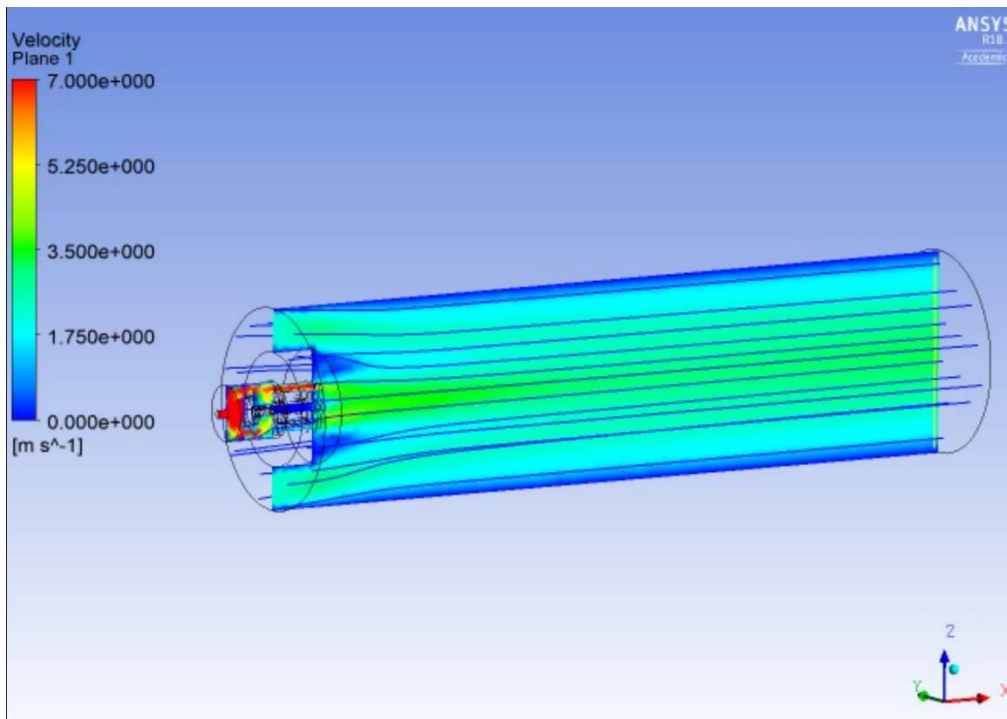
Compound Class	Formula	MW	Precursor	SIMPOL C* ( $\mu\text{g m}^{-3}$ )
HN	C <sub>6</sub> H <sub>13</sub> NO <sub>4</sub>	163	Hexanol	3.56E+04
HN	C <sub>8</sub> H <sub>17</sub> NO <sub>4</sub>	191	Octanol	5.49E+03
HN	C <sub>9</sub> H <sub>19</sub> NO <sub>4</sub>	205	Nonanol	2.14E+03
HN	C <sub>10</sub> H <sub>21</sub> NO <sub>4</sub>	219	Decanol	8.30E+02
HN	C <sub>12</sub> H <sub>25</sub> NO <sub>4</sub>	247	Dodecanol	1.23E+02
DHN	C <sub>6</sub> H <sub>13</sub> NO <sub>5</sub>	179	Hexanol	2.46E+02
DHN	C <sub>8</sub> H <sub>17</sub> NO <sub>5</sub>	207	Octanol	3.76E+01
DHN	C <sub>9</sub> H <sub>19</sub> NO <sub>5</sub>	221	Nonanol	1.46E+01
DHN	C <sub>10</sub> H <sub>21</sub> NO <sub>5</sub>	235	Decanol	5.57E+00
DHN	C <sub>12</sub> H <sub>25</sub> NO <sub>5</sub>	263	Dodecanol	8.29E-01
DHC	C <sub>8</sub> H <sub>16</sub> O <sub>3</sub>	160	Octanol	5.09E+02
DHC	C <sub>9</sub> H <sub>18</sub> O <sub>3</sub>	174	Nonanol	2.02E+02
DHC	C <sub>10</sub> H <sub>20</sub> O <sub>3</sub>	188	Decanol	7.96E+01
DHC	C <sub>12</sub> H <sub>24</sub> O <sub>3</sub>	216	Dodecanol	1.22E+01

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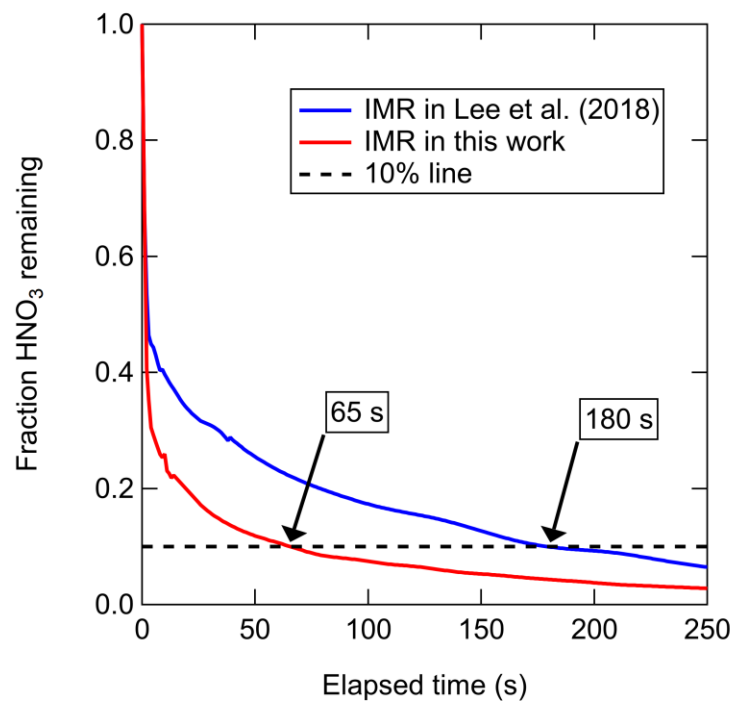


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8 **Figure S1.** Two example fluid dynamics simulations run in ANSYS Fluent Release 18.2, colored by the  
 9 magnitude of the velocity of the gas (without regard to direction, simply to illustrate turbulence) with  
 10 streamlines shown: a) a case where both the sample flow and ion flows are turbulent upon entering the  
 11 drift region. Turbulence leads to enhanced wall interactions in the drift region; and b) a case where the  
 12 sample flow passes through a laminizer element and the ion flow was initialized as laminar coming into  
 13 the boundary. These examples are not to scale with the actual design of the IMR presented herein, but  
 14 the results of such simulations informed the IMR design. Images used courtesy of ANSYS, Inc.



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16 **Figure S2.** Delay time measurements for HNO<sub>3</sub> in the Lee et al. (2018) IMR compared with the new IMR  
 17 presented herein. The delay time in the new IMR is approximately a factor of three shorter, indicating  
 18 reduced effects of wall interactions.

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20 **References**

- 21 Lee, B. H., Lopez-Hilfiker, F. D., Veres, P. R., McDuffie, E. E., Fibiger, D. L., Sparks, T. L., Ebben, C. J.,  
22 Green, J. R., Schroder, J. C., Campuzano-Jost, P., Iyer, S., D'Ambro, E. L., Schobesberger, S., Brown, S. S.,  
23 Wooldridge, P. J., Cohen, R. C., Fiddler, M. N., Bililign, S., Jimenez, J. L., Kurtén, T., Weinheimer, A. J.,  
24 Jaegle, L. and Thornton, J. A.: Flight Deployment Of A High-Resolution Time-Of-Flight Chemical Ionization  
25 Mass Spectrometer: Observations Of Reactive Halogen And Nitrogen Oxide Species, *J. Geophys. Res.*  
26 *Atmos.*, doi:10.1029/2017JD028082, 2018.
- 27 Liu, X., Deming, B., Pagonis, D., Day, D. A., Palm, B. B., Talukdar, R., Roberts, J. M., Veres, P. R., Krechmer,  
28 J. E., Thornton, J. A., de Gouw, J. A., Ziemann, P. J. and Jimenez, J. L.: Effects Of Gas-Wall Interactions On  
29 Measurements Of Semivolatile Compounds And Small Polar Molecules, *Atmos. Meas. Tech.*, 12, 3137–  
30 3149, doi:10.5194/amt-12-3137-2019, 2019.

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