Supplemental Information for: Performance of a new co-axial ion-molecule reaction region for low-pressure chemical ionization mass spectrometry with reduced instrument wall interactions

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

Compound Class	Formula	MW	Precursor	SIMPOL *C** ($\mu g\ m^{-3}$)
HN	$C_6H_{13}NO_4$	163	Hexanol	3.56E+04
HN	$C_8H_{17}NO_4$	191	Octanol	5.49E+03
HN	$C_9H_{19}NO_4$	205	Nonanol	2.14E+03
HN	$C_{10}H_{21}NO_4$	219	Decanol	8.30E+02
HN	$C_{12}H_{25}NO_4$	247	Dodecanol	1.23E+02
DHN	$C_6H_{13}NO_5$	179	Hexanol	2.46E+02
DHN	$C_8H_{17}NO_5$	207	Octanol	3.76E+01
DHN	$C_9H_{19}NO_5$	221	Nonanol	1.46E+01
DHN	$C_{10}H_{21}NO_5$	235	Decanol	5.57E+00
DHN	$C_{12}H_{25}NO_5$	263	Dodecanol	8.29E-01
DHC	$C_8H_{16}O_3$	160	Octanol	5.09E+02
DHC	$C_9H_{18}O_3$	174	Nonanol	2.02E+02
DHC	$C_{10}H_{20}O_3$	188	Decanol	7.96E+01
DHC	$C_{12}H_{24}O_3$	216	Dodecanol	1.22E+01

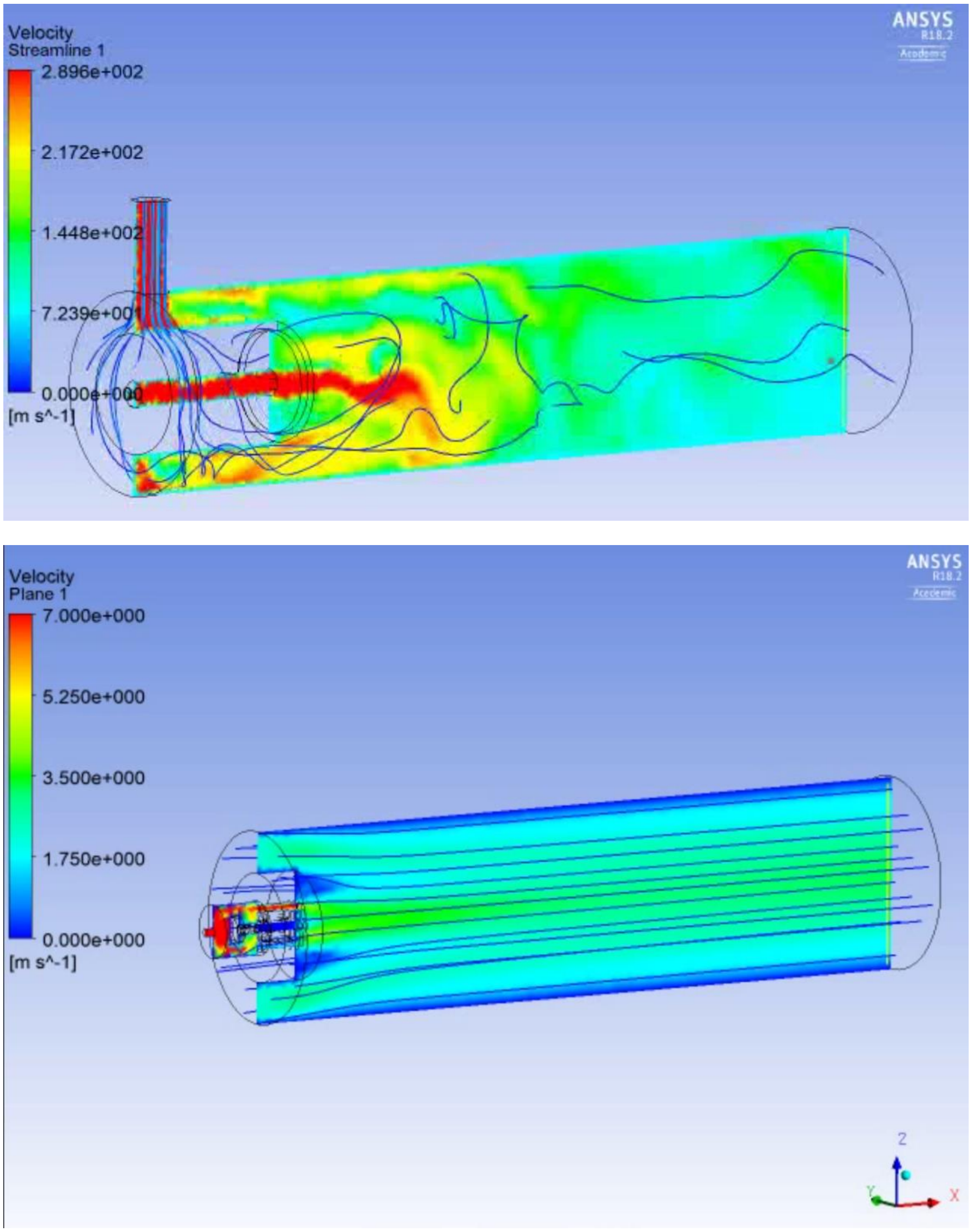

Figure S1. Two example fluid dynamics simulations run in ANSYS Fluent Release 18.2, colored by the magnitude of the velocity of the gas (without regard to direction, simply to illustrate turbulence) with streamlines shown: a) a case where both the sample flow and ion flows are turbulent upon entering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

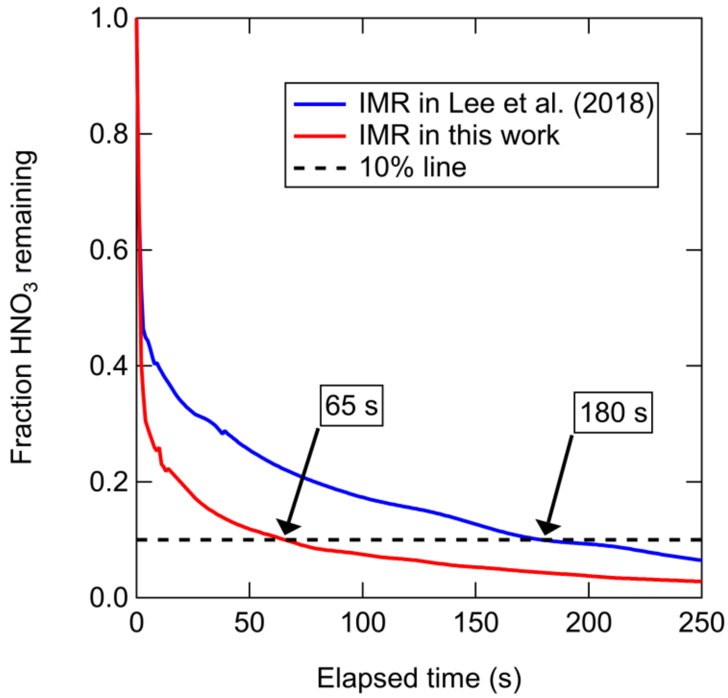

Figure S2. Delay time measurements for HNO_3 in the Lee et al. (2018) IMR compared with the new IMR presented herein. The delay time in the new IMR is approximately a factor of three shorter, indicating reduced effects of wall interactions.

References

Lee, B. H., Lopez-Hilfiker, F. D., Veres, P. R., McDuffie, E. E., Fibiger, D. L., Sparks, T. L., Ebben, C. J., Green, J. R., Schroder, J. C., Campuzano-Jost, P., Iyer, S., D'Ambro, E. L., Schobesberger, S., Brown, S. S., Wooldridge, P. J., Cohen, R. C., Fiddler, M. N., Bililign, S., Jimenez, J. L., Kurtén, T., Weinheimer, A. J., Jaegle, L. and Thornton, J. A.: Flight Deployment Of A High-Resolution Time-Of-Flight Chemical Ionization Mass Spectrometer: Observations Of Reactive Halogen And Nitrogen Oxide Species, J. Geophys. Res. Atmos., doi:10.1029/2017JD028082, 2018.

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