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Curriculum Vitae

Research interests:

Kinetics, non-Arrhenius behaviour, absorption cross sections, analytical chemistry, structure-activity relationships, CIMS, missing reactivities, field measurements.

Professional experience:

10/10 – present: Research Scientist at NOAA, working with Dr. Jim Burkholder.
10/07 – 10/10: PDRA at University of Manchester, UK, working with Prof. Carl Percival.

University education:

The University of Manchester, UK: 09/04–10/07. PhD, Chemical kinetics.
Keele University, UK: 09/00–07/04. MGeoscience (1st class honours).

Publications:

Papadimitriou, V.C., **McGillen, M.R.**, Smith, S.C., Jubb, A.M., Portmann, R.W., Hall, B.D., Fleming, E.L., Jackman, C.H. and Burkholder, J.B. (2013) 1,2-Dichlorohexafluoro-Cyclobutane (1,2-c-C₄F₆Cl₂, R-316c) a Potent Ozone Depleting Substance and Greenhouse Gas: Atmospheric Loss Processes, Lifetimes, and Ozone Depletion and Global Warming Potentials for the (E)- and (Z)- Stereoisomers, *accepted, Journal of Physical Chemistry A*.

McGillen, M.R., Fleming, E.L., Jackman, C.H. and Burkholder, J.B. (2013) CFCl₃ (CFC-11): UV absorption spectrum temperature dependence measurements and the impact on atmospheric lifetime and uncertainty, *accepted, Geophysical Research Letters*, DOI: 10.1002/grl.50915.

McGillen, M.R., Baasandorj, M. and Burkholder, J.B. (2013) Gas-Phase Rate Coefficients for the OH + *n*-, *i*-, *s*-, and *t*-Butanol Reactions Measured Between 220 and 380 K: Non-Arrhenius Behavior and Site-Specific Reactivity, *Journal of Physical Chemistry A*, **117**, 4636–4656.

Papadimitriou, V.C., **McGillen, M.R.**, Fleming, E.L., Jackman, C.H. and Burkholder, J.B. (2013) NF₃: UV Absorption spectrum temperature dependence and the atmospheric and climate forcing implications, *Geophysical Research Letters*, **40**, 440–445.

Le Breton, M., **McGillen, M.R.**, Muller, J.B.A., Shallcross, D.E., Xiao, P., Huey, L.G., Tanner, D. and Percival, C.J. (2012) Airborne observations of formic acid using a chemical ionisation mass spectrometer, *Atmospheric Measurement Techniques*, **5**, 3029–3039.

Booth, A.M., Banan, T., **McGillen, M.R.**, Barley, M.H., Topping, D.O., McFiggans, G., Percival, C.J. (2012) The role of *ortho*, *meta*, *para* isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids, *RSC Advances*, **2**, 4430–4443.

Ghalaieny, M., Bacak, A., **McGillen, M.**, Martin D., Knights, A.V., O'Doherty, S., Shallcross, D.E. and Percival, C.J. (2012) Determination of gas-phase ozonolysis rate coefficients of a number of sesquiterpenes at elevated temperatures using the relative rate method, *Physical Chemistry Chemical Physics*, **14**, 6596–6602.

Leather, K.E., **McGillen, M.R.**, Cooke, M.C., Utembe, S.R., Archibald, A.T., Jenkin, M.E., Derwent, R.G., Shallcross, D.E. and Percival, C.J. (2012) Acid-yield measurements of the gas-phase ozonolysis of ethene as a function of humidity using Chemical Ionisation Mass Spectrometry (CIMS), *Atmospheric Chemistry and Physics*, **12**, 469–479.

Bacak, A., Cooke, M.C., Bardwell, M.W., **McGillen, M.R.**, Archibald, A.T., Huey, L.G., Tanner, D., Utembe, S.R., Jenkin, M.E., Derwent, R.G., Shallcross, D.E. and Percival, C.J. (2011) Kinetics of the HO₂ + NO₂ Reaction: On the impact of new gas-phase kinetic data for the formation of HO₂NO₂ on HO_x, NO_x and HO₂NO₂ levels in the troposphere, *Atmospheric Environment*, **45**, 6414–6422.

McGillen, M.R., Ghalaieny, M. and Percival, C.J. (2011) Determination of gas-phase ozonolysis rate coefficients of C_{8–14} terminal alkenes at elevated temperatures using the relative rate method, *Physical Chemistry Chemical Physics*, **13**, 10965–10969.

Leather, K.E., **McGillen, M.R.**, Ghalaieny, M., Shallcross, D.E. and Percival, C.J. (2011) Temperature-dependent kinetics for the ozonolysis of selected chloroalkenes in the gas phase, *International Journal of Chemical Kinetics*, **43**, 120–129.

McGillen, M.R., Archibald, A.T., Carey, T.J., Leather, K.E., Percival, C.J., Shallcross, D.E. and Wenger, J.C. Structure-activity relationship (SAR) for the prediction of gas-phase ozonolysis rate coefficients: an extension towards heteroatomic unsaturated species, *Physical Chemistry Chemical Physics*, **13**, 2842–2849.

Leather, K.E., **McGillen, M.R.** and Percival, C.J. (2009) Temperature-dependent ozonolysis kinetics of selected alkenes in the gas phase: an experimental and structure-activity relationship (SAR) study, *Physical Chemistry Chemical Physics*, **12**, 2935–2943.

Booth, A.M., Markus, T., McFiggans, G., Percival, C.J., **McGillen, M.R.** and Topping, D.O. (2009) Design and construction of a simple Knudsen effusion mass spectrometer (KEMS) system for vapour pressure measurements of low volatility organics, *Atmospheric Measurement Techniques*, **2**, 355–361.

Bobruzki, K., Blom, M., Braban, C., Coe, H., Famulari, D., Gallagher, M.W., Geddes, J., Ghalaieny, M., Jones, S., **McGillen, M.R.**, Mohacsi, A., Murphy, J., Percival, C.J., Pogany, A., Popescu, R., Rantanen, S., Whitehead, J. M., Sutton, M.A., Nemitz, E.G. (2009) An Intercomparison of ten ammonia measurement techniques during a field experiment. *Atmospheric Measurement Techniques Discussions*, **2**, 1783–1836.

Last, D.J., Najera, J., Wamsley, R., Jackson, G., **McGillen, M.R.**, Percival, C.J. and Horn, A.B. (2009) Ozonolysis of organic compounds and mixtures in solution. Part I: Oleic, maleic, nonanoic and benzoic acids, *Physical Chemistry Chemical Physics*, **11**, 1427–1440.

Percival C.J. and **McGillen, M.R.** (2008) Structure Activity Relationship Methods, *NATO Science for Peace and Security Series –C: Environmental Security*, 47–59.

McGillen, M.R., Percival, C.J., Archibald, A.T., Carey, T.J., Wenger, J.C. and Shallcross, D.E. (2008) Structure-activity relationship (SAR) for the gas-phase ozonolysis of aliphatic alkenes and dialkenes, *Physical Chemistry Chemical Physics*, **10**, 1757–1768.

Archibald, A.T. **McGillen, M.R.**, Taatjes, C.A., Percival, C.J. and Shallcross, D.E. (2007) The atmospheric transformation of enols: a potential source of carboxylic acids in the urban atmosphere, *Geophysical Research Letters*, **34**: L21801, doi:10.1029/2007GL031032.

McGillen, M.R. and Percival, C.J. (2007) A kinetic study of the reaction of OH with alkenes. *Physical Chemistry Chemical Physics*, **9 (31)**: 4349-4356.

Raventos, M.T., Percival C.J., **McGillen, M.R.**, Hamer, P.D. and Shallcross D.E. (2007) Kinetics and mechanism of the reaction between $C_2H_5O_2 + HO_2$. *Physical Chemistry Chemical Physics*, **9**, 4338-4348.

McGillen, M.R., Percival, C.J., Pieterse, G., Watson, L.A. and Shallcross, D.E. (2007) Predicting arene rate coefficients with respect to hydroxyl and other free radicals: a simple and effective method using a single topological descriptor. *Atmospheric Chemistry and Physics*, **7**, 3559-3569.

Raventos, M.T., **McGillen, M.R.**, Percival C.J., Hamer, P.D. and Shallcross D.E. (2007) Kinetics and mechanism of the reaction between $CH_3O_2 + HO_2$. *International Journal of Chemical Kinetics*, **39**, 571-579.

McGillen, M.R., Crosier, J., Percival, C.J., Sanchez-Reyna, G. and Shallcross, D.E. (2006) Can topological indices be used to predict gas-phase rate coefficients of importance to tropospheric chemistry? Reactions of alkenes with OH, NO_3 and O_3 . *Chemosphere*, **65**, 2035-2044.

Reynolds, J.C., Last, D.J., **McGillen, M.R.**, Nijs, A., Horn, A.B., Percival, C., Carpenter, C. and Lewis, A.C. (2006) Structural analysis of oligomeric molecules formed from the reaction products of oleic acid ozonolysis, *Environmental Science and Technology*, **40**, 6674-6681.

McGillen, M.R., Percival, C.J., Raventos-Duran, T., Sanchez-Reyna, G. and Shallcross, D.E. (2006) Can topological indices be used to predict gas-phase rate coefficients of importance to tropospheric chemistry? *Atmospheric Environment*, **40**, 2488-2500.

McGillen, M.R. and Fairchild, I.J. (2005) An experimental study on the controls on incongruent dissolution of $CaCO_3$ under analogue glacial conditions. *Journal of Glaciology*, **51**, 383.

Experience and skills:

- I have used a variety of analytical methods including CIMS, FTIR, LIF, GC/FID, GC/ECD, GC/MS, quantum cascade laser (QCL) and UV spectroscopy, and have used these techniques to detect a variety of trace species in flow tubes, reaction chambers, absorption cells and in the field.
- I have gained experience in building scientific apparatus including:
 - The EXTreme RAnge (EXTRA) chamber, A 123 L Teflon-coated stainless steel reaction chamber which is a static system for measuring rate coefficients and product yields between the temperatures of 188–473 K.
 - A CIMS rack, which operates aboard the BAe 146 research aircraft for measuring acids, organic acids and nitrate radicals.
 - A catalytic total combustion system for quantifying hydrocarbon concentrations absolutely using FTIR.

- I have field experience using CIMS to detect ammonia and acids in a variety of environments including a rural site in Edinburgh, Scotland, and airborne measurements of gaseous acids covering much of the UK.
- I am experienced in various types of kinetic experiments including temperature-dependent kinetic measurements and product branching ratios in flowtubes and static reaction chambers using CIMS, LIF, FTIR and GC apparatus for detection.
- I am proficient in a broad variety of vacuum and compressed gas applications, and have worked successfully with many difficult-to-handle species, be they condensable, corrosive, short-lived or thermally unstable. I am also adept at making gas standards for use in calibrations, including high precision gas mixtures and permeation tubes.
- I am experienced in programming with Igor Pro and use it routinely for data analysis, calculations and preparing figures for publications.
- I maintain strong connections with my previous colleagues and collaborators, and have on-going research collaborations with many of them.

Teaching experience:

I have instructed and directed the research of a number of post-graduate project students of various levels of education, ranging from undergraduate students to PhD students.

Awards and prizes:

- 09/07: GEIA funding to attend the *Surface Emissions and Prediction of Atmospheric Composition Changes* summer school (Ile d'Oléron, France).
- 12/06: INTROP travel grant of €3500 awarded for the purpose of acquiring experimental data for the augmentation of a theoretical work on ozonolysis reactions.
- 11/04: NERC bursary award to attend the *European Research Course on Atmospheres* (ERCA) (Grenoble, France).
- 05/02: Nuffield Foundation undergraduate research bursary.

Personal:

Nationality: British.

Currently holding a US J1 visa.

Referees:

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