Nomination Statement

The CIRES chemical ionization mass spectrometer (CIMS) team of Andy Neuman and Rich McLaughlin showed sustained scientific and engineering excellence in identifying and pursuing a scientific vision, and overcame major challenges to carry out an airborne global-scale "voyage of discovery" that has yielded exciting insights into new atmospheric chemical processes that influence air quality and climate.

Criteria

Criteria 1: Development of new scientific, engineering and/or software tools or models directly resulting in novel research valuable to CIRES and the wider scientific community.

A systematic effort to realize their scientific vision.

Three years ago, the CIRES CIMS team of Andy Neuman (Research Scientist III) and Rich McLaughlin (Senior Associate Scientist), with the participation of Patrick Veres (a CIRES Research Scientist II during this effort, but now a Federal employee, thus ineligible for this award), articulated their scientific vision: to exploit the untapped capability of a new generation of time-of-flight mass spectrometer (ToF-MS) detectors by carrying out a systematic large-scale airborne survey to fill key gaps in our understanding of the chemistry of the global atmosphere. This vision had two essential requirements: a ToF-MS detector, and a "ride" around the world. At that point, they had neither. Undeterred, and by working diligently over several years, they overcame these challenges to realize their vision. Their initial results have already begun to influence, and in novel ways to reshape, our scientific understanding of the natural and human-affected atmosphere on a global scale, as described below.

In pursuit of their scientific vision, this team began in 2015 by approaching the NOAA Chemical Sciences Division (CSD) Director to successfully advocate for the purchase of a new ToF-MS detector. This major purchase ($400K), which took over a year to complete, was approved based on their proven track record of successful airborne mass spectrometric measurements and interpretation. Looking ahead, the CIMS team immediately identified the NASA Atmospheric Tomography (ATom) airborne field mission as their first deployment priority. ATom uses the NASA DC-8 research aircraft to systematically sample the atmosphere in continuous airborne vertical profiles, from 500 feet over the ocean surface to 42,000 feet into the upper troposphere and lower stratosphere, from Arctic to Antarctic in the Pacific and Atlantic oceans, once in each season for a total of four complete circuits of the globe. However, at that point, the ATom-1 and ATom-2 global circuits had already been completed, and the DC-8 aircraft was completely full and at its maximum takeoff weight with existing ATom instruments, scientists, aircrew, spares, and fuel.

By highlighting the unique science expected from their portfolio of planned measurements, over the course of multiple discussions with NASA management in 2016 and early 2017 the CIRES CIMS team was able to successfully negotiate the inclusion of their new CIMS instrument in ATom-3. Their new ToF-MS measurement capabilities, focused on halogen oxide and reactive nitrogen species, were deemed of sufficient interest and quality to become mission-essential. As a result, NASA DC-8 managers went to great lengths to reconfigure the existing ATom payload to permit this inclusion, despite an increase in overall mission risk and a reduction in aircraft vertical-profiling capability. This inclusion is a tribute to the initiative and persuasiveness of the CIRES CIMS team in successfully articulating their scientific vision to NASA ATom management and engineering staff.

Criteria 2: Uncommon initiative, resourcefulness, and/or scientific creativity conducting research with potential to expand or change the direction of a particular field or discipline.

(a) Engineering excellence under extreme time pressure.

The CIRES CIMS team now faced another challenge: integrate their new ToF-MS detector into a rugged field-deployable airborne instrument in time to meet the ambitious ATom-3 field deployment schedule. In a remarkable show of grace under pressure, the CIRES team carried out a major systems-engineering effort that met stringent ATom aircraft payload limits on weight, configuration, and power consumption (Figure 1 in the Supplement, attached as “2018 CIRES CIMS team supplement.pdf”). This effort included designing calibration and zeroing systems for the sampling inlet; developing and characterizing flight-capable sample gas handling and vacuum systems; and writing and debugging the instrument interface and data analysis software. As one example of CIRES CIMS team innovation, they developed a novel inlet and sampling scheme (Figure 2 in the Supplement) that provided a constant sample mass flow with exceptional pressure stability, within 1 part in 10,000, in the ion-molecule reactor despite routine drastic changes in inlet pressure encountered during continuous airborne profiling between 500 and 42,000 feet in altitude. Their pressure control scheme provided rock-solid instrument sensitivity independent of aircraft altitude over the course of the entire ATom airborne mission, leading to greatly improved accuracy in the resulting CIRES CIMS data compared with other airborne CIMS systems.

The overall level of CIRES CIMS engineering excellence led to a picture-perfect ATom-3 integration and deployment, a notable accomplishment for any instrument and especially for one of this complexity. This is in stark contrast to the usual “teething pains” expected of new-build flight instruments, and to the instrument issues that routinely affect more mature instruments on ATom-3. The level of success in this regard is best illustrated by an anecdote: the CIRES CIMS instrument performed so reliably that many people on the ATom project, including some of the senior science team, never realized this was its first deployment.

(b) Initial results with far-reaching scientific impact.

The CIRES CIMS team was able to provide science-quality data for a wide range of gas-phase reactive nitrogen and halogen oxide compounds through the full flight envelope of the NASA DC-8 research aircraft over the course of all 12 flights making up the 78,000-km ATom global circuit, spanning the Arctic and Antarctic in both the Pacific and Atlantic oceans (Figure 2 in the Supplement). The scientific impact of this novel work has been immediately apparent in several ways, as described below.

Global-scale distributions of N_2O_5 and $ClNO_2$. In another first, the CIRES CIMS team in ATom measured N_2O_5 and $ClNO_2$, chemicals linking the atmospheric reactive nitrogen and reactive chlorine cycles through heterogeneous chemistry on atmospheric particulate matter. The CIRES CIMS efforts provided a uniquely valuable global-scale data set to quantify these linkages and their effects on the oxidation chemistry that determines ozone and methane lifetimes in the atmosphere. Their N_2O_5 and $ClNO_2$ data in the lower stratosphere are being examined for evidence of novel acid-mediated heterogeneous chemistry on aerosol particles, with implications for potential future solar radiation management efforts involving aerosol injection to the stratosphere (see Figure 3 in the Supplement).

Halogen oxides and the background ozone budget. Earlier pioneering measurements by CU/CIRES and NSF investigators in the 2012 TORERO and 2014 CONTRAST airborne field missions quantified a variety of halogen oxides in the tropical and midlatitude marine atmosphere and measured their atmospheric vertical profiles. The CIRES CIMS team data in ATom extend these earlier observations, providing the first global-scale data set to guide implementation of halogen chemistry parameterizations in 3-dimensional chemical-transport models (CTMs). Comparisons show that three widely used CTMs – GEOS-Chem (Harvard), CAM-Chem (NCAR), and CMAQ (EPA) – predict very different impacts on background tropospheric ozone from halogen oxide chemistry. As a result, the CIRES CIMS team initiated active collaborations with multiple research groups, in the U.S. and abroad, responsible for implementing and evaluating halogen chemistry in these models. These collaborations using the CIRES CIMS data are expected to significantly improve CTM simulations of the role of halogen oxides in determining background ozone levels around the globe.

An unexpected discovery – a new marine source of reactive sulfur. The combination of a extremely powerful analytical tool, expert practitioners, and an unprecedented atmospheric sampling strategy provided fertile ground for the unexpected during ATom-3. In this case, a major surprise was the discovery by the CIRES CIMS team of a ubiquitous, previously unreported, reactive sulfur compound emitted at the ocean surface. The discovery was triggered by subtle differences in the mass spectra obtained during flight that depend on the high-resolution performance specification of the new ToF-MS detector and required the expertise of the CIRES CIMS team to diagnose and recognize as potentially important.

Marine emissions of sulfur compounds play a major role in new particle formation and growth to cloud-active sizes, with substantial effects on processes influencing cloud formation, albedo, and lifetimes. The atmospheric chemistry of marine sulfur compounds is a mature and extensively studied field. Following their discovery in the field, the CIRES team carried out exacting laboratory work in Boulder to definitively identify this compound's chemical structure and quantify its detection sensitivity in the CIMS instrument. Further, the team began work with laboratory kineticists and experts in atmospheric sulfur chemistry to determine the role this newly-discovered compound plays in the sulfur cycle near the ocean surface, and its potential effect on the state of understanding of biochemical sulfur sources, marine clouds, and their coupled effects on climate.

Criteria 3: Participation in collaborative and/or multidisciplinary research that engages a broader cross-section than the nominee's typical scientific or engineering community.

The value of the successes achieved by the CIRES CIMS team on this voyage of discovery can be framed in a broader perspective. First, a major advance for this team came as a result of needing to "step up" to the NASA DC-8 research aircraft. Instrument operation aboard the DC-8 demands a substantially higher level of engineering refinement than this team had needed in operating legacy instruments on the lower-altitude, lower-Mach number WP-3D and C-130 turboprop research aircraft. Second, the CIRES CIMS team successfully contributed to a major, multi-agency collaborative effort to study human effects on atmospheric chemistry on a global scale, greatly expanding their previous scope which had focused on the smaller scales attendant to local and regional chemical processing. Third, and most importantly, the CIRES CIMS team in ATom has established direct and significant collaborations with multiple members of the global-scale chemical-transport modeling (CTM) community, and is guiding several efforts to critically test chemical representations in a broad range of global-scale CTMs. These successes represent a major expansion of the normal breadth of their scholarship, which now includes global Earth system model validation and improvement efforts that are principal deliverables of the ATom science plan and at the heart of the CIRES science mission. As a result, the initial science products from the CIMS team have found a new audience, and have earned a new level of international recognition for CIRES research.