Proposed Title:

Non-Intrusive Testing Techniques to Analyze Aerosols in the Exhaust from Rockets and Hypersonic Vehicles

Applicant (Principal Investigator)

Marcos Fernandez-Tous, Assistant Professor.

University of North Dakota, Grand Forks, ND

John D. Odegard School of Aerospace Sciences

Space Studies Department

Collaborator (co-Principal Investigator)

Hallie B. Chelmo, Assistant Professor.

University of North Dakota, Grand Forks, ND

College of Engineering and Mines

Mechanical Engineering Department

Topic number: 2- Agile Science of Test and Evaluation.

Program Officer: Dr. Brett Pokines.

Abstract

There is a need to quantify particle emission from rockets and hypersonic aircraft, which are indicators of incomplete combustion processes within rocket chambers and aircraft motors. As the number of vehicles crossing at high altitudes exponentially increases, these particle emissions result in an increase of suspended particles in the atmosphere called aerosols. The amount and composition of aerosols within the upper atmosphere that results from rocket and hypersonic flights is not fully understood. To address this need, a ground-based system is developed that uses sensors to measure the thermodynamic, physical and chemical properties of the rockets exhausts. Specifically, **the objective is to improve the theory relating particle emissions with rocket motors performance using a controlled environment.** Such a theorical understanding enables the impact of rockets and hypersonic aircraft flights on the stratospheric environment to be evaluated. Important potential impacts include the radiative forcing from black carbon aerosols and stratospheric ozone reductions.

Although past theoretical studies do show impacts of rockets and aviation activity on aerosol emissions in the stratosphere, in-situ measurements are scarce and their high values inconsistent with the theory. To date, observations in the stratosphere have either not discriminated among the sources or they have focused on different aerosols sources –such as wildfires or volcanic eruptions. No research to the best of our knowledge has validated a match of aerosol concentrations and aviation or rocket performance either. In order to analyze rockets and aviation contributions, we need to measure rocket exhaust thermodynamic, mechanical and chemical properties; this will enable an analysis of aerosol concentrations –number of particles per volume–, as they vary along a rocket's trail. For this reason, this project requires previous experimental setup and tests in a controlled environment, which is what we propose to develop.

A key advantage of our techniques is their non-intrusive nature. We use thermocouples and pressure transducers to obtain information in harsh environments such as those found in the chamber and at the nozzle exit. These techniques will be evaluated in a test setup at UND with different fuel compositions and rocket configurations. The focus is on solid fuels; however, results may be extrapolated to liquid fuels as well. The aerosol size distribution, the number of suspended particles at size intervals, and particle composition will be measured. The aerosols size is important for determining atmospheric lifetime and composition is important for atmospheric chemical changes via reactions between particles and gas molecules.

This research will be conducted by a multi-disciplinary team at the University of North Dakota (UND) that includes propulsion, engineering, and atmospheric science experts. UND is the first member of the Space Force University Partnership Program, as well as an upcoming member of the University Consortium of Applied Hypersonics (UCAH). This project will greatly contribute to the University's strategic focus on national security and the Aerospace College's focus on the stratosphere. Finally, the applicant and collaborators will greatly benefit from this project to boost DoD relevant research and participate in international fora within the research area.

Program description narrative

Background: small particles must be quantified

The present proposal constitutes an interdisciplinary approach **to quantify particle emissions from rocket and hypersonic vehicle exhaust that enables evaluation of rocket motors performance and potential environmental impacts, such as radiative forcing from black carbon aerosols and stratospheric ozone reductions.** The focus is on solid rocket motors in a broad speed range including hypersonics, which are typically speeds above Mach 5. The project focuses on black carbon aerosols –suspended solid and liquid particles in the size range of 1 to 10,000 nm– due to link to stratospheric ozone concentration. The presence of black carbon is symptomatic of less-than-optimum combustion processes in the motor chamber, which has an immediate effect on the rocket's operational performance. The project's double focus on rocket performance and environmental impact through aerosols exhaust is illustrated in **Fig. 1**.

Improving rocket exhaust testing is expected to become more significant as the number and types of rockets crossing the atmosphere increases. Recent publications forecast an increasing trend for the space industry since new start-ups accumulated an investment of $21.8 billion between 2000 and 2018. Inevitably, with more space traffic comes **an explosive increase in the number of vehicles that cross the stratosphere;** hence, the importance of quantification of exhaust emissions. Some researchers have already signaled potential impacts of exhaust emissions at certain altitudes. Potential impacts due to the release of aerosols from aerospace vehicles has two key detrimental effects to the ozone layer: **ozone catalytic reactions** with nitrogen oxide particles and condensation of sulfuric acid on their surface, and enhanced radiation from space to Earth's surface, or **radiative forcing**.

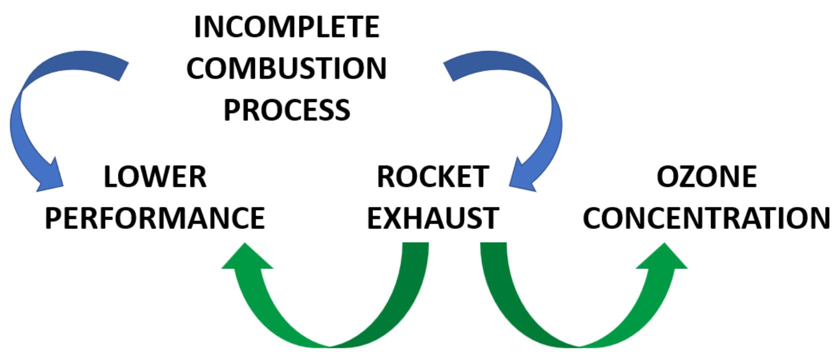

Fig. 1 The project's objective is to relate rocket exhaust particles produced by incomplete combustion to fuel amount and rocket type.

Black carbon aerosols, also known as soot, are typically found in plume from organic fuel such as solid hydroxyl-terminated polybutadiene (HTPB) and liquid kerosene. Such emissions can be traced back to incomplete combustion processes, which also impact the motor performance. These non-optimum oxidation processes can be related to pressure and temperature within the combustion chamber, as well as the concentration and chemical composition of the propellants. However, exhaust soot can also have a different origin, which is from ingredients used as stabilizers for paraffin-based propellants and opacifiers in other solid fuel compositions. In this case, the soot is not related to a specific combustion process. In summary, it is not necessarily straightforward to correlate the aerosols size distribution and motor performance.

Researchers started measuring the concentration of black carbon aerosols in the stratosphere due to aviation exhausts in the 1990s. Unfortunately, some of these experiments were complex and indicated higher concentrations than expected from theory. A recent estimation of the emissions from kerosene and solid propellants, both producing black carbon aerosols in different concentrations, is presented in **Fig. 2**, showing a concerning positive correlation between rocket launches and black carbon emissions around the world. Laboratory tests have been using intrusive techniques to measure thermodynamic parameters in the plumes and the chamber. This project will concentrate on non-intrusive techniques, since they will not affect mass flows and aerosols velocities readings.

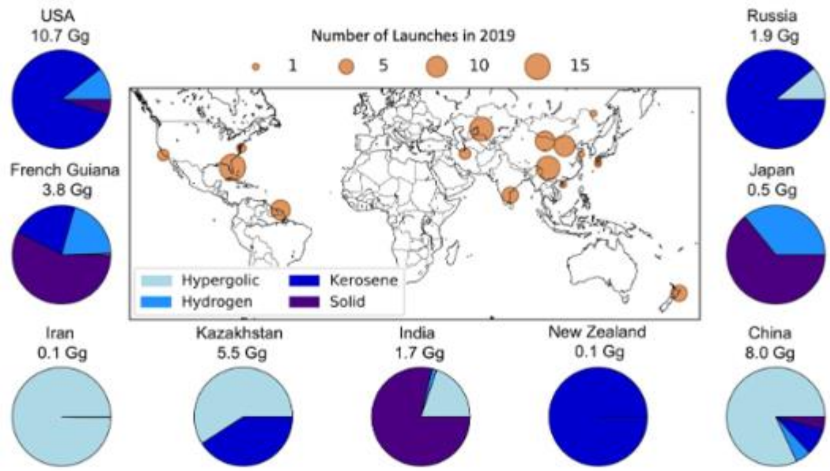

Fig. 2. Diagram showing the emissions of most used propellants in different regions in the world (Ryan et al, 2022).

Objective

This project aims at **setting up and validating a theory that correlates the presence and distribution of aerosols in rockets and hypersonic vehicles with their operational performance and potential to impact ozone concentration.** A validation test will be setup using non-intrusive controlled techniques to measure aerosol emissions characteristics from different rocket fuel and fuel configurations. The first phase will consist of the development of a theory relating the aerosols to these two phenomena (see **Fig. 1** above). The second phase is an investigation of the best nonintrusive techniques to measure thermodynamic parameters in the chamber. Ultimately, the two phases of research will yield improved measurement techniques that will enable accurate, rapid and reliable test data collection of physical, chemical, mechanical, and flow parameters in extreme environments.

A list of planned test measurements on the rocket exhaust and their corresponding techniques is presented: a) thermodynamic properties in the combustion chamber; b) the use of pressure transducers, ultrasound transducers to measure burning rates, thermocouples, infrared (IR) thermography, or IR pyrometry will be explored; c) exhaust **composition**. The best techniques are spectroscopy in the ultraviolet and visible spectrum range (UV-VIS), and infrared (IR) signature; d) exhaust **particles size distribution**. The aerosol size distribution is measured using a scanning mobility particle sizer from TSI Incorporated. This instrument scans across particle diameters and counts the number of particles at each size, producing quantitative information of particle number concentrations and sizes; e) **shock waves geometry**, for which we propose to use visual methods.

Solid propellants of various compositions will be tested. For the booster phase of a hypersonic vehicle, several fuel compositions will be considered. Traditional composite mixtures consist of hydroxyl terminated polybutadiene and ammonium perchlorate, using aluminum as a fuel. A propellant able to deliver better performance while keeping a lower environmental impact than with organic fuels using a mixture of ammonium dinitramide, glycidyl azide polymer and aluminum/magnesium alloy fibers has been obtained in the past. Zirconium in nitrocellulose/nitroglycerine double base propellants has also demonstrated very high burn rates.

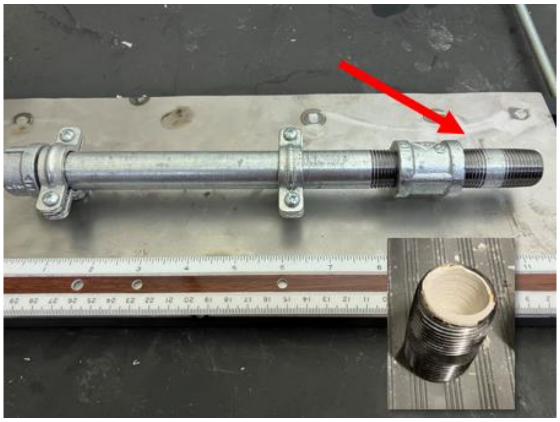

Fig. 3. Picture showing test stand in the lab, ready to ignite. On the bottom right we can observe one of the nozzles specifically made for the project -placed where the arrow points.

The validation of measurement techniques will be performed in the controlled lab environment shown in **Fig. 3**. Different nozzle configurations – made of ceramics– will be used to obtain different propulsion efficiencies. This setup is already prepared for such tests, on the UND campus site outdoors for safety reasons. An example of the test stand generating the rocket emissions is presented in **Fig. 3**.

DoD relevance

Space technology and hypersonics were recently listed as critical technology areas by the National Defense Science and Technology strategy. This project therefore addresses the DoD's top technical priorities. The outcome of the present project has two direct applications. First, as an indirect measure of the rocket or vehicle performance. Second, as an indication on the concentration of ozone. The techniques developed and results obtained can easily be applied to liquid propellants, thus covering a broader spectrum of chemical propulsion systems. We stress the fact that although the stratospheric in-situ measurements are beyond the scope of this project, the non-intrusive techniques developed here will facilitate a future incorporation into flying models.

Approximate yearly costs

This project will cost $200k/year for a total of $600k, with at least 60% going to the Applicant/PI and at most 40% going to the Collaborator/co-PI. Dr. Delene and Dr. Majdi will receive salary support from either share. Two to three grad students will also be supported. The present project has been planned so that initial costs are limited. This coincides with the need to develop an experimental phase at project's start, where different setups will be safely tested in a controlled testing environment. Decisions will be made on the best approach to incorporate measurement probes both in the chamber and at the nozzle exit. These forecasts include yearly trips to DEPSCoR-related activities, attendance to a project review in Washington DC area and at least attendance to one additional conference.

Collaboration composition statement

Through the duration of the project, the ultimate objective of the relationship between the trainee/Applicant and the mentor/Collaborator is to establish the former as an independent researcher, hence this will be the driving target between both researchers. This relationship will be dramatically reinforced by the fact that both of them work in the same institution, the University of North Dakota, and both are on tenured-track positions as assistant professors, and thus share similar experiences. The complementary professional expertise of Dr. Chelmo and Dr. Fernandez-Tous will also offer a unique opportunity of collaboration between their respective colleges, the College of Engineering and Mines –Dr. Chelmo– and John D. Odegard School of Aerospace Sciences –Dr. Fernandez-Tous. Moreover, their extensive and significant previous experience in different research roles in their fields guarantees a successful outcome.

Within the first month of the project, the Applicant will set up a kick-off meeting with the Collaborator where a proposed schedule will be discussed and approved. The schedule will include the project's key milestones and a brief description of the tasks and the effort in man-weeks into which the project will be divided. A dedicated folder will be set up in OneDrive, and shared will all researchers involved. There will also be regular meetings through the project –monthly or bi-monthly, to be agreed during the kick-off meeting. Both the Applicant and Collaborator are highly experienced with web-based tools for project management, whose use will be tailored to the project's complexity.

The buildup of the Applicant as an independent researcher will include:

- Discussions with the Collaborator on appropriate fora to present intermediate results. At the end of the project, an article will be published in a prestigious journal in the area where the results will be analyzed and further work outlined.
- Attendance to conferences and presentations is considered key to contact other researchers working in similar projects, sharing experiences and optimizing limited resources.
- Regular contacts between the Applicant and the Collaborator will also serve to counsel the former on his career development, search for additional opportunities of collaboration and exchange research and teaching methodologies.
- A healthy work environment will be promoted, based on mutual trust, common interests and ethical behavior. In order to preserve this environment, specific rules on data ownership, access and management will be discussed between both sides at the start of the project.

A note on the interdisciplinarity of the research team**:** Dr. Chelmo, Dr. Delene, and Dr. Majdi have an extensive experience with aerosols. Dr. Chelmo will also bring in her expertise on the chemical composition and fluid mechanical properties of nanoparticles. Dr. Delene is world expert in conducting in-situ cloud and aerosol measurements, having lead the in-situ cloud probe team for the NASA IMPACTS project and the DOD funded CAPE2015 and CapeEx19 field projects . Dr. Majdi is has experience modeling atmospheric aerosols, include smoke emissions. Dr. Fernandez-Tous research field is rocket propulsion systems and works closely with other members of the Department of Space Studies on rocket projects.

Basic research statement

The present proposal constitutes a systematic study on the impact of aerosols emissions over the stratosphere. It aims at setting up a rocket test stand that would gather comprehensive information of thermodynamic, chemical and kinetic properties of exhaust plumes of several rocket designs, defined by specific nozzle profiles and solid fuel configurations, as well as hypersonic vehicles using both liquid and solid propellants. In this sense, we go beyond the standard composition of liquid hydrogen for vehicles flying above Mach 5. A common component of reactions, black carbon, also known as soot, manifests as aerosols sizes of less than a micron on the exhaust gases, and it has been identified as a major agent of ozone depletion and radiation forcing in the atmosphere. Tests will be specifically designed to increase our understanding of the fundamental aspects of this phenomenon.

This project constitutes a multidisciplinary approach at the crossroads of atmospheric sciences, environment sciences, and aeronautical and space engineering. Its outcomes will help the Department of Defense in better understanding combustion processes of hypersonic vehicles. Moreover, it will also help other federal agencies, such as the Environmental Protection Agency in defining more efficient policies to protect the ozone layer. This layer acts as a sunscreen for the Sun's harmful ultraviolet radiation with the potential to affect both crops and humans.

The information obtained will be used to better understand the processes that take place in the stratosphere, a region less understood than the troposphere because it is more difficult to access. Understandably, most of the research to date has focused on atmospheric regions easily reachable with balloons and unmanned air vehicles (UAVs) duly equipped with a variety of sensors. What we present here constitutes a critical step towards integrating measurement techniques in vehicles that will fly at higher altitudes. In this sense, this project offers a high payoff research, and constitutes a unique opportunity to prevent disastrous consequences for life on our planet. Moreover, the development of techniques to measure chemical composition, and thermodynamic and kinetic properties of rockets and hypersonic vehicles exhaust will allow a better understanding of these processes, thus allowing the development of greener practices and a more efficient design of propulsion systems without impairing thrust and power drivers. The presence of certain aerosols such as black carbon in the rocket exhausts is not only detrimental to the environment, but it also hinders a more efficient use of the energy released through chemical reactions in the combustion processes. Minimizing its presence in the plumes is thus of capital interest to the industry and scientific community. It is in this sense that the proposed research meets the definition of basic research, as it appears in paragraph 1.5.1 of chapter 5 of the Financial Management Regulation of the Department of Defense, volume 2B, chapter 5.

Curriculum Vitae, Marcos Fernandez-Tous, Ph.D. (Applicant)

Summary

Passionate Aerospace and Aeronautical professor, I hold a broad background experience embracing all levels of research, from the development of the proposal through project management. Broad research interests, including rocket propulsion systems, hypersonic aerodynamics and in-space maintenance. More than 20 years of professional experience in the industry, having worked for universities and colleges, Civil Aviation Administrations, international aviation organizations, and air transport consultancies in the U.S. and abroad. Training experience in a wide variety of cultural environments, including the U.S., Europe, South Korea, Morocco, Jordan, Mauritania, and Nepal. Instructor of rocket propulsion, hypersonic aerodynamics, air navigation, communications and surveillance systems.

Experience

Space Studies Assistant Professor University of North Dakota, Department of Space Studies	Aug 2022- present Grand Forks, ND
NASA Intern Marshall Space Flight Center	Jun 2022-Aug 2022 Huntsville, AL
NASA Grant Applicant University of North Dakota, Department of Space Studies	Mar 2022-Jun 2022 Grand Forks, ND
Graduate Research Assistant for ASSURE A54 project University of North Dakota, Department of Aviation	Jan 2022-Jul 2022 Grand Forks, ND
Graduate Research Assistant for ASSURE A25 project University of North Dakota, Department of Aviation	Jul 2020-Jan 2022 Grand Forks, ND
Instructor or Rocket Propulsion Systems University of North Dakota, Department of Space Studies	Jan 2021-May 2021 Grand Forks, ND
Trainee University of North Dakota, Department of Aviation	Feb 2020-Aug 2020 Grand Forks, ND
Graduate Student Assistant University of North Dakota, Research Institute for Unmanned Systems	Dec 2018-Aug 2019 Grand Forks, ND
Adjunct Professor Vaughn College of Aeronautics	Sep 2017-May 2018 New York, NY
Air Transport Operations Expert Freelance	Jul 2016-Aug 2018 New York, NY

Air Navigation Safety and Quality Auditor Jan 2009-Jun 2016
SENASA Madrid, Spain

Single European Sky Expert May 2008-Jan 2009
INECO –seconded to Aena Madrid, Spain

Delegate to the European Union Sep 2004-May 2008
INECO Brussels, Belgium

Advisor to the Director General Sep 2002-Sep 2004
INECO –seconded to EUROCONTROL Brussels, Belgium

Member of Automatic Dependent Surveillance Group Jun 2001-Sep 2002
INECO –seconded to Aena Madrid, Spain

Education

Doctor of Philosophy in Space Sciences May 2022
University of North Dakota –Grand Forks, ND
Master of Science in Aerospace Engineering Nov 2001
Polytechnic University of Madrid –Madrid, Spain

Honors and Awards

North Dakota Space Grant Consortium, *September 2021*.
Daniel and JoEmily Nieuwsma Scholarship award, *May 2019.*

Published articles

Adjekum, D. K. & Fernandez-Tous, M. (2020). Assessing the relationship between organizational management factors and a resilient safety culture in a collegiate aviation program with Safety Management Systems (SMS). *Safety Science, 131*, 1-16. https://doi.org/10.1016/j.ssci.2020.104909.

Adjekum, D. K.& Fernandez-Tous, Marcos. (2020). Assessing cultural drivers of safety resilience in a collegiate aviation program. Collegiate *Aviation Review International, 38*(1), 122-147. Retrieved from http://ojs.library.okstate.edu/osu/index.php/CARI/article/view/8012/7386

Fernandez-Tous, M. (2022, October 26-29). *A Receiver-Only time Synchronization protocol for UAS. Simulation results*. [Conference Session] 2022 IEEE 13th Annual Ubiquitous Commuting, Electronics and Mobile Communication Conference (UEMCON), virtual conference. Awarded best paper certificate in the session Robotics; Cloud networks.

Hallie Boyer Chelmo, PhD
Mechanical Engineering, College of Engineering and Mines
University of North Dakota, Grand Forks, ND 58201
Phone: 701-777-6515, E-mail: Hallie.chelmo@und.edu

(a) Professional Preparation

Macalester College	Physics	BA, 2008
University of Minnesota	Mechanical Engineering	PhD, 2017
Carnegie Mellon University, Pittsburgh, PA	Environmental Chemistry	PD 2017-2019

(b) Appointments

8/2019–present, Assistant Professor, University of North Dakota, Grand Forks, USA.
8/2017–7/2019, Camille and Henry Dreyfus Environmental Chemistry Postdoctoral Fellow, Carnegie Mellon University, USA.
6/2014–5/2017, National Science Foundation Graduate Research Fellow, University of Minnesota, USA.
8/2012-5/2014, Graduate Research Fellow/Teaching Assistant, University of Minnesota, USA.

(c) Relevant publications (published as Boyer as of 2021)

1. Boyer, H., Wexler, A.S., Dutcher, C.S. Parameter Interpretation and Reduction for a Unified Statistical Mechanical Surface Tension Model. *Journal of Physical Chemistry Letters*, 6 (17), pp 3384 - 3389 (2015) DOI: 10.1021/acs.jpclett.5b01346.
2. Boyer, H.C., and Dutcher, C.S. Statistical Thermodynamic Model for Surface Tension of Aqueous Organic Acids with Consideration of Partial Dissociation. *Journal of Physical Chemistry A*, 120 (25), pp 4368 - 4375 (2016) DOI: 10.1021/acs.jpca.6b01469.
3. Boyer, H.C., Bzdek, B., Reid, J.P., and Dutcher, C.S. A Statistical Thermodynamic Model for Surface Tension of Organic and Inorganic Aqueous Mixtures. *Journal of Physical Chemistry A*, 121 (1), pp 198 - 205 (2017) DOI: 10.1021/acs.jpca.6b10057.
4. Boyer, H.C. and Dutcher, C.S. Atmospheric Aqueous Aerosol Surface Tensions: Isotherm-based Modeling and Biphasic Microfluidic Measurements. Feature Article in *Journal of Physical Chemistry A*, 121 (25), 4733 - 4742 (2017) DOI: 10.1021/acs.jpca.7b03189.
5. Boyer, H. C., Gorkowski, K., and Sullivan, R.C. In Situ pH Measurements of Individual Levitated Microdroplets Using Aerosol Optical Tweezers, *Analytical Chemistry* 92(1), p. 1089-1096, (2020) DOI :10.1021/acs.analchem.9b04152.
6. Sullivan, R. C.; Boyer-Chelmo, H.; Gorkowski, K.; Beydoun, H. Aerosol Optical Tweezers Elucidate the Chemistry, Acidity, Phase Separations, and Morphology of Atmospheric Microdroplets. *Acc. Chem. Res.* 2020, *2017* (21). DOI:10.1021/acs.accounts.0c00407.

(d) Synergistic Activities

1. Employed, mentored, and trained 7 UND students: 7 undergraduate students (2 juniors, 5 seniors) and 3 graduate students (thesis supervisor to 2 masters students) on optical tweezers chamber design and thermodynamic modeling.

2. Conference organizer:
Organizer of conference section Aerosol Physics at the 39th American Association for Aerosol Research (Albuquerque, NM October 2021).
Co-Organizer of conference section Aerosol Physics at the 38th American Association for Aerosol Research (virtual event, October 2020).

3. Developed two new graduate courses and three undergraduate courses at UND that were never previously taught at this institution. Topics included aerosol engineering (dynamics, filtration, nucleation) and molecular gas dynamics (kinetic theory, statistical mechanics). Developed three undergraduate courses for individual study for two undergraduate students.

4. Outreach activities through a state-sponsored program (summer camps and on-site visits) for American Indian college students, including the Nurturing American Tribal Undergraduate Research and Education (NATURE) camp in summer 2021 and 2022. Supervised a student from Nueta Hidatsa Sahnish College to model pollutant dispersion from methane plumes in oil and gas fields. Served as lead coordinator of the NATURE University summer camp in summer 2022.

5. Community outreach: ND regional science fair judge (March, 2021); Advised Grand Forks based UAS company, SkyScopes, Inc., on disinfectant spray via drone (summer 2020).

6. Service: Peace Corps Volunteer in Ghana, West Africa, (2010-2012); Taught high school physics in a remote village, integrated into their culture, and spoke two local languages.

Lists of all previous DoD research relevant funding active between 1 October 2016 and 30 September 2023

The Applicant has never received DoD funding.

Dr. Chelmo's DoD research relevant funding active between 1 October 2016 and 30 September 2023:

- Investigating the formation and impacts of ice crystals aggregates on hypersonic vehicles.
  - Award number: N00014-23-1-2269.
  - P.I.: Hallie Boyer Chelmo.
- An Ecosystem of High-Performance Defense Sensitive Materials Research at University of North Dakota.
  - Award number: FA9550-22-1-0274.
  - P.I.: Jon Mihelich.
  - Key personnel/senior scientist: Hallie B. Chelmo.