ND EPSCoR
Established Program to Stimulate Competitive Research

News & Notes

July 2019

Bashful no longer

Summertime reflections are a favorite pastime, and one that often leads to fresh inspiration, thoughtful changes, and greater awareness of and gratitude for the many good things in our lives.

Although our current NSF Track-1 cooperative agreement has been extended, July marks the end of the fifth year of research and outreach for the project. What are the accomplishments? What benefits have resulted from the thousands of hours of effort? What is different in North Dakota because of these research, education outreach, and workforce efforts?

In looking through the annual report, you see many names, research topics and outreach projects, written in academic prose. But the reality of what the Center for Regional Climate Studies (CRCS), and the Center for Sustainable Materials Science (CSMS), have accomplished is amazing. Their insightful work has changed, (and will continue to impact), the way we see our state/world, the way we function on a daily basis, and the information we use to make vital decisions.

In short, it is time to stop being "North Dakota bashful" about the accomplishments of the researchers, students, mentors, and staff who worked diligently to make a difference throughout these past five years.

Thanks to CRCS, there are a host of new models and insights about the land, water, and climate for use by the agricultural community and those who depend on that industry.

- Researchers at Dickinson State University have focused on soil health, foundational to our state's economy. Others across the state, including Nueta Hidatsa Sahnish and United Tribes Technical Colleges, have looked at pollinators and insect predators to find the "why" behind declines in bee and bat populations.
- At UND and NDSU, researchers have developed better models to predict winter blizzards, monitor watershed impacts, and expand hydrology and economic crop models.
- Water and air quality analyses have been a statewide emphasis, and is resulting in better data for use in the state's forecasting and long-range planning.

Thanks to CSMS, many novel biobased materials using ND's agricultural products or byproducts have been developed. Not only will farmers benefit, but the environment of our state and country can potentially gain from these scientific advances.

- Innovative uses of agricultural products have been researched to replace petrochemical ingredients in coatings, plastics, resins, and a host of other commercial-ready products.
- At Mayville State and Minot State Universities, researchers and students have developed new processes that change how biobased materials are processed or incorporated into new applications.
- At NDSU, a researcher has taken the computational tool—QSAR—developed by another North Dakotan (Corwin Hansch of Kenmare), and used it to create a new, highly efficient method for analyzing properties of new polymers. Thousands of experiments can now be modeled via computer, saving both time and money, to predict the best combinations of materials and therapies.

Finally, from my perspective, the most important impact is with the students involved in the research and other programs like Nurturing American Tribal Undergraduate Research and Education (NATURE). Many students acknowledge—reflected in some of this (and prior) issue's articles—that their research experience has changed their career focus or broadened their outlook. With over half of the TC and ND University System (NDUS) graduates choosing to stay in state after graduation, it means we have created a talented and well-trained workforce that will be an economic driver in our state for years to come.

No need to be bashful. The work done through ND EPSCoR's Track-1 and other programs produces results in which we can all take pride.
Regards,

Kelly A. Rusch, Ph.D., P.E., BCEE
ND EPSCoR Executive Director

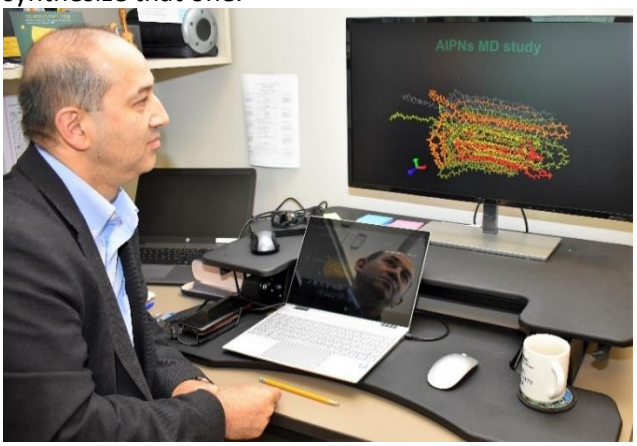
Timesaving innovation

A researcher and his team are developing new avenues of discovery with novel and complex materials—biobased polymers. **Bakhtiyor Rasulev**, a CSMS researcher (a new faculty hire during this award) and assistant professor in Coatings and Polymeric Materials (CPM) at NDSU, has been able to build predictive models that help researchers model different properties of polymeric materials.

"It's a mathematical way to investigate materials," Rasulev said. "There are several approaches to building predictive models, such as a statistical approach, quantum chemistry, molecular modeling, or a combination of approaches such as QSAR (Quantitative Structure-Activity Relationship) modeling. It's a way of digitizing properties of polymers or other materials to predict an endpoint of interest."

The value of this research effort is a huge efficiency boost, he said. Rather than thousands of individual lab experiments to determine which material will react with another substance in a desired manner or have a particular property, Rasulev's team conducts a computerized analysis of the polymer components and provides predictions about which materials will work best, saving hundreds of hours of time and material costs. "It eliminates many routine steps," he said, "and speeds the process of finding a polymer with the right properties."

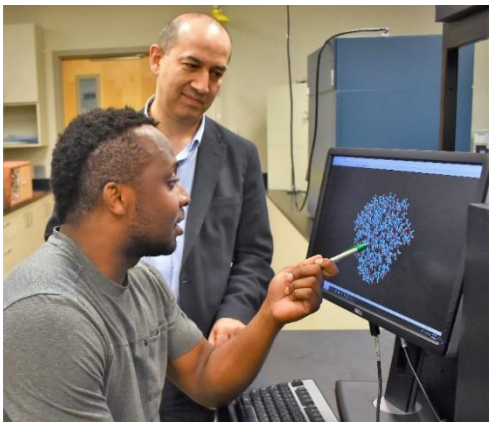
Within CSMS, many of the biobased polymers are so new, they don't have well-known characteristics, as do many of the traditional petrochemical-based polymers. "We can now help predict for researchers a particular polymer that has the properties they want," Rasulev (below) noted. "We take all the components involved and virtually screen all possible variations, so they can select the one with the desired properties, and synthesize that one."



Rasulev's background includes extensive work with nanotechnologies, data analysis, and high performance computing. He's using those skills in refining this new predictive modeling system, and, in the process, also helping train graduate students. Recently, he tested over 1,000 proteins to see their interaction with 170 nanomaterials. For those proteins that interacted with only one nanomaterial (i.e., the nanomaterial selectively inhibits activity of this protein), it opens the door for identifying a system that may have distinctive commercial uses, such as delivering a substance to a specific cell type. The practical benefit? If a material appears to react with only one protein, it may reduce side effects in delivering a medication. On the flip side, a nanomaterial that reacts with almost all the proteins may be beneficial for a different commercial application. The developed methodology based on this study can then be extended to predict interactions of polymeric materials with biomolecules.

Once identified computationally, results are confirmed in lab experiments. By building correlations between the computer simulation and lab experiments, the model continues to increase accuracy and reliability, Rasulev noted. The final step is being able to predict the properties of new polymers, just by knowing their structural characteristics.

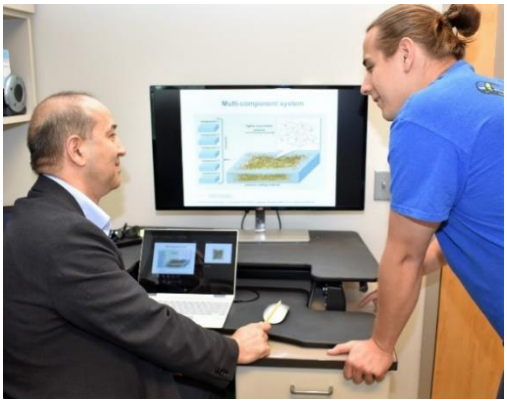
Student work



Kweeni Iduoku (left, with Rasulev, right), graduate student in CPM and CSMS researcher, is using the QSAR as a means to optimize the physical and molecular properties to predict how polymeric micelles (a collection of molecules that make up a larger particle) can be used to deliver specific compounds to cells. The practical application could be useful in agriculture or medical applications, as the micelles are used to carry microscopic amounts of compounds to the right cells, and then release their contents.

With biobased polymers, one of the key questions asked by commercial users is "if" and "how" the polymers will degrade. **Meade Erickson**, a doctoral graduate student in CPM and CSMS researcher, is trying to predict how the polymers will degrade when exposed to various conditions, including thermal degradation

(changes in temperature or heat), photo degradation (a combined action of sunlight and air), or bio-degradation (how the polymer degrades when exposed to the environment). Once those properties are known, they can be used to develop mathematical models to make these polymers more efficient, such as more easily degradable or inversely, make them more stable.



Rasulev (left), with Erickson (right), discussing a model of a multi-component system.

"To my knowledge, no one has done this type of high throughput screening with polymers before," Rasulev said. He is following in the footsteps of another North Dakotan: Corwin Hansch, who is credited as the "father" of QSAR modeling. Hansch, a Kenmare native, was the first one who developed a system that builds the quantitative correlation between the structures of selected molecules with their physicochemical properties or biological activities. That QSAR model approach is an important part of the toolkit Rasulev's team uses in their predictive modeling.

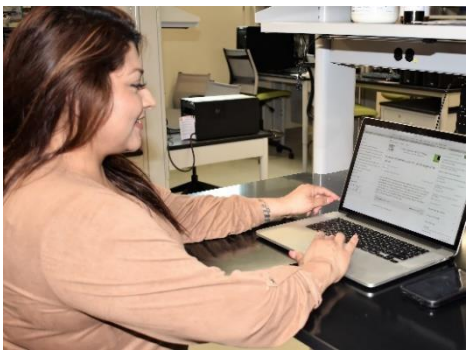
"To date, no one else is using QSAR for crosslinked polymers," Rasulev said, "but it has great potential and can dramatically change the whole direction of science in developing biopolymers."

Impacting how biopolymers are studied, conserving researcher resources, and helping develop a highly skilled workforce: some of the CSMS research benefits for our state.

The value of research

A senior in Environmental Science at Nueta Hidatsa Sahnish College (NHSC), **Lizette Alvarez**, spent part of her summer break learning more about research techniques and gaining a greater appreciation for biobased nanoparticles, especially cellulose nanoparticles. **Dilpreet Bajwa**, professor in NDSU's Mechanical Engineering department and an ND EPSCoR Emerging Areas Seed collaborator with **Kerry Hartman**, academic dean at NHSC, have joined forces to study how a corn-based polymer, poly(lactic acid) (PLA), can use cellulose nanocrystals to create a better biobased packaging.

"I am intrigued by plant science, especially ethnobotany, and I like the research aspects," Alvarez (left) said. "I was attracted by the concept last year, when my mentor, Kerry Hartman, talked about it." With her background in Environmental Science, she has studied the impact of traditional plastic on the oceans, soil and animals. "This kind of research will make a difference," she said. "It's amazing to work with a plastic that is biobased and biodegradable."



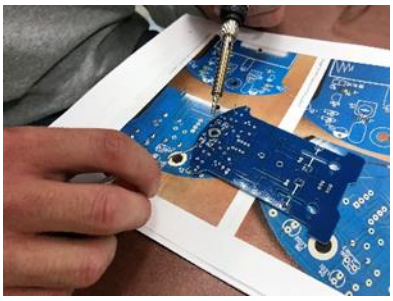
In her work at the NDSU lab, Alvarez is taking the opportunity to "do everything" from attempting to create uniformly dispersed nanocrystals in the PLA, to studying its antimicrobial properties, to testing the mechanical properties of the films for water absorption, color changes, strength, and crystalline properties that will help protect package contents.

"It's important for students to have hands-on learning," Bajwa said. "The research experience is essential." He has hosted other students in the past, and both he and his post-doctoral assistant, **Jamileh Shojaeiarani**, Mechanical Engineering, are working with Alvarez to build her research skills.

Alvarez (left) shows the results of a test protocol to Bajwa (right).

"Since I've started doing research, even my son has gotten interested," Alvarez noted. "He has participated in the NATURE Sunday Academy program at NHSC, and said the hands-on research made it interesting." For Alvarez, this short-term experience could open doors to other career or educational avenues, a direct result of spending time in an emerging area of research.

Bridges and smart cars



Students at the Nurturing American Tribal Undergraduate Research and Education (NATURE) Bridges camp, held at Turtle Mountain Community College (TMCC), assembled smart car components (above) during an engineering segment. The multi-day camp, piloted at TMCC, is designed to foster STEM interest for students.

Students solder components for the smart cars (seated from left to right) ***Lyle Lunday, Jr.****,* ***Dario Vega****,* ***Bryghton Peltier****, and* ***Hunter Gladue****.* ***Danny Luecke****, mentor, is standing.*

Something's in the air

"Understanding how particles behave in the atmosphere will improve the accuracy of atmospheric models used to predict climate change," said **Frank Bowman**, CRCS researcher and UND associate professor and chair of Chemical Engineering. "The goal is to make more informed choices."

Initially, Bowman's research looked at the effects of diesel exhaust under the ND EPSCoR Track-1 cooperative agreement. "Our work on air quality in ND helps us better understand how much (or how little) impact oil and gas development activities have on air quality related to health and visibility," Bowman said.

Bowman started modeling with clean air, then added diesel exhaust with particulates and vapor. When exposed to ultraviolet (UV) rays, present in sunlight, there's a reaction, which can change the gas compounds, turning them from gas to liquid. That liquid may adhere to the diesel's soot particles so they grow. The growth in particles is then measured over time.

"We are particularly interested in how these diesel particles behave in forming cloud droplets, or cloud condensation nuclei (CCN)," he said. What they found in the lab was interesting: when the diesel soot is "fresh," it's very oily, so the particles don't attract water. But as the particles get more coated, they get bigger and also become more tolerant of water, making it easier for them to form cloud droplets.

Bowman's modeling work looks at baseline air quality simulations from 2010 and will compare it with similar model predictions using 2015 emissions information. "We're very fortunate that ND, in general, has air that's pretty clean," he said. "When we look at the model differences between 2010 and 2015, we will be able to remove the effects of natural variability and see what changes come from oil production. With the computer model, we're able to look at a whole region instead of just a narrow list of locations."

Air quality is a key factor in health issues, from respiratory functions to heart disease and other health concerns, Bowman said, and the particulates can also impact visibility and overall air quality. "Historically ND's air is clean, and we want to make sure it stays that way. The models consider the sources of particulates, what impacts there might be, and what steps we can take to mitigate. When we have more accurate models," he noted, "we can make better plans for the future."

From diesel, Bowman is now focusing on other organic compounds in the test chamber (below): Alpha-humulene which is emitted by sunflowers and pine trees, and beta-farnesene which is emitted from potatoes and corn. Bowman said the next laboratory studies will focus on how particle growth is affected by temperature changes.

In addition to creating better models, Bowman noted that the majority of his work also provides research training for students. "Beyond the scientific information, the state also benefits from having a more educated technical workforce," Bowman said, "like **Carlos Bucaram Carbo**, who came to UND to study for his master's degree. He returned home, then came back to work on his doctorate as an air quality modeler—a career he didn't know existed before coming to UND."

Better information, better models, and a well-trained workforce: just a few of the benefits of the CRCS research efforts for North Dakota.

NATURE closing ceremony

Native American students from across the state took the stage on June 14 at UND's Gorecki Alumni Center to present the research they had been involved in during NATURE University Summer Camp. The research ranged from studying fossils to learning about using poly(lactic) acid in 3D printing, studying water quality, as well as the use of aerial photography to learn about ecological changes.

One common theme was the value of learning more about potential career choices. "These two weeks helped me decide what I want to do next," said **Mhaddie Poitra**, (pictured above left) presenting with **Curtis Ferris**. Her experience, along with mentoring from **Taufique Mahmood**, UND assistant professor in Geology & Geological Engineering, helped her decide on a geology major.

Other students, including **Peyton Davis**, commented that they now "felt more comfortable in doing research," learning about different computer programs, or discovering a field they wanted to explore. The positive attitude of the instructors and mentors was cited as a significant influence. "To think that we're the first ones to do research on this particular topic is exciting," said **Aliya Martinez**. "We're solving some of the questions about why and how and who for others who will come after us."

Brian Tande (left), UND interim dean of the College of Engineering and Mines, talked about the goal of engineers and scientists in his keynote address. "What do engineers and scientists do?" he asked. "They solve problems, and our world doesn't have a shortage of problems." He encouraged the students to explore and look at both UND and NDSU as places where they could be successful. "Each of these universities has a lot of mentors who are invested in your future and want to see you succeed," he said. "It may not always be easy, but it will be worth it."

For the students who participated, as well as the faculty and mentors, it was a celebration of effort and exploration.

Softball to soils

The draw to Dickinson State University (DSU) for this Bismarck native was a softball scholarship. She wasn't sure what direction to take until she started with Environmental Science. "It was a 'wow' moment," **Karissa Bohn** recalled. "I fell in love."

Bohn is a ND EPSCoR's Research Experience for Undergraduates (REU) awardees this past year, and has had the opportunity to work in both lab and field under the guidance of two CRCS researchers: **Eric Brevik**, professor of Geology and Soils, and **Josh Steffan**, assistant professor in Agriculture and in Biology. "I like the mix of field work and lab analysis of soil samples," she said. "It's been a great learning experience."

The field research has helped her better understand information gained from coursework on soil, she noted. "Working out in the field helps you see what's going on," Bohn said. "You can apply the theory, and it helps with the assessments and analysis." As a part of her REU

experience, Bohn (left) has done the "dirty work" of soil analysis as well as operating specialized equipment. She is currently working on a joint paper for publication. Her project relates to the photosynthesis of plants in the test plots at the leaf, canopy and satellite levels.

Preparing for her senior year, Bohn is also active on campus, as the student assistant director of the Honors Program, a recipient of the Theodore Roosevelt Honors award, adding a minor in leadership studies, and working part-time this summer with the US Forest Service. When asked about post-graduation interests, she said she is considering graduate school, having developed a special interest in conservation and ecology.

Although softball is still a favorite sport, the career focus has shifted and expanded, opening doors that Bohn didn't know existed just a few years ago. Brevik said the value of the REU is helping students make informed decisions. "Most people—including me—don't have any idea what research involves," Bohn said. "The REU has given me a chance to see what a research scientist does, and to see the importance of that work."

Activities of note

Keshab Thapa (on right), DDA awardee and NDSU graduate student in Civil and Environmental Engineering, took second place in the American Society of Civil Engineers(ASCE) Geo-Institute poster competition held during the Engineering Mechanics Institute and Geo-Institute joint conference at Caltech in June. The title of his poster was *Role of Clay-Fluids Molecular Interactions on the Compression of Swelling Clays*. The poster described results from molecular dynamics simulations of compression of swelling clay, providing a potential molecular basis for macroscopic behavior of such clays. Thapa's advisor is **Dinesh Katti**. The photograph was taken at the awards banquet.

Khwaja Hossain, CSMS researcher at Mayville State University and professor in Biology, was featured in the Grand Forks Herald for his research on wheat bran. https://www.grandforksherald.com/news/education/2735218-Mayville-State-research-finds-wheat-bran-could-be-used-to-treat-water-clean-oil-spills

A group of engineers collaborated in a panel discussion for the NATURE Bridges students, focusing on engineering career paths. Pictured above (left to right) are **Terri Ann Allery, Ann Vallie, Gabe Brien, Rachel Gourneau, April Walker** and **Austin Allard**. All are from the Turtle Mountain Band of Chippewa Reservation, and all now have a professional career in engineering.

New Corn Oil-Based Monomer Synthesis for Latex Applications in Coatings and Paints by **Andriy Voronov**, CSMS researcher and associate professor in CPM at NDSU, received a grant of $52,522 by the North Dakota Corn Utilization Council to include synthesis of new corn oil-based monomers (COM) and their evaluation for biobased latexes that will be prepared from COM.

Valorization of Corn as a Feedstock for Designing of High Value Functional Materials by Emerging Seed Area awardees **Surojit Gupta**, assistant professor in Mechanical Engineering, and **Yun Ji**, graduate program director in Chemical Engineering (both UND), received a grant of $90,600, from the ND Corn Council. Average net cash farm income for farms specializing in corn production is expected to decrease, creating an urgent need for new corn-based products for markets.

Center for Regional Climate Studies (CRCS) publications

Evaluating Sensitivities of Economic Factors through Coupled Economics-ALMANAC Model System by **Jon Starr**, **Haochi Zheng**, **Jianglong Zhang** (all UND), and Jeffrey Reid, in Journal of Agronomy, 2019. DOI:10.2134/agronj2018.08.

Emerging Areas Seed publications

On the Development of a Bio-based Dielectric Material was an abstract presented by **Sima Noghanian**, **Ali Alshami**, **Ala Ali Alemaryeen**, and **Meysam Haghshenas**, (all UND), along with A. Tesser and J. Lewis at the URSI Commission B International Symposium on Electromagnetic Theory (EMTS 2019), May 27-31, 2019.

Doctoral Dissertation Assistantship (DDA) publications

Genome-wide RNA Pol II Initiation and Pausing in Neural Progenitors of the Rat by **Sergei Nechaev** (UND), with Adam Scheidegger, Carissa Dunn, Ann Samarakkody, Nii Koney-Kwaku Koney, Danielle Perley, and Ramendra Saha in BMC Genomics, 2019, 20: 477. DOI: 10.1186/s12864-019-5829-4

Upcoming events

- **CRCS and CSMS monthly meetings:** Hosted via IVN to all campuses, with dates posted on the websites.
- **Tribal College summer camps:**
  - NHSC will be July 15-19, 2019
  - TMCC's third camp will be July 15-26, 2019

Stay in touch

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