Khaled Mosharraf Mukut, Ph.D.

Postdoctoral Associate, Department of Mechanical Engineering, University of Minnesota Twin Cities
Minneapolis, MN, USA
kmukut@umn.edu linkedin.com/in/kmmukut github.com/kmmukut kmmukut.github.io
ORCID

Professional Summary

Accomplished Postdoctoral Associate with a Ph.D. in Mechanical Engineering, specializing in **CFD, Molecular Dynamics, and High-Performance Computing**. Proven track record of developing **novel computational frameworks** for soot formation and multi-scale modeling. Recipient of a **$22,000 research fellowship** with a strong portfolio of high-impact publications. Experienced mentor to undergraduate and graduate students, passionate about advancing research in sustainable energy and computational engineering.

Research Interests

Electrochemical and Plasma-Assisted Reacting Flows • Soot Formation and Morphology • Molecular Dynamics (MD) • Computational Fluid Dynamics (CFD) • Data-Driven Engineering-Scale Modeling • Radiative Heat Transfer • Interdisciplinary Collaboration

Education

Ph.D. in Mechanical Engineering
Aug 2019 – Aug 2025
Marquette University, Milwaukee, WI, USA

- Dissertation: Fundamental Exploration of Soot Formation and Morphology from a Molecular Modeling Perspective
- Advisor: Dr. Somesh Roy

M.S. in Mechanical Engineering
Aug 2017 – May 2019
Marquette University, Milwaukee, WI, USA

- Thesis: Effect of Radiation and EGR on Pollutant Formation in High-Pressure Constant Volume Spray Combustion
- Advisor: Dr. Somesh Roy

B.S. in Mechanical Engineering
Feb 2011 – May 2016
Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh

- Thesis: Numerical Investigation on Active Control for Drag Reduction in NACA 4412 Airfoil
- Advisor: Dr. Mohammad Ali

Professional Experience

Postdoctoral Associate
Sep 2026 – Present
Computational Reactive Flow & Energy Lab (CRFEL), Department of Mechanical Engineering, University of Minnesota Twin Cities, Minneapolis, MN, USA

- Developing OpenFOAM-based solvers for **electrochemical and plasma-assisted reacting flows**, resolving charged, reacting transport in electrolytes.
- Coupling multi-species **Poisson–Nernst–Planck transport** with homogeneous chemistry, electrode kinetics, electrical double layers, flow with electro-osmotic effects, and gas–liquid interfaces.
- Mentor: Dr. Suo Yang

Postdoctoral Research Fellow
Oct 2025 – Sep 2026
Marquette University, Computational Combustion Lab (CCL), Milwaukee, WI, USA

- Leading research on **advanced microclimate modeling** at a city-block scale using **high-fidelity CFD**.
- Developing a novel framework for optimizing **load balancing** in large-scale **Lagrangian-Eulerian simulations** within HPC environments.
- Mentor: Dr. Somesh Roy

Graduate Research Assistant *Aug 2017 – Aug 2025*
Department of Mechanical Engineering, Marquette University, Milwaukee, WI, USA

- Conducted **reactive molecular dynamics (RMD)** simulations of soot formation, delivering detailed in situ insights into particle morphology and evolution.
- Developed **novel computational methods** for RMD simulations, aiding in advanced analysis of soot particle dynamics and morphology.
- Characterized multi-physics interactions in spray combustion devices using **macro-scale CFD, soot models, and radiation models**, enhancing understanding of soot particle interactions and radiative heat transfer.
- Collaborated with interdisciplinary teams and presented research findings at international conferences, resulting in high-impact publications and exchange knowledge within the research community.

Graduate Assistant *Mar 2016 – Aug 2017*
Department of Mechanical Engineering, Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh

- Performed molecular dynamics simulations of explosive boiling characteristics, providing critical insights into phase transition mechanisms.
- Characterized critical heat flux density and inherent metastability in nano-scale boiling heat transfer.
- Studied the effects of nano-structures on liquid boiling, enhancing heat transfer models.
- Standardized numerical parameters for thermally stratified co-axial jet flow, increasing simulation reliability and accuracy.

Industry Experience

Operation Engineer (Export) *Jun 2016 – Dec 2016*
PRAN-RFL Group, Dhaka, Bangladesh

- Actively participated in the "Automatic Conveyor Control System in Production Line" project, increasing production efficiency.
- Collaborated with the operation and maintenance team for Injection and Blow Molding Machines.

Maintenance Engineer (Intern) *Feb 2016 – Apr 2016*
Khulna Power Company LTD. (KPCL), Khulna, Bangladesh

- Gained hands-on experience with large diesel and HFO-based power plants.

Teaching and Mentoring

Graduate Research Assistant (mentoring) *Aug 2017 – Aug 2025*
Department of Mechanical Engineering, Marquette University, Milwaukee, WI, USA

- Co-supervised 6 undergraduates in designing affordable air quality monitoring devices for their senior project.
- Mentored 3 summer undergraduate researchers in developing ML–based image segmentation algorithms for HRTEM soot images; one received the WSGC fellowship and joined my lab as a graduate student.
- Guided fresh graduate students on interdisciplinary projects, leading to publications and improved collaboration; one earned the WSGC fellowship.

Graduate Teaching Assistant *Aug 2018 – May 2020*
Department of Mechanical Engineering, Marquette University, Milwaukee, WI, USA

- Conducted lab sessions for Materials Science (MEEN 2460), enhancing hands-on learning experiences for over 30 students each semester.
- Prepared and delivered lectures on Heat Transfer (MEEN 3330) for junior-level undergraduates.
- Served as a grader for Fluid Mechanics, Thermodynamics, and Heat Transfer courses, providing timely and constructive feedback to students.

Graduate Assistant (mentoring) *Mar 2016 – Aug 2017*
Department of Mechanical Engineering, Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh

- Mentored two groups totaling seven undergraduate seniors in their thesis projects, leading to three student-led presentations at national conferences and two publications.

Leadership and Service

Organizer & Mentor, Python Workshop for High School Students *Jul 2023 & Jul 2025*
Marquette University

- Mentored 15 high school seniors with no prior programming experience, enabling them to write basic Python programs and create their own air quality visualization code by the end of the workshop.
- The detailed course material is available on my GitHub repository: https://github.com/c4c-2023/code4climate.git

Organizer & Mentor, Entangled Air: an exhibition bringing together the art of Tomás Saraceno and my research *Jan 2022 – May 2022*
Marquette University

- Co-supervised a group of 4 undergraduate and 2 graduate students in developing an interactive exhibition on air quality and climate change.
- A series of social outreach raising awareness about air quality and climate change through art and science.
- Developed artwork and scientific content for the exhibition, advocating for environmental sustainability.
- The exhibition was a huge success and received a lot of positive media coverage in Milwaukee, WI.

President, Bangladeshi Student Association at Marquette University (BSAMU) *Jun 2021 – May 2023*
Marquette University

- Organized a number of cultural events and community service activities to promote Bangladeshi culture and heritage as well as bring together the Bangladeshi community at Marquette University.
- Led an executive board of 10 members and ran bi-weekly meetings to oversee progress in essential parts of the organization.

Honors and Awards

Richard W. Jobling Distinguished Research Fellowship *Aug 2023 – May 2024*
Marquette University

- Awarded **$22,000** to conduct research on the impact of soot and particulate matter on air quality and climate change.

Outstanding Research Assistant Award *Mar 2021*
Opus College of Engineering Honors Convocation, Marquette University

- Recognized for exceptional performance as a Graduate Research Assistant.

Cover Feature for Publication *Vol. 24(3), 2020*
Combustion Theory and Modelling

- My manuscript was featured on the journal's cover.

Best Poster Award *Apr 2018*
Annual Graduate Poster Exhibition, Marquette University

- Awarded for excellence among more than 60 participating graduate students.

Dean's List Scholarship *2011 & 2012*
Bangladesh University of Engineering and Technology (BUET)

- Awarded to the top three students each year of undergraduate study.

Professional Memberships

American Society of Mechanical Engineers (ASME) *Jan 2023 – Present*
American Physical Society (APS) *Jan 2023 – Present*

The Combustion Institute (CI) *Mar 2018 – Present*
The American Association for Aerosol Research (AAAR) *Jun 2018 – Present*

Software and Numerical Tools

1. **Mukut**, **K. M.** *PyPack: A Python toolkit for building molecular simulation systems* GitHub. Version 1.0.0. Aug. 10, 2025. https://github.com/kmmukut/PyPack.
2. Day, T. P., **Mukut**, **K. M.**, Klacik, L., O'Donnell, R., Wasilewski, J. & Roy, S. P. SAGE: A machine learning model for primary particle segmentation in TEM images of soot aggregates. *Proc. Combust. Inst.* **41,** 105821. DOI: 10.1016/j.proci.2025.105821 (Jan. 2025).
3. **Mukut**, **K. M.** & Roy, S. P. *StereoFractAnalyzer: A Python package for analyzing fractal dimensions of 3D surfaces and 2D images* PyPI. Version 1.0.0. Documentation available at https://comp-comb.github.io/StereoFractAnalyzer/. Mar. 2, 2024. https://pypi.org/project/StereoFractAnalyzer/.
4. **Mukut**, **K. M.** & Roy, S. P. *Molecular arrangement and fringe identification and analysis from molecular dynamics (MAFIA-MD): A tool for analyzing the molecular structures formed during reactive molecular dynamics simulation of hydrocarbons* Mendeley Data. Version 1.0.0. https://github.com/comp-comb/MAFIA-MD. Jan. 26, 2022. https://doi.org/10.17632/s7dsk553fh.1.

Technical Skills

Programming: **Python**, **C/C++**, **Fortran**, MATLAB, Bash, LaTeX, Gnuplot, Git
Engineering tools: **LAMMPS**, **OpenFOAM**, CONVERGE CFD, ANSYS, COMSOL, Tecplot
HPC, systems and cloud: **MPI**, OpenMP, SLURM, Docker, Linux (Headless/Server), Networking (Tailscale, Proxy), Self-Hosting
CFD solver development: Finite-volume CFD, Lagrangian-Eulerian multiphase modeling, Soot, Radiation, Flamelet combustion, Compressible/incompressible flow, MPI load balancing, ParaView/VTK
Methods: CFD, Reactive molecular dynamics, Radiative heat transfer, Chemical kinetics, Machine learning

Publications

Journal Articles

1. **Mukut**, **K. M.**, Goudeli, E., Kelesidis, G. A. & Roy, S. P. Elucidating pore and surface features of soot nanoparticles using molecular dynamics simulations. *Fuel* **406,** 136692. DOI: 10.1016/j.fuel.2025.136692 (Feb. 2026).
2. Ganguly, A., **Mukut**, **K. M.**, Roy, S., Kelesidis, G. & Goudeli, E. Investigation of soot precursor molecules during inception by acetylene pyrolysis using reactive molecular dynamics. *Aerosol Research* **3,** 185–203. DOI: 10.5194/ar-3-185-2025 (Apr. 2025).
3. Day, T. P., **Mukut**, **K. M.**, Klacik, L., O'Donnell, R., Wasilewski, J. & Roy, S. P. SAGE: A machine learning model for primary particle segmentation in TEM images of soot aggregates. *Proc. Combust. Inst.* **41,** 105821. DOI: 10.1016/j.proci.2025.105821 (Jan. 2025).
4. **Mukut**, **K. M.**, Ganguly, A., Goudeli, E., Kelesidis, G. A. & Roy, S. P. Physical, chemical and morphological evolution of incipient soot obtained from molecular dynamics simulation of acetylene pyrolysis. *Fuel* **373,** 132197. DOI: 10.1016/j.fuel.2024.132197 (Oct. 2024).
5. **Mukut**, **K. M.**, Ganguly, A., Goudeli, E., Kelesidis, G. A. & Roy, S. P. Internal Structure of Incipient Soot from Acetylene Pyrolysis Obtained via Molecular Dynamics Simulations. *J. Phys. Chem. A* **128,** 5175–5187. DOI: 10.1021/acs.jpca.4c01548 (July 2024).
6. **Mukut**, **K. M.**, Roy, S. & Goudeli, E. Molecular arrangement and fringe identification and analysis from molecular dynamics (MAFIA-MD): A tool for analyzing the molecular structures formed during reactive molecular dynamics simulation of hydrocarbons. *Comput. Phys. Commun.* **276,** 108325. DOI: 10.1016/j.cpc.2022.108325 (July 2022).
7. Sharma, A., **Mukut**, **K. M.**, Roy, S. P. & Goudeli, E. The coalescence of incipient soot clusters. *Carbon* **180,** 215–225. DOI: 10.1016/j.carbon.2021.04.065 (Aug. 2021).

8. **Mukut**, **K. M.** & Roy, S. P. Effect of O_2 concentration in ambient mixture and multiphase radiation on pollutant formation in ECN spray-A. *Combust. Theory. Model.* **Featured on the journal cover**. DOI: 10.1080/13647830.2020.1721561 (May 2020).

9. Hasan, M. N., Shavik, S. M., Rabbi, K. F., **Mukut**, **K. M.** & Alam, M. M. Thermal transport during thin-film argon evaporation over nanostructured platinum surface: A molecular dynamics study. *Proceedings of the Institution of Mechanical Engineers, Part N: Journal of Nanomaterials, Nanoengineering and Nanosystems* **232,** 83–91. DOI: 10.1177/2397791418802498 (June 2018).

10. Hasan, M. N., Shavik, S. M., **Mukut**, **K. M.**, Rabbi, K. F. & Faisal, A. H. M. Atomistic modelling of thin film argon evaporation over different solid surfaces at different wetting conditions. *Micro Nano Lett.* **13,** 351–356. DOI: 10.1049/mnl.2017.0198 (Mar. 2018).

11. Hasan, M. N., Shavik, S. M., Rabbi, K. F., **Mukut**, **K. M.** & Morshed, A. Phase Change Characteristics of Ultra-Thin Liquid Argon Film over different Flat Substrates at High Wall Superheat for Hydrophilic/Hydrophobic Wetting Condition: A Non-Equilibrium Molecular Dynamics Study. *J. Chem. Engg.* **29,** 49–55. DOI: 10.3329/jce.v29i1.33820 (Aug. 2017).

Conference Proceedings

1. **Mukut**, **K. M.**, Ganguly, A., Goudeli, E., Kelesidis, G. & Roy, S. P. *Characterization of Nascent Soot Particles from Acetylene Pyrolysis: A Molecular Modeling Perspective* in *13th US National Combustion Meeting* (Mar. 2023). https://par.nsf.gov/biblio/10410208.

2. **Mukut**, **K. M.**, Sharma, A., Goudeli, E. & Roy, S. *A Closer Look into the Formation of Soot Particles: A Molecular Dynamics Study* in *12th U.S. National Combustion Meeting* (Texas A&M University, College Station, TX, USA, May 2021). https://www.researchgate.net/publication/353548199_A_Closer_Look_into_the_Formation_of_Soot_Particles_A_Molecular_Dynamics_Study/stats.

3. **Mukut**, **K. M.** & Roy, S. *An Investigation of Soot Evolution in High-pressure Spray Combustion* in *11th US National Combustion Meeting* (Pasadena, CA, Mar. 2019), 1–9. https://epublications.marquette.edu/mechengin_fac/310/.

4. **Mukut**, **K. M.** & Roy, S. P. *A Sensitivity Study on Soot and NO_x Formation in High Pressure Combustion System* in *2018 Spring Technical Meeting of Central States Section of the Combustion Institute* (Minneapolis, MN, USA, Apr. 2018). https://www.researchgate.net/publication/333356994_A_Sensitivity_Study_on_Soot_and_NOx_Formation_in_High_Pressure_Combustion_System.

5. Hasan, M. N., Rabbi, K. F., **Mukut**, **K. M.**, Tamim, S. I. & Faisal, A. H. M. *Nano scale dynamics of bubble nucleation in confined liquid subjected to rapid cooling: Effect of solid-liquid interfacial wettability* in *7th BSME International Conference on Thermal Engineering* **1851** (AIP Publishing, June 2017). DOI: 10.1063/1.4984729.

6. Rabbi, K. F., Tamim, S. I., Faisal, A. H. M., **Mukut**, **K. M.** & Hasan, M. N. *A molecular dynamics study on thin film liquid boiling characteristics under rapid linear boundary heating: Effect of liquid film thickness* in *7th BSME International Conference on Thermal Engineering* **1851** (AIP Publishing, June 2017). DOI: 10.1063/1.4984731.

Thesis and Dissertation

1. **Mukut**, **K. M.** *Fundamental Exploration of Soot Formation and Morphology from a Molecular Modeling Perspective* PhD dissertation (Marquette University, Milwaukee, Wisconsin, Aug. 2025). https://www.proquest.com/dissertations-theses/fundamental-exploration-soot-formation-morphology/docview/3231789390/se-2.

2. **Mukut**, **K. M.** *Effect of Radiation and EGR on Pollutant Formation in High-Pressure Constant Volume Spray Combustion* MS thesis (Marquette University, 2019). https://epublications.marquette.edu/theses_open/543/.

Conference Presentations

Oral Presentations

1. Roy, S., Day, T. & **Mukut**, **K. M.** *Utilizing Machine Learning to Analyze Soot Morphology in Microscopic Images* in *APS March Meeting Abstracts* **2024** (Mar. 2024), A62.007. https://ui.adsabs.harvard.edu/abs/2024APS..MARA62007R/abstract.

2. **Mukut**, **K. M.**, Ganguly, A., Goudeli, E., Kelesidis, G. A. & Roy, S. P. *Physicochemical Analysis of Soot Particles Obtained from Molecular Dynamics Simulation of Acetylene Pyrolysis* in *AAAR 40th Annual Conference* Oral Presentation (Virtual, Oct. 2022).
3. **Mukut**, **K. M.**, Sharma, A., Ganguli, A., Goudeli, E. & Roy, S. P. *A Reactive Molecular Dynamics-based Exploration of Soot Inception Pathways in Combustion* in *AAAR 39th Annual Conference* Oral Presentation (Virtual, Sept. 2021).
4. **Mukut**, **K. M.**, Sharma, A., Goudeli, E. & Roy, S. P. *A Molecular Dynamics Study of Nucleation of Soot* in *European Aerosol Conference-EAC2021* Oral Presentation (Virtual, Aug. 2021).
5. **Mukut**, **K. M.** & Roy, S. P. *Effect of EGR and Radiation on Soot Morphology in ECN Spray-A Combustion Chamber* in *17th International Conference on Numerical Combustion* Oral Presentation (Aachen, Germany, July 2019).
6. Hasan, N., **Mukut**, **K. M.**, Rabbi, K., Alam, M., Mitsutake, Y. & Monde, M. *Atomistic and Macroscopic Perspective of Thin Film Boiling* in *10th International Conference on Boiling and Condensation Heat Transfer* (Nagasaki, Japan, Mar. 2018).
7. **Mukut**, **K. M.**, Roy, S., Fernandez, S., Haworth, D. & Modest, M. *Soot and Radiation Models in Prediction of Pollutant Formation from Practical Combustion Scenarios* in *10th International Aerosol Conference* (St. Louis, MO, Mar. 2018).
8. **Mukut**, **K. M.**, Hasan, N. & Ali, M. *Numerical Study of Turbulent Co-Axial Free Jets* in *ICMEAS 2017* (Dhaka, Bangladesh, Feb. 2017).

Poster Presentations

1. Day, T., **Mukut**, **K.** & Roy, S. *Utilizing Machine Learning to Analyze Soot Morphology in Microscopic Images* in *Bulletin of the American Physical Society* [Online; accessed 3. May. 2024] (Apr. 2024). https://meetings.aps.org/Meeting/MAR24/Session/A62.7.
2. **Mukut**, **K. M.** & Roy, S. P. *Effect of EGR and Radiation on Soot Morphology in ECN Spray-A Combustion Chamber* in *17th International Conference on Numerical Combustion* Oral Presentation (Aachen, Germany, July 2019).
3. **Mukut**, **K. M.**, Roy, S., Fernandez, S., Haworth, D. & Modest, M. *Soot and Radiation Models in Prediction of Pollutant Formation from Practical Combustion Scenarios* in *10th International Aerosol Conference* (St. Louis, MO, Mar. 2018).

References

Available upon request.