Khaled Mosharraf Mukut

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Professional Summary

Highly motivated Mechanical Engineering PhD candidate with extensive expertise in Computational Fluid Dynamics (CFD), Molecular Dynamics, Programming (Python, C++), Software Development, High-Performance Computing (HPC), and data-driven statistical analysis using Python. Demonstrates leadership and collaboration within interdisciplinary research teams. Successfully secured a $22,000 research fellowship and authored several impactful publications in reputable journals. Possesses substantial teaching experience, delivering courses and mentoring both undergraduate and graduate students. Seeking a tenure-track position to spearhead innovative research initiatives and contribute to academic excellence through interdisciplinary teamwork and technological advancement.

Education

Ph.D. in Mechanical Engineering (Energy Systems) *Expected May 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 (Energy Systems) *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

Teaching and Mentoring Experience

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

- 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 *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 presentations at national conferences and two publications.

Research Interests

- **Soot Formation and Morphology**
- **Molecular Dynamics (MD)**
- **Computational Fluid Dynamics (CFD)**
- **Data-Driven Engineering-Scale Modeling**
- **Radiative Heat Transfer**
- **Interdisciplinary Collaboration**

Research Experience

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

- Conduct reactive molecular dynamics (RMD) simulations of soot formation, delivering detailed *in situ* insights into particle morphology and evolution.
- Develop and validate novel post-processing methods for RMD simulations, aiding in advanced analysis of soot particle dynamics and morphology.
- Characterize 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.
- Collaborate with interdisciplinary teams and present research findings at international conferences, resulting in high-impact publications and exchange knowledge within the research community.
- Mentored undergraduate and graduate students in interdisciplinary research projects, leading to student-led publications and enhanced team collaboration.

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

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

Professional 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.

Technical Skills

Programming Languages & Tools:	C/C++, Python, Fortran, LaTeX, MATLAB, Gnuplot, Bash
CAD/Engineering Tools:	AutoCAD, SolidWorks, LAMMPS, Tecplot, OpenFOAM, Converge CFD, Ansys, COMSOL Multiphysics
Operating Systems:	Linux, macOS, Windows
High-Performance Computing:	MPI, OpenMP, SLURM, HPC Clusters

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

- A figure from my paper on Spray-A 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.

Leadership and Service

Student Member

- 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*

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

- Mentored 15 high school students 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

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

- 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 run bi-weekly meetings to oversee progress in essential parts of the organization.

Organizer/Volunteer/Mentor *Jan 2022 – May 2022*
Entangled Air | *An exhibition bringing together the art of TOMÁS SARACENO and my research at CCL*

- 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.

Publications

Thesis and Dissertation

[1] **Mukut K.M.** "Fundamental Exploration of Soot Formation and Morphology from a Molecular Modeling Perspective (in Preparation)". PhD dissertation. Milwaukee, Wisconsin: Marquette University, 2024.

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

Journal Articles

[1] **Mukut K.M.** Ganguly Anindya Goudeli Eirini Kelesidis Georgios A. Roy Somesh P. "Internal Structure of Incipient Soot from Acetylene Pyrolysis Obtained via Molecular Dynamics Simulations". In: *J. Phys. Chem. A* 128.26 (July 2024), pp. 5175–5187. ISSN: 1089-5639. DOI: 10.1021/acs.jpca.4c01548.

[2] **Mukut K.M.** Ganguly Anindya Goudeli Eirini Kelesidis Georgios A. Roy Somesh P. "Physical, chemical and morphological evolution of incipient soot obtained from molecular dynamics simulation of acetylene pyrolysis". In: *Fuel* 373 (Oct. 2024), p. 132197. ISSN: 0016-2361. DOI: 10.1016/j.fuel.2024.132197.

[3] **Mukut K.M.** Roy Somesh Goudeli Eirini. "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". In: *Comput. Phys. Commun.* 276 (July 2022), p. 108325. ISSN: 0010-4655. DOI: 10.1016/j.cpc.2022.108325.

[4] Sharma Akaash **Mukut K.M.** Roy Somesh P. Goudeli Eirini. "The coalescence of incipient soot clusters". In: *Carbon* 180 (Aug. 2021), pp. 215–225. ISSN: 0008-6223. DOI: 10.1016/j.carbon.2021.04.065.

[5] **Mukut K.M.** Roy Somesh P. "Effect of O_2 concentration in ambient mixture and multiphase radiation on pollutant formation in ECN spray-A". In: *Combust. Theory. Model.* (May 2020). **Figure featured on the journal cover**. DOI: 10.1080/13647830.2020.1721561. URL: https://www.tandfonline.com/doi/full/10.1080/13647830.2020.1721561.

[6] Hasan Mohammad Nasim Shavik Sheikh Mohammad **Mukut K.M.** Rabbi Kazi Fazle Faisal A. H. M. "Atomistic modelling of thin film argon evaporation over different solid surfaces at different wetting conditions". In: *Micro Nano Lett.* 13.3 (Mar. 2018), pp. 351–356. ISSN: 1750-0443. DOI: 10.1049/mnl.2017.0198.

[7] Hasan Mohammad Nasim Shavik Sheikh Mohammad Rabbi Kazi Fazle **Mukut K.M.** Alam Md. Muntasir. "Thermal transport during thin-film argon evaporation over nanostructured platinum surface: A molecular dynamics study". In: *Proceedings of the Institution of Mechanical Engineers, Part N: Journal of Nanomaterials, Nanoengineering and Nanosystems* 232.2-3 (June 2018), pp. 83–91. ISSN: 2397-7914. DOI: 10.1177/2397791418802498.

[8] Hasan Mohammad Nasim Shavik S. M. Rabbi K. F. **Mukut K. M.** Morshed Akmm. "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". In: *J. Chem. Engg.* 29.1 (Aug. 2017), pp. 49–55. ISSN: 2408-8617. DOI: 10.3329/jce.v29i1.33820.

[9] Rabbi Kazi Fazle Tamim Saiful Islam Faisal A. H. M. **Mukut K. M.** Hasan Mohammad Nasim. "A molecular dynamics study on thin film liquid boiling characteristics under rapid linear boundary heating: Effect of liquid film thickness". In: *AIP Conf. Proc.* 1851.1 (June 2017). ISSN: 0094-243X. DOI: 10.1063/1.4984731.

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. URL: https://par.nsf.gov/biblio/10410208.

[2] **Mukut K. M.** Sharma Akaash Goudeli Eirini Roy Somesh. "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. URL: 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 Somesh. "An Investigation of Soot Evolution in High-pressure Spray Combustion". In: *11th US National Combustion Meeting*. Pasadena, CA, Mar. 2019, pp. 1–9. URL: https://epublications.marquette.edu/mechengin_fac/310/.

[4] **Mukut K. M.** Roy Somesh 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. URL: https://www.researchgate.net/publication/333356994_A_Sensitivity_Study_on_Soot_and_NOx_Formation_in_High_Pressure_Combustion_System.

Articles in Preparation

[1] **Mukut K.M.** Ganguly Anindya Goudeli Eirini Kelesidis Georgios A. Roy Somesh P. "Surface and Pore Properties of Primary Soot Particles Based on Molecular Dynamics Simulations". In: *TBD* (2024).

Conference Presentations

Oral Presentations

[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. URL: https://par.nsf.gov/biblio/10410208.

[2] **Mukut K.M.** Ganguly Anindya Goudeli Eirini Kelesidis Georgios A. Roy Somesh 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 Akaash Goudeli Eirini Roy Somesh. "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. URL: https://www.researchgate.net/publication/353548199_A_Closer_Look_into_the_Formation_of_Soot_Particles_A_Molecular_Dynamics_Study/stats.

[4] **Mukut K.M.** Sharma A. Ganguli A. Goudeli Eirini Roy Somesh P. "A Reactive Molecular Dynamics-based Exploration of Soot Inception Pathways in Combustion". In: *AAAR 39th Annual Conference*. Oral Presentation. Virtual, Sept. 2021.

[5] **Mukut K.M.** Sharma A. Goudeli Eirini Roy Somesh P. "A Molecular Dynamics Study of Nucleation of Soot". In: *European Aerosol Conference-EAC2021*. Oral Presentation. Virtual, Aug. 2021.

[6] **Mukut K. M.** Roy Somesh. "An Investigation of Soot Evolution in High-pressure Spray Combustion". In: *11th US National Combustion Meeting*. Pasadena, CA, Mar. 2019, pp. 1–9. URL: https://epublications.marquette.edu/mechengin_fac/310/.

[7] **Mukut K.M.** Roy Somesh 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.

[8] Hasan Nasim **Mukut K. M.** Rabbi K.F. 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.

[9] **Mukut K. M.** Roy S.P. Fernandez S.F. Haworth D.C. 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.

[10] **Mukut K. M.** Roy Somesh 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. URL: https://www.researchgate.net/publication/333356994_A_Sensitivity_Study_on_Soot_and_NOx_Formation_in_High_Pressure_Combustion_System.

[11] **Mukut K. M.** Hasan Nasim Ali M.T. "Numerical Study of Turbulent Co-Axial Free Jets". In: *ICMEAS 2017*. Dhaka, Bangladesh, Feb. 2017.

Poster Presentations

[1] Day T. **Mukut K.M** Roy S.P. "Utilizing Machine Learning to Analyze Soot Morphology in Microscopic Images". In: *Bulletin of the American Physical Society*. [Online; accessed 3. May. 2024]. Apr. 2024. URL: https://meetings.aps.org/Meeting/MAR24/Session/A62.7.

[2] **Mukut K.M.** Roy Somesh 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.P. Fernandez S.F. Haworth D.C. 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.

Softwares and Numerical Tools

[1] **Mukut K.M.** Roy Somesh P. *StereoFractAnalyzer*. PyPI. Version 1.0.0. https://github.com/comp-comb/StereoFractAnalyzer. Mar. 2, 2024. URL: https://pypi.org/project/StereoFractAnalyzer/.

[2] **Mukut K.M.** Roy Somesh 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. URL: https://doi.org/10.17632/s7dsk553fh.1.

References

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Additional references available upon request.