

# Khaled Mosharraf Mukut

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## Professional Summary

Motivated Mechanical Engineering PhD candidate with competence in CFD, Molecular Dynamics, Python, C++, software development, HPC, and Python-based data-driven statistical analysis. Leads and collaborates in multidisciplinary research. Obtained a **\$22,000** research fellowship and published influential articles in recognized journals. Has extensive teaching and mentoring experience with undergraduate and graduate students. Seeking a tenure-track job to lead research, develop interdisciplinary collaboration, and mentor students in advancing technology and sustainability.

## Research Interests

- 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 (Energy Systems)**  
Marquette University, Milwaukee, WI, USA

*Expected May 2025*

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

**M.S. in Mechanical Engineering (Energy Systems)**  
Marquette University, Milwaukee, WI, USA

*Aug 2017 – May 2019*

- 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

## 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 &amp; 2012

Bangladesh University of Engineering and Technology (BUET)

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

## Research Experience

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**Graduate Research Assistant**

Aug 2017 – Present

Department of Mechanical Engineering, Marquette University, Milwaukee, WI

- 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.

## Publications

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**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). **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 Rabbi Kazi Fazle **Mukut K. M.** Tamim Saiful Islam Faisal A. H. M. “Nano scale dynamics of bubble nucleation in confined liquid subjected to rapid cooling: Effect of solid-liquid interfacial wettability”. In: *AIP Conf. Proc.* 1851.1 (June 2017). ISSN: 0094-243X. DOI: 10.1063/1.4984729.
- [9] 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.
- [10] 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](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/](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](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).

## 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/](https://epublications.marquette.edu/theses_open/543/).

## Conference Presentations

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### 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. “Physico-chemical 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](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/](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](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.

## Software 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>.

## Teaching and Mentoring Experience

### Graduate Research Assistant

Aug 2017 – Present

Department of Mechanical Engineering, Marquette University, Milwaukee, WI

- 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 the lab as a graduate student.
- Guided fresh graduate students on interdisciplinary projects, leading to publications and improved collaboration; one earned the [WSGC fellowship](#).

### Organizer & Mentor

Jul 2023

#### Python Workshop for High School Students, 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

Jan 2023 – May 2023

#### Entangled Air | An exhibition bringing together the art of TOMÁS SARACENO and my research

- 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.

**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-led presentations at national conferences and two publications.

**Technical Skills****Programming Languages & Tools:** C/C++, Python, Fortran, L<sup>A</sup>T<sub>E</sub>X, 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**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.

**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*

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

## References

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**Dr. Somesh Roy**

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**Additional references available upon request.**