Danyal Mohaddes

Senior research scientist · Computational physics · Complex reacting flows

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I develop models to simulate complex systems, implement efficient code and deploy on highly parallelized architectures to generate large datasets. I use LLMs to accelerate my workflow and deep learning to model my data.

Education

Stanford University — Stanford, USA
Ph.D. in Mechanical Engineering — 2017–2022

- Thesis: *Numerical Simulation of Hot Surface Ignition and Combustion of Fuel Sprays*
- Advisor: Prof. Matthias Ihme
- Coursework: Numerical mathematics, reacting flow physics, parallel and GPU programming, deep learning

Stanford University — Stanford, USA
M.Sc. in Mechanical Engineering — 2016–2018

- Concentration: Flow Physics and Computational Engineering

University of Toronto — Toronto, Canada
B.A.Sc. in Mechanical Engineering (High Honors, 3.9/4.0) — 2011–2016

- Concentrations: Energy, Solid mechanics

Experience

FM, Research Division — Boston, USA
Senior Research Scientist, Fire Modeling — 2022–

- Developed and implemented (C++) physics-based computational models of fire propagation for deployment on cloud-based (AWS) and on-premises high-performance computing (HPC) architectures [Open Source]
- Derived the first theoretical model of thermal runaway propagation (TRP) in lithium-ion battery (LIB) stacks [Paper]; collaborated with experimentalists on further development and validation [Paper] [Open Source]
- Developed a large language model (LLM) agent in LangChain/LangGraph to inspect simulation software using retrieval-augmented generation (RAG), and to set up, execute, and post-process fire dynamics simulations on HPC systems. Led and mentored an intern who contributed to the implementation. [NeurIPS workshop paper]
- Developed generative (GAN) and regressive (CNN) machine learning (ML) approaches (in PyTorch) and applied foundation models for image analysis (Meta AI's SAM2) for physical modeling of multiphase reacting fluid flows
- Served as the representative for the Research Division on FM's Responsible AI (RAI) Oversight Group, which gives guidance and feedback to teams implementing major AI projects across the company
- Implemented a development workflow across multiple research teams in Azure DevOps: version control, issue tracking, containerization (Docker), continuous integration, documentation

Arbury Labs, Inc. — Seattle, USA
Scientific Advisor (Remote) — 2023–2024

- Provided research services to a startup developing a coaching application for sports leveraging computer vision and LLMs
- Developed interfaces to LLMs for app integration and implemented one/few-shot learning approaches for data analysis, human-machine-human interaction and feedback, synthetic data generation and program logic

Stanford University — Stanford, USA
Graduate Research Assistant under Prof. Matthias Ihme — 2016–2022

- Extended a dynamic modeling framework and applied a global optimization algorithm for computationally efficient and physically accurate modeling of multiphase chemical effects in combustion simulations [Paper]
- Conducted high-fidelity modeling of flow physics using massively-parallel simulations [Paper], [Paper]
- Performed parallelized (C++/MPI/OpenMP) simulations of a Lagrangian-Eulerian system with over 6M degrees of freedom to model ignition of fuel leaks in aircraft in collaboration with Boeing [Paper]
- Developed a parallelized (C++/OpenMP) solver for highly stiff and coupled combustion PDEs [Open Source]
- Employed machine learning -based data analysis techniques in Python (TensorFlow) to analyze parametric sensitivities in numerical simulations of combustion problems [Paper]

Technische Universität München — Munich, Germany
Visiting Student Researcher under Prof. Oskar Haidn — Summer 2019

- Performed high-fidelity numerical modeling for gas turbine and rocket propulsion using C++-based software
- Supported by Stanford Graduate Internship and Research Program in Germany

Amec Foster Wheeler (now Wood plc.) — Toronto, Canada
Engineering Intern, Canadian Nuclear Division — Summer 2015

- Programmed databases in Visual Basic for Applications (VBA) for risk analysis of thermal power plants

Syncrude Canada Ltd. — Edmonton, Canada
Research Intern, Division of Research and Development — 2014-2015

- Performed economic analysis and developed business cases for upgrades to heavy industrial machinery

University of Toronto — Toronto, Canada
Undergraduate Research Assistant under Prof. David Sinton and Prof. Nasser Ashgriz — Summer 2013/2014

- Developed image-processing software for identifying and tracking droplet behavior in nuclear engineering experiments [Open Source, over 700 downloads]
- Developed and conducted microfluidic experiments for CO_2 sequestration [Paper]

University of Manitoba — Winnipeg, Canada
Undergraduate Research Assistant under Prof. Zahra Moussavi — Summer 2012

- Developed software and performed 3D graphics design for a custom C++-based virtual reality simulator for experiments in the early detection of Alzheimer's disease [Paper]

Awards, Grants and Honors

Most Collaborative Participant, Stanford FLAME AI Workshop — 2023

Boeing Research & Technology Strategic Universities Program, *grant awarded to PI's lab to support my PhD* — 2018–2022

Natural Sciences and Engineering Research Council of Canada (NSERC) Postgraduate Scholarship — 2019–2020

Graduate Internship and Research Program in Germany — 2019

Departmental Graduate Engineering Fellowship Award — 2016–2017

Editors' Choice article published in *Analytical Chemistry* — 2014

Eight undergraduate research and academic scholarships — 2011–2016
NSERC summer research award, U. Toronto Excellence Award for summer research, ASME student scholarship, SPE Canada student scholarship, SPE Calgary section student scholarship, Otto Holden scholarship, WJT Wright scholarship, Faculty admission scholarship

Publications

Journal papers

Mohaddes, D., Wang, Y., "Theory and analysis of module-scale thermal runaway propagation," *Combustion and Flame*, vol. 279, p. 114 327, 2025. DOI: https://doi.org/10.1016/j.combustflame.2025.114327

Zeng, D., **Mohaddes, D.**, Gagnon, L., Wang, Y., "Modeling initiation and propagation of thermal runaway in pouch li-ion battery cells: Effects of heating rate and state-of-charge," *Proceedings of the Combustion Institute*, vol. 40, no. 1, p. 105 316, 2024. DOI: https://doi.org/10.1016/j.proci.2024.105316

Mohaddes, D., Brouzet, D., Ihme, M., "Cost-constrained adaptive simulations of transient spray combustion in a gas turbine combustor," *Combustion and Flame*, vol. 249, p. 112 530, 2023. DOI: 10.1016/j.combustflame.2022.112530

Mohaddes, D., Ihme, M., "Wall heat transfer and flame structure transitions in stagnating spray flames," *Proceedings of the Combustion Institute*, vol. 39, no. 2, pp. 2683–2692, 2023. DOI: 10.1016/j.proci.2022.08.037

Mohaddes, D., Ihme, M., "On the hot surface ignition of a wall-stagnating spray flame," *Combustion and Flame*, vol. 240, p. 111 988, 2022. DOI: 10.1016/j.combustflame.2022.111988

Dodd, M. S., **Mohaddes, D.**, Ferrante, A., Ihme, M., "Analysis of droplet evaporation in isotropic turbulence through droplet-resolved DNS," *International Journal of Heat and Mass Transfer*, vol. 172, p. 121 157, 2021. DOI: 10.1016/j.ijheatmasstransfer.2021.121157

Mohaddes, D., Boettcher, P., Ihme, M., "Hot surface ignition of a wall-impinging fuel spray: Modeling and analysis using large-eddy simulation," *Combustion and Flame*, vol. 228, pp. 443–456, 2021. DOI: 10.1016/j.combustflame.2021.02.025

Mohaddes, D., Xie, W., Ihme, M., "Analysis of low-temperature chemistry in a turbulent swirling spray flame near lean blow-out," *Proceedings of the Combustion Institute*, vol. 38, no. 2, pp. 3435–3443, 2021. DOI: 10.1016/j.proci.2020.08.030

Sobhani, S., Muhunthan, P., Boigné, E., **Mohaddes, D.**, Ihme, M., "Experimental feasibility of tailored porous media burners enabled via additive manufacturing," *Proceedings of the Combustion Institute*, vol. 38, no. 4, pp. 6713–6722, 2021. DOI: 10.1016/j.proci.2020.06.120

Watson, L. M., Dunham, E. M., **Mohaddes, D.**, Labahn, J., Jaravel, T., Ihme, M., "Infrasound Radiation From Impulsive Volcanic Eruptions: Nonlinear Aeroacoustic 2D Simulations," *Journal of Geophysical Research: Solid Earth*, vol. 126, no. 9, pp. 1–28, 2021. DOI: 10.1029/2021JB021940

Mohaddes, D., Chang, C. T., Ihme, M., "Thermodynamic cycle analysis of superadiabatic matrix-stabilized combustion for gas turbine engines," *Energy*, vol. 207, p. 118 171, 2020. DOI: 10.1016/j.energy.2020.118171

Boigne, E., Muhunthan, P., **Mohaddes, D.**, Wang, Q., Sobhani, S., Hinshaw, W., Ihme, M., "X-ray computed tomography for flame-structure analysis of laminar premixed flames," *Combustion and Flame*, vol. 200, pp. 142–154, 2019. DOI: 10.1016/j.combustflame.2018.11.015

Sobhani, S., **Mohaddes, D.**, Boigne, E., Muhunthan, P., Ihme, M., "Modulation of heat transfer for extended flame stabilization in porous media burners via topology gradation," *Proceedings of the Combustion Institute*, vol. 37, no. 4, pp. 5697–5704, 2019. DOI: 10.1016/j.proci.2018.05.155

Nguyen, P., **Mohaddes, D.**, Riordon, J., Fadaei, H., Lele, P., Sinton, D., "Fast Fluorescence-Based Microfluidic Method for Measuring Minimum Miscibility Pressure of CO2 in Crude Oils," *Analytical Chemistry*, vol. 87, no. 6, pp. 3160–3164, 2015. DOI: 10.1021/ac5047856

Byagowi, A., **Mohaddes, D.**, Moussavi, Z., "Design and Application of a Novel Virtual Reality Navigational Technology (VRNChair)," *Journal of Experimental Neuroscience*, vol. 8, no. 1, JEN.S13448, 2014. DOI: 10.4137/JEN.S13448

PhD thesis

Mohaddes, D., *Numerical simulation of hot surface ignition and combustion of fuel sprays*, Stanford University, 2022.

Conference podium presentations

Mohaddes, D., Wang, Y., *Fire Dynamics and Inter-Module Thermal Runaway Propagation in Battery Energy Storage Systems*, International Conference on Numerical Combustion, 2025.

Mohaddes, D., Wang, Y., *Module-scale thermal runaway propagation: Theory and analysis*, 14th US National Combustion Meeting, 2025.

Mohaddes, D., Wang, Y., *Toward fire dynamics simulations of thermal runaway propagation in battery energy storage systems*, 20th OpenFOAM Workshop, 2025.

Mohaddes, D., Zeng, D., Gagnon, L., Krisman, A., Ren, N., *Lithium-ion battery modeling: From cell-level thermal runaway to multi-module fires*, FM Global Open Source CFD Fire Modeling Workshop, 2024.

Mohaddes, D., *Numerical simulation of hot surface ignition and combustion of fuel sprays*, Stanford University, 2022.

Mohaddes, D., Ihme, M., *Adaptive combustion modeling of a gas turbine engine near lean blow-out*, International Conference on Numerical Combustion, 2022.

Mohaddes, D., Ihme, M., *Analysis of the hot surface ignition limits of a wall-stagnating fuel spray*, Spring Meeting of the Western States Section of the Combustion Institute, 2022.

Mohaddes, D., Ihme, M., *Wall heat transfer and flame structure transitions in stagnating spray flames*, 39th International Symposium on Combustion, 2022.

Mohaddes, D., Ihme, M., *Parametric study of hot surface ignition of an impinging fuel spray using large-eddy simulation*, APS Division of Fluid Dynamics Annual Meeting, 2020.

Mohaddes, D., Xie, W., Ihme, M., *Analysis of low-temperature chemistry in a turbulent swirling spray flame near lean blow-out*, 38th International Symposium on Combustion, 2020.

Mohaddes, D., Ihme, M., *Resolution requirements for LES modeling of a methanol pool fire*, FM Global Open Source CFD Fire Modeling Workshop, 2019.

Mohaddes, D., Ihme, M., Damazo, J., Boettcher, P., Moravec, B., *Computational modeling of compartment fires for aircraft safety*, International Conference on Numerical Combustion, 2019.

Mohaddes, D., Xie, W., Ihme, M., *Flame structure analysis and flame stabilization in a turbulent swirling spray flame*, APS Division of Fluid Dynamics Annual Meeting, 2019.

Mohaddes, D., Ihme, M., *Computational modeling of accidental fire spread in under-ventilated compartments*, APS Division of Fluid Dynamics Annual Meeting, 2018.

Mohaddes, D., Sobhani, S., Boigne, E., Muhunthan, P., Ihme, M., *Experimental investigation of flame stability in porous media burners*, APS Division of Fluid Dynamics Annual Meeting, 2017.

Mohaddes, D., Asghriz, N., *Study of vapor bubbles in horizontal PHWR cores*, Canadian Society for Mechanical Engineering International Congress, 2014.

Other conference contributions

Xiao, T., **Mohaddes, D.**, Brown, W., Xiong, G., Wang, Y., *Modeling of small pouch li-ion battery cells: Thermal runaway initiation and propagation*, 14th US National Combustion Meeting, 2025.

Xu, L., **Mohaddes, D.**, Wang, Y., "LLM agent for fire dynamics simulations," in *Neurips 2024 Workshop Foundation Models for Science: Progress, Opportunities, and Challenges*, 2024.

Zeng, D., **Mohaddes, D.**, Gagnon, L., Wang, Y., *Modeling initiation and propagation of thermal runaway in pouch Li-ion battery cells: Effects of heating rate and state-of-charge*, 40th International Symposium on Combustion, 2024.

Mohaddes, D., Lu, X., Krisman, A., Ren, N., *Devops for fire modeling research*, FM Global Open Source CFD Fire Modeling Workshop, Poster, 2023.

Mohaddes, D., Ren, N., Wang, Y., *Firefoam simulation of the macfp-3 parallel-panel target*, 3rd Workshop of the Measurement and Computation of Fire Phenomena (MaCFP) Database, Poster, 2023.

Bonanni, M., **Mohaddes, D.**, Ly, N., Perakis, N., Hardi, J., Börner, M., Ihme, M., "Toward Numerical Investigation of Ignition and Combustion Transition in a Subscale LOX/Methane Rocket Combustor," in *AIAA Scitech Forum*, 2021. DOI: 10.2514/6.2021-1141

Sobhani, S., Muhunthan, P., Boigné, E., **Mohaddes, D.**, Ihme, M., *Experimental feasibility of tailored porous media burners enabled via additive manufacturing*, 38th International Symposium on Combustion, 2020.

Muhunthan, P., Sobhani, S., Boigne, E., **Mohaddes, D.**, Ihme, M., *Experimental investigation of combustion in porous media burners with tailored matrix-structure using additive manufacturing*, APS Division of Fluid Dynamics Annual Meeting, 2019.

Sobhani, S., Muhunthan, P., **Mohaddes, D.**, Boigne, E., Cheng, Z., Ihme, M., *Enabling tailored porous media burners via additive manufacturing*, Proceedings of the 11th US National Combustion Meeting, 2019.

Ihme, M., **Mohaddes, D.,** *Toward the modeling and analysis of oxygen-controlled turbofan engine fan case compartment fires*, FM Global Open Source CFD Fire Modeling Workshop, 2018.

Sobhani, S., **Mohaddes, D.**, Boigne, E., Muhunthan, P., Ihme, M., *Modulation of heat transfer for extended flame stabilization in porous media burners via topology gradation*, 37th International Symposium on Combustion, 2018.

Boigne, E., Muhunthan, P., **Mohaddes, D.**, Sobhani, S., Parkinson, D., Barnard, H., Ihme, M., *Pore-scale and topology analysis of flame stabilization inside inert porous media using x-ray microtomography*, APS Division of Fluid Dynamics Annual Meeting, 2017.

Muhunthan, P., Sobhani, S., Boigne, E., **Mohaddes, D.**, Hinshaw, W., Ihme, M., *Calibration of x-ray computed tomography (xct) using a flat flame burner*, APS Division of Fluid Dynamics Annual Meeting, 2017.

Sobhani, S., Muhunthan, P., Boigne, E., **Mohaddes, D.**, Ihme, M., *Investigation of pore-scale flow physics in porous media burners*, APS Division of Fluid Dynamics Annual Meeting, 2017.

Byagowi, A., **Mohaddes, D.**, McLeod, R. D., *Accidental emergence within an agent based model: Simulation of agent interactions in an emergency situation*, Proceedings of the 17th International Conference on Computer Games (CGAMES), 2012. DOI: 10.1109/CGames.2012.6314574

Public repositories

khod-kaar – (Python) An early (∼2023) implementation of an LLM-based SWE agent with shell control from scratch.

spray-HSI – (C++) Parallelized solver for unsteady multiphase reacting flows that are wall-impinging.

Professional service

Peer review

Proceedings of the Combustion Institute	8 reviews since 2022
Fire Safety Journal	7 reviews since 2023
Combustion and Flame	4 reviews since 2021
Combustion Science and Technology	2 reviews since 2023

International Journal of Thermal Sciences — 1 review since 2024

International Journal of Hydrogen Energy — 1 review since 2023

Fuel — 1 review since 2022

Journal of Engineering for Gas Turbines and Power — 2 reviews since 2022

AIMS Energy — 1 review since 2021

Session chair appointments

14th US National Combustion Meeting: Computational and ML/AI-Data Driven Combustion — 2025

Mentorship

Leidong Xu, AI/ML Ph.D. summer intern at FM Research — 2024

Matthew Bonanni, Ph.D. candidate at Stanford — 2019–2022

Wai Tong Chung, Ph.D. candidate at Stanford — 2018–2022

Priyanka Muhunthan, Ph.D. candidate at Stanford — 2016–2019

Advisorship

Stanford Graduate School of Business, Gukomeza Sprayer team, Technical advisor — 2018

Teaching and Invited Talks

From Combustion Fundamentals to Fire Modeling, Combustion Processes, Cornell University (Guest Lecture) — 2024

Computational Fluid Dynamics in C++, Computing for Geomatics Engineers, U. Calgary (Guest Lecture) — 2023

Fidelity-Adaptive Modeling for Spray Combustion, Saudi Aramco (Invited talk) — 2022

Modeling Hot Surface Ignition with C++, Computing for Geomatics Engineers, U. Calgary (Guest Lecture) — 2022

Modern Applications of Combustion Science, Combustion Processes, Cornell University (Guest Lecture) — 2021

Hot Surface Ignition of Wall-Impinging Fuel Sprays, FM Global Research (Job Talk) — 2021

Gas Turbine Design and Analysis, Stanford University (Teaching Assistant) — 2020

Skills

Technology

Programming: Object-oriented C/C++, Python, Matlab

HPC: MPI, OpenMP, CUDA

Frameworks: Numpy, SciPy, Pandas, scikit-learn, TensorFlow, PyTorch

Toolbox: Linux, vim, git, bash, zsh, slurm, mongodb, Docker

Design: SolidWorks, ANSYS

Experiments: LabVIEW, Arduino

Human Languages

English: Native language

French: Fluent (C1/C2 level)

German: Fluent (C1 level)

Persian: Fluent (native-level speaking ability, competent in reading and writing)

Interests and Activities

Linguistics, especially phonology and writing systems; poetry and its analysis, especially ancient; history, foreign policy analysis and grand strategy; freestyle wrestling; classical guitar.