

Clayton R. Mulvihill

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Education

- Ph.D. in Mechanical Engineering** 2019
Texas A&M University
College Station, TX
Advisor: Eric L. Petersen
Dissertation: "H₂O laser absorption and OH* chemiluminescence measurements of H₂-NO₂ oxidation in a shock tube"
- M.S. in Mechanical Engineering** 2015
Texas A&M University
College Station, TX
Advisor: Eric L. Petersen
Thesis: "Shock-tube time-history measurements of H₂O in the H₂/O₂ system using IR laser absorption spectroscopy"
- B.S. in Mechanical Engineering** 2013
Texas A&M University
College Station, TX
Minor in Mathematics
GPA: 3.85

Research Interests

Chemical kinetics
Laser diagnostics
Quantum chemistry
Gas dynamics
Transition state theory
Spin-forbidden reactions

Journal Publications

Summary: 32 total, 11 as first author, h-index=14

32. Cho, J., Mulvihill, C.R., Klippenstein, S.J., Sivaramakrishnan, R. "Bimolecular peroxy radical (RO₂) reactions and their relevance in radical initiated oxidation of hydrocarbons" *Journal of Physical Chemistry A* 127 (2023) 300-315.
31. Couch, D.E., Mulvihill, C.R., Sivaramakrishnan, R., Au, K., Taatjes, C.A., Sheps, L. "Quantification of key peroxy and hydroperoxide intermediates in the low-temperature oxidation of dimethyl ether" *Journal of Physical Chemistry A* 126 (2022) 9497-9509.

30. Maffei, L.P., Moore III, K.B., Georgievskii, Y., Mulvihill, C.R., Elliott, S.N., Sivaramakrishnan, R., Faravelli, T., Klippenstein, S.J., Cho, J. "Automated identification and calculation of prompt effects in kinetic mechanisms using statistical models" *Combustion and Flame* (2022, in press).
29. Cooper, S.P., Marshall, P., Mathieu, O., Pinzón, L.T., Mulvihill, C.R., Glarborg, P., Petersen, E.L. "Experimental and modeling study of water time histories during H₂S-N₂O combustion in a shock tube" *Proceedings of the Combustion Institute* 39 (2023) 487-497.
28. Yan, C., Zhao, H., Wang, Z., Song, G., Lin, Y., Mulvihill, C.R., Jasper, A.W., Klippenstein, S.J., Ju, Y. "Low-and intermediate-temperature oxidation of dimethyl ether up to 100 atm in a supercritical pressure jet-stirred reactor" *Combustion and Flame* 243 (2022) 112059.
27. Mulvihill, C.R., Danilack, A.D., Goldsmith, C.F., Demireva, M., Sheps, L., Georgievskii, Y., Elliott, S.N., Klippenstein, S.J. "Non-Boltzmann effects in chain branching and pathway branching for diethyl ether oxidation" *Energy & Fuels* 35 (2021) 17890-17908.
26. Danilack, A.D., Mulvihill, C.R., Klippenstein, S.J., Goldsmith, C.F. "Diastereomers and low-temperature oxidation" *The Journal of Physical Chemistry A* 125 (2021) 8064-8073.
25. Cooper, S.P., Mulvihill, C.R., Mathieu, O., Petersen, E.L. "Isopropanol dehydration reaction rate kinetics measurements using H₂O time histories" *International Journal of Chemical Kinetics* 53 (2021) 536-547.
24. Alturaifi, S., Mulvihill, C.R., Mathieu, O., Petersen, E.L. "Speciation measurements in shock tubes for validation of complex chemical kinetics mechanisms: Application to 2-methyl-2-butene oxidation" *Combustion and Flame* 225 (2021) 196-213.
23. Mulvihill, C.R., Alturaifi, S., Petersen, E.L. "A shock-tube study of the N₂O + M \rightleftharpoons N₂ + O + M (M=Ar) rate constant using N₂O laser absorption near 4.6 μ m" *Combustion and Flame* 224 (2021) 6-13.
22. Atherley, T., de Persis, S., Chaumeix, N., Fernandes, Y., Bry, A., Comandini, A., Mathieu, O., Alturaifi, S., Mulvihill, C.R., Petersen, E.L. "Laminar flame speed and shock-tube multi-species laser absorption measurements of dimethyl carbonate oxidation and pyrolysis near 1 atm" *Proceedings of the Combustion Institute* 38 (2021) 977-985.
21. Mathieu, O., Chaumeix, N., Yamamoto, Y., Abid, S., Paillard, C.-E., Tezuka, T., Nakamura, H., Mulvihill, C.R., Petersen, E.L. "Nitromethane pyrolysis in shock tubes and a micro flow reactor with a controlled temperature profile" *Proceedings of the Combustion Institute* 38 (2021) 1007-1015.
20. Cooper, S.P., Mulvihill, C.R., Mathieu, O., Petersen, E.L. "Isopropanol dehydration reaction rate kinetics measurement using H₂O time histories" *International Journal of Chemical Kinetics* 53 (2021) 536-547.
19. Mulvihill, C.R., Juárez, R., Mathieu, O., Petersen, E.L. "A shock-tube study of the rate constant of PH₃ + M \rightleftharpoons PH₂ + H + M (M = Ar) using PH₃ laser absorption" *Journal of Physical Chemistry A* 124 (2020) 7380-7387.
18. Mathieu, O., Cooper, S.P., Alturaifi, S., Mulvihill, C.R., Atherley, T.M., Petersen, E.L. "Shock-tube laser absorption measurements of CO and H₂O during iso-octane combustion" *Energy and Fuels* 34 (2020) 7533-7544.
17. Mulvihill, C.R., Petersen, E.L. "OH* chemiluminescence in the H₂-NO₂ and H₂-N₂O systems" *Combustion and Flame* 213 (2020) 291-301.

16. Mathieu, O., Pinzón, L.T., Atherley, T.M., Mulvihill, C.R., Schoegl, I., Petersen, E.L. "Experimental study of ethanol oxidation behind reflected shock waves: Ignition delay time and H₂O laser-absorption measurements" *Combustion and Flame* 208 (2019) 313-326.
15. Cooper, S.P., Mulvihill, C.R., Mathieu, O., Petersen, E.L., Crofton, M.W., Lam, K.Y. "CH kinetics measurements and their importance for modeling prompt NO_x formation in gas turbines" *Journal of Engineering for Gas Turbines and Power* 142 (2020) 041007.
14. Mulvihill, C.R., Mathieu, O., Petersen, E.L. "H₂O time histories in the H₂-NO₂ system for validation of NO_x hydrocarbon kinetics mechanisms" *International Journal of Chemical Kinetics* 51 (2019) 669-678.
13. Mulvihill, C.R., Crofton, M.W., Arnold, D.G., Petersen, E.L., Lam, K.Y. "A laser diagnostic at 427 nm for quantitative measurements of CH in a shock tube" *Applied Physics B* 125 (2019) 78.
12. Pinzón, L.T., Mathieu, O., Mulvihill, C.R., Schoegl, I., Petersen, E.L. "Ignition delay time and H₂O measurements during methanol oxidation behind reflected shock waves" *Combustion and Flame* 203 (2019) 143-156.
11. Pinzón, L.T., Mathieu, O., Mulvihill, C.R., Schoegl, I., Petersen, E.L. "Ethanol pyrolysis kinetics using H₂O time history measurements behind reflected shock waves" *Proceedings of the Combustion Institute* 37 (2019) 239-247.
10. Mulvihill, C.R., Keesee, C.L., Sikes, T., Teixeira, R.S., Mathieu, O., Petersen, E.L. "Ignition delay times, laminar flame speeds, and species time histories in the H₂S/CH₄ system at atmospheric pressure" *Proceedings of the Combustion Institute* 37 (2019) 735-742.
9. Mulvihill, C.R., Petersen, E.L. "Concerning shock-tube ignition delay times: An experimental investigation of impurities in the H₂/O₂ system and beyond" *Proceedings of the Combustion Institute* 37 (2019) 259-266.
8. Mathieu, O., Mulvihill, C.R., Petersen, E.L., Curran, H.J. "NO_x-hydrocarbon kinetics model validation using measurements of CO and H₂O in shock-heated CH₄/C₂H₆ mixtures with O₂ or NO₂ as oxidant" *Journal of Engineering for Gas Turbines and Power* 141 (2019) 041007.
7. Mathieu, O., Mulvihill, C.R., and Petersen, E.L. "Assessment of modern detailed kinetics mechanisms to predict CO formation from methane combustion using shock-tube laser-absorption measurements" *Fuel* 236 (2018) 1164-1180.
6. Mulvihill, C.R., Mathieu, O., Petersen, E.L. "The unimportance of the reaction $\text{H}_2 + \text{N}_2\text{O} \rightleftharpoons \text{H}_2\text{O} + \text{N}_2$: A shock-tube study using H₂O time histories and ignition delay times" *Combustion and Flame* 196 (2018) 478-486.
5. Mulvihill, C.R., Alturaifi, S.A., Petersen, E.L. "High-temperature He- and O₂-broadening of the R(12) line in the 1←0 band of carbon monoxide" *Journal of Quantitative Spectroscopy and Radiative Transfer* 217 (2018) 432-439.
4. Mulvihill, C.R., Petersen, E.L. "High-temperature argon broadening of CO₂ near 2190 cm⁻¹ in a shock tube" *Applied Physics B* 123 (2017) 255.
3. Mathieu, O., Mulvihill, C.R., Zhang, Y., Curran, H.J., and Petersen, E.L. "CO and H₂O time-histories in shock-heated blends of methane and ethane for assessment of a chemical kinetics model" *Journal of Engineering for Gas Turbines and Power* 139 (2017) 121507.

2. Mathieu, O., Mulvihill, C.R., and Petersen, E.L. “Shock-tube water time-histories and ignition delay time measurements for H₂S near atmospheric pressure” *Proceedings of the Combustion Institute* 36 (2017) 4019-4027.
1. Mathieu, O., Hargis, J., Camou, A., Mulvihill, C.R., and Petersen, E.L. “Ignition delay time measurements behind reflected shock-waves for a representative coal-derived syngas with and without NH₃ and H₂S impurities” *Proceedings of the Combustion Institute* 35 (2015) 3143-3150.

Awards

Distinguished Graduate Student	2020
1 of only 8 awardees out of all university-wide Ph.D. students for excellence in research	
Peters Award (37th International Symposium on Combustion)	2018
Best student paper out of ~50 eligible student authors	
Best Student Paper Winner (31st International Symposium on Shock Waves)	2017
1 of only ~10 awardees	
NSF Graduate Research Fellowship	2014
University and Foundation Honors	2013
Only member of graduating class of ~120 to receive both honors	
National Merit Scholar	2008

Teaching

Heat Transfer Operations (CHEN 323)	2020
Department of Chemical Engineering, Texas A&M University 90 students, 2 TAs	
Thermodynamics I (CHEN 205)	2019
Department of Chemical Engineering, Texas A&M University 29 students, 1 TA	
Principles of Thermodynamics (MEEN 315)	2018
Department of Mechanical Engineering, Texas A&M University 81 students, 1 TA, 1 undergraduate grader	

Positions

Assistant Professor	2023–Present
Department of Mechanical Engineering Baylor University Waco, TX	

Postdoctoral Researcher	2020–2023
Chemical Sciences and Engineering Argonne National Laboratory Lemont, IL Advisor: Stephen J. Klippenstein	
Lecturer	2019–2020
Department of Chemical Engineering Texas A&M University College Station, TX	
Graduate Research Assistant	2013–2019
Department of Mechanical Engineering Texas A&M University College Station, TX Advisor: Eric L. Petersen	
Summer Research Intern	2014
Combustion Lab GE Global Research Schenectady, NY	
Undergraduate Research Assistant	2010–2013
Department of Mechanical Engineering Texas A&M University College Station, TX	
Service	
Peer Reviewer	2018–Present
Combustion and Flame; Computational and Theoretical Chemistry; Industrial and Engineering Chemistry Research; Proceedings of the Combustion Institute; Fuel	
Visiting Computer Scientist (St. Alphonsus School, Lemont, IL)	2022
Taught local 5 th and 6 th graders about the benefits and basics of computer programming	
Session Chair	2022
Central States Meeting of the Combustion Institute	
Session Chair	2021
US Meeting of the Combustion Institute	
Mentor for NSF Research Experience for Undergraduates (REU)	2017–2018
Mentored 3 visiting undergraduate researchers in the laboratory	
Session Chair	2018
Central States Meeting of the Combustion Institute	
Career Day Presenter (Navarro Elementary, Bryan, TX)	2016, 2017
Presented to local 5 th graders about my work as a scientist	
Mentor to Researchers	2016–2020
Mentored 4 Ph.D., 2 M.S., and 2 undergraduate students in the laboratory	

Panelist and Mentor to NSF GRFP Applicants 2015–2018

Served as panelist and/or mentor for prospective applicants to the NSF GRFP

Coordinator and Volunteer, Pioneers 2009–2018

Served as overall coordinator, transportation coordinator, and general volunteer in a children's outreach every Friday night for 18 consecutive semesters with ~120 children and ~40 volunteers

Conference Presentations

Presented by first author unless otherwise noted. Oral presentations unless otherwise noted.

35. Mulvihill, C.R., Georgievskii, Y., Klippenstein, S.J. "Improvements to non-adiabatic statistical theories: Application to N₂O decomposition" *13th U.S. National Combustion Meeting*, March 19-22, 2023, College Station, Texas.
34. Klippenstein, S.J., Mulvihill, C.R., Glarborg, P. "Theoretical kinetics predictions for reactions on the NH₂O potential energy surface" *13th U.S. National Combustion Meeting*, March 19-22, 2023, College Station, Texas.
33. Cooper, S.P., Marshall, P., Mathieu, O., Pinzón, L.T., Mulvihill, C.R., Glarborg, P., Petersen, E.L. "Experimental and modeling study of water time histories during H₂S-N₂O combustion in a shock tube" *39th International Symposium on Combustion*, July 24-29, 2022, Vancouver, Canada.
32. Mulvihill, C.R., Moore III, K.B., Jasper, A.W., Klippenstein, S.J. "N₂O decomposition: New perspectives on a historically challenging system" *Technical Meeting of the Central States Section of the Combustion Institute*, May 15-17, 2022, Detroit, Michigan.
31. Moore III, K.B., Elliott, S.N., Copan, A.V., Mulvihill, C.R., Maffei, L.P., Klippenstein, S.J. "Automated construction of fully representative stereochemical reaction mechanisms" *Technical Meeting of the Central States Section of the Combustion Institute*, May 15-17, 2022, Detroit, Michigan. (Presented by S.N. Elliott.)
30. Mulvihill, C.R., Klippenstein, S.J., Danilack, A.D., Goldsmith, C.F., Demireva, M., Sheps, L. "A modeling, experiment, and theory approach to low-temperature diethyl ether oxidation" *12th U.S. National Combustion Meeting*, May 24-26, 2021, College Station, Texas (virtual).
29. Danilack, A.D., Mulvihill, C.R., Klippenstein, S.J., Goldsmith, C.F. "Enhancing reactivity of low-temperature oxidation mechanisms via inclusion of diastereomers" *12th U.S. National Combustion Meeting*, May 24-26, 2021, College Station, Texas (virtual).
28. Parajuli, P., Mulvihill, C.R., Wang, Y., Petersen, E.L., Kulatilaka, W.D. "Laser-induced fluorescence and infrared absorption diagnostics of potential PO₂ precursors" *12th U.S. National Combustion Meeting*, May 24-26, 2021, College Station, Texas (virtual). (Presented by C.R. Mulvihill.)
27. Mathieu, O., Nakamura, H., Keesee, C.L., Yamamoto, Y., Tezuka, T., Mulvihill, C.R., Petersen, E.L. "A comprehensive experimental investigation of nitromethane oxidation kinetics using a wide array of techniques" *12th U.S. National Combustion Meeting*, May 24-26, 2021, College Station, Texas (virtual).

26. Mathieu, O., Pinzón, L.T., Mulvihill, C.R., Marshall, P., Glarborg, P., Petersen, E.L. "Water time histories during combustion of H₂S-N₂O mixtures in a shock tube" *12th U.S. National Combustion Meeting*, May 24-26, 2021, College Station, Texas (virtual).
25. Atherley, T., de Persis, S., Chaumeix, N., Fernandes, Y., Bry, A., Comandini, A., Mathieu, O., Alturaifi, S., Mulvihill, C.R., Petersen, E.L. "Laminar flame speed and shock-tube multi-species laser absorption measurements of dimethyl carbonate oxidation and pyrolysis near 1 atm" *38th International Symposium on Combustion*, January 24-29, 2021, Adelaide, Australia.
24. Mathieu, O., Chaumeix, N., Yamamoto, Y., Abid, S., Paillard, C.-E., Tezuka, T., Nakamura, H., Mulvihill, C.R., Petersen, E.L. "Nitromethane pyrolysis in shock tubes and a micro flow reactor with a controlled temperature profile" *38th International Symposium on Combustion*, January 24-29, 2021, Adelaide, Australia.
23. Mulvihill, C.R., Alturaifi, S., Mathieu, O., Petersen, E.L. "A N₂O laser absorption diagnostic near 4.6 μm for shock-tube chemical kinetics studies" *AIAA SciTech 2020*, January 6-10, 2020, Orlando, Florida.
22. Mulvihill, C.R., Mathieu, O., Petersen, E.L. "Development of a high-temperature diagnostic for the PO₂ radical using laser absorption near 7.4 microns" *Gordon Research Conference on Laser Diagnostics in Energy and Combustion Science*, June 23-28, 2019, Les Diablerets, Switzerland. (Poster presentation.)
21. Mathieu, O., Mulvihill, C.R., Petersen, E.L. "CO formation from dimethyl-carbonate pyrolysis behind reflected shock waves" *11th International Conference on Chemical Kinetics*, June 23-27, 2019, Orléans, France.
20. Mathieu, O., Cooper, S., Alturaifi, S., Mulvihill, C.R., Petersen, E.L. "Shock-tube measurements of CO concentration time-histories during iso-octane oxidation" *11th International Conference on Chemical Kinetics*, June 23-27, 2019, Orléans, France.
19. Mulvihill, C.R., Mathieu, O., Petersen, E.L. "NO_x-hydrocarbon kinetics model validation against new H₂O shock-tube measurements in the H₂-NO₂ system" *11th Mediterranean Combustion Symposium*, June 16-20, 2019, Costa Adeje, Spain.
18. Mulvihill, C.R., Crofton, M.W., Arnold, D.G., Petersen, E.L., Lam, K.Y. "Quantitative measurements of CH in a shock tube using laser absorption at 427 nm" *11th U.S. National Combustion Meeting*, March 24-27, 2019, Pasadena, California.
17. Atherley, T.M., Pinzón, L.T., Mathieu, O., Mulvihill, C.R., Schoegl, I., Petersen, E.L. "Kinetics study of ethanol oxidation behind reflected shock waves: Ignition delay times, H₂O measurements, and detailed kinetics model comparisons" *11th U.S. National Combustion Meeting*, March 24-27, 2019, Pasadena, California. (Presented by O. Mathieu.)
16. Pinzón, L.T., Mathieu, O., Mulvihill, C.R., Schoegl, I., Petersen, E.L. "Ethanol pyrolysis kinetics using H₂O time history measurements behind reflected shock waves" *37th International Symposium on Combustion*, July 29-August 3, 2018, Dublin, Ireland.
15. Mulvihill, C.R., Keese, C.L., Sikes, T., Teixeira, R.S., Mathieu, O., Petersen, E.L. "Ignition delay times, laminar flame speeds, and species time histories in the H₂S/CH₄ system at

- atmospheric pressure” *37th International Symposium on Combustion*, July 29-August 3, 2018, Dublin, Ireland.
14. Mulvihill, C.R., Petersen, E.L. “Concerning shock-tube ignition delay times: An experimental investigation of impurities in the H₂/O₂ system and beyond” *37th International Symposium on Combustion*, July 29-August 3, 2018, Dublin, Ireland.
 13. Mulvihill, C.R., Mathieu, O., Petersen, E.L. “A shock-tube study of the H₂-N₂O system using H₂O absorption and ignition delay times” *Technical Meeting of the Central States Section of the Combustion Institute*, May 20-22, 2018, Minneapolis, Minnesota.
 12. Mulvihill, C.R., Keese, C.L., Sikes, T., Teixeira, R.S., Mathieu, O., Petersen, E.L. “Ignition delay times, laminar flame speeds, and species time histories in the H₂S/CH₄ system at atmospheric pressure” *Technical Meeting of the Central States Section of the Combustion Institute*, May 20-22, 2018, Minneapolis, Minnesota.
 11. Pinzón, L.T., Mathieu, O., Mulvihill, C.R., Schoegl, I., Petersen, E.L. “Ignition delay times and H₂O measurements during methanol oxidation behind reflected shock waves” *Technical Meeting of the Central States Section of the Combustion Institute*, May 20-22, 2018, Minneapolis, Minnesota.
 10. Mathieu, O., Mulvihill, C.R., Petersen, E.L. “Experimental study of nitromethane oxidation: CO and H₂O time-histories behind reflected shock waves” *26th International Colloquium on the Dynamics of Explosions and Reactive Systems*, July 30 - August 4, 2017, Boston, Massachusetts.
 9. Mulvihill, C.R., Mathieu, O., Petersen, E.L. “CO and H₂O time-histories in a shock-heated H₂S/CH₄ blend near atmospheric pressure” *31st International Symposium on Shock Waves*, July 9-14, 2017, Nagoya, Japan.
 8. Mathieu, O., Mulvihill, C.R., Petersen, E.L. “Shock-tube measurements by laser absorption of CO and H₂O time-histories during nitromethane pyrolysis” *10th U.S. National Combustion Meeting*, April 23-26, 2017, College Park, Maryland. (Presented by C.R. Mulvihill.)
 7. Mulvihill, C.R., Mathieu, O., Petersen, E.L. “Shock-tube time-history measurements of CO and H₂O using IR laser absorption” *AIAA SciTech*, January 9-13, 2017, Grapevine, Texas.
 6. Mathieu, O., Mulvihill, C., and Petersen, E.L. “Shock-tube water time-histories and ignition delay time measurements for H₂S near atmospheric pressure” *36th International Symposium on Combustion*, July 31-August 5, 2016, Seoul, Korea. (Presented by E.L. Petersen.)
 5. Mulvihill, C.R., Petersen, E.L. “A shock-tube study of the effects of impurities on ignition within the H₂/O₂ system using tunable diode laser absorption at 1.38 microns” *Technical Meeting of the Central States Section of the Combustion Institute*, May 15-17, 2016, Knoxville, Tennessee.
 4. Mulvihill, C.R., Petersen, E.L. “Shock-tube time-history measurements of H₂O in the H₂/O₂ system using IR laser absorption spectroscopy” *9th U.S. National Combustion Meeting*, May 17-20, 2015, Cincinnati, Ohio.
 3. Mathieu, O., Hargis, J., Camou, A., Mulvihill, C., and Petersen, E.L. “Ignition delay time measurements behind reflected shock-waves for a representative coal-derived syngas with and

- without NH₃ and H₂S impurities” *35th International Symposium on Combustion*, August 3-8, 2014, San Francisco, California.
2. Mulvihill, C.R., Aul, C.J., Thion, S., Petersen, E.L. “Using UV absorption spectroscopy to measure the time history of the hydroxyl radical in a shock tube” *Technical Meeting of the Central States Section of the Combustion Institute*, March 16-18, 2014, Tulsa, Oklahoma.
 1. Mathieu, O., Hargis, J., Camou, A., Mulvihill, C., and Petersen, E.L. “Ignition delay time measurements behind reflected shock-waves for a representative coal-derived syngas with and without NH₃ and H₂S impurities” *Technical Meeting of the Central States Section of the Combustion Institute*, March 16-18, 2014, Tulsa, Oklahoma.