Nicole Labbe
Curriculum Vitae

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Research:

As our need for energy and need for alternative energy sources continue to grow, so does the need for understanding the behavior in flame and combustion systems. My research specializes in the kinetics and thermodynamics of combustion and flame applications, spanning from soot formation kinetic mechanisms, exploring the chemistry of new biofuels, and the chemistry of hypergolic rocket fuels. My work entails using ab initio molecular simulation to derive thermodynamics and kinetics for organic species found in flames and deriving combustion mechanisms for fuels for wide ranges of pressure and temperature conditions. Tools used include Gaussian, CHEMKIN, PolyRate, Multiwell, ChemRate, and Fortran. Currently I am looking for post-doctoral positions in molecular simulation and kinetics, especially in the area of chemical kinetics.

Education:

University of Massachusetts Amherst, Amherst, Massachusetts
Ph.D. Degree in Progress, Chemical Engineering
Advisors: Dr. Philip Westmoreland (NCSU) and Dr. David Ford
Grade Point Average: 3.56/4.0

Worcester Polytechnic Institute, Worcester, Massachusetts
B.S. in Chemical Engineering; awarded May 2006
Grade Point Average: 3.76/4.0 (graduated with high distinction)

Teaching Experience:

Fall 2008 TA for Eng 101: Introduction to Chemical Engineering
Fall 2009 TA for Eng 101: Introduction to Chemical Engineering

Honors and Awards:

- National Defense Science and Engineering Graduate Fellowship Recipient, 2009
- Combustion Energy Frontier Research Center (CEFRC) Summer Program on Combustion participant. Princeton University, 2010
- Presidents IQP Award for project entitled “Erosion and Flood Control in Otjomuise” (Authors: N. Labbe, N. McBride, E. Ray), Worcester Polytechnic Institute, 2007
- Sigma Xi MQP Award for project entitled “Ab Intio Studies of Cyclohexane Adsorption in Zeolites,” Worcester Polytechnic Institute, 2006
- Charles O. Thompson Scholar Award for the most outstanding first year student, Worcester Polytechnic Institute, 2004
- David Todd Scholarship, 2004
- Walter S. Barr Scholarship, 2004
- St. Ann Society Scholarship, received twice, 2003 and 2004
- WPI Presidential Scholarship, 2003
- Worcester Polytechnic Institute Award in Leadership and Innovation in Math and Science, 2003

Memberships and Affiliations:

- AIChE
- Sigma Xi
- Omega Chi Epsilon

Publications, Posters, and Presentations:

1. N. Labbe and P.R. Westmoreland. “Reaction Kinetics for TMEDA as an Alternative Hypergolic Rocket Fuel.” Reaction Engineering for Combustion and Pyrolysis II, 2011 AIChE National Meeting, Minneapolis, MN, Oct. 2011.
2. N. Labbe and P.R. Westmoreland. “Reaction Kinetics for TMEDA combustion with Red Fuming Nitric Acid.” Eastern States Section of the Combustion Institute Fall Technical Meeting, Storrs, CT, Oct. 2011.
3. A. Lucassen, N. Labbe, P.R. Westmoreland, K. Kohse-Höinghaus. “Structure of a Laminar Premixed Flame of Morpholine as an Oxygen- and Nitrogen- Containing Model Biofuel – Experiment and Simulation.” Combustion and Flame, 158 (2011) 1647-1666.

4. P.R. Westmoreland, N.J. Labbe, W. Li, M.E. Law, T. Kasper, N. Hansen, A. Lucassen, K. Kohse-Höinghaus. “Extrapolating Flame Kinetics from Cyclohexane to Heteroatomic Rings." 7th International Conference on Chemical Kinetics, Cambridge, MA, July 2011.
5. N. Labbe, A. Lucassen, P. Westmoreland, K. Kohse-Höinghaus. “Mechanistic Insights into Nitrogen Fate in a Morpholine Flat Flame.” 7th US National Combustion Meeting, Atlanta, GA, March 2011.
6. A. Lucassen, P. Oßwald, N. Labbe, K. Kohse-Höinghaus, P. Westmoreland. “Combustion Behavior of Nitrogen Containing Model Biofuels.” DGMS 2011, Dortmund, Germany. March 2011.
7. N. Labbe and P. Westmoreland. “Kinetics of Nitrogen Containing Fuels.” 29th Annual Meeting on Kinetics and Dynamics, Amherst, MA. Jan. 2011.
8. P. Westmoreland and N. Labbe “Task 3.2 Reaction Kinetics Studies” MURI Hypergolic Rocket Fuel Review Meeting, Aberdeen, MD. Nov. 2010
9. N. Labbe, Y. Kim, and P. Westmoreland. “ Mechanism Development for Hypergolic Propellant Systems: MMH and DMAZ.” Reaction Path Analysis I, 2010 AIChE National Meeting, Salt Lake City, UT, Nov. 2010
10. N. Labbe, Y. Kim, and P. Westmoreland. “Computational Mechanism Development for Hypergolic Propellant Systems: MMH and DMAZ.” CoMSEF Poster Session, 2010 AIChE National Meeting, Salt Lake City, UT, Nov. 2010
11. N. Labbe and P. Westmoreland. “Combustion of Nitrogen Containing Fuels: Morpholine and Hypergolic MMH.” 28th Regional Meeting on Kinetics and Dynamics, Trinity College, Jan. 2010
12. N. Labbe, P. Westmoreland, A. Lucassen. P. Oßwald, U. Struckmeier, K. Kohse-Hoeinghaus, T. Kasper, N. Hansen, and T. Cool. “Mechanism Development for Combustion of Morpholine, a Model Compound for Oxygen- and Nitrogen-Containing Fuels.” Chemistry and Kinetics Integrated CFD Modeling, 2009 AIChE National Meeting, Nashville, TN, Nov. 2009
13. N. Labbe, P. Westmoreland, A. Lucassen. P. Oßwald, U. Struckmeier, K. Kohse-Hoeinghaus, T. Kasper, N. Hansen, and T. Cool. “Mechanism Development for Combustion of Morpholine” CoMSEF Poster Session, 2009 AIChE National Meeting, Nashville, TN, Nov. 2009
14. W. Li, N. Labbe, P. Westmoreland, B. Yang, J. Wang, T. Cool. T. Kasper, N. Hansen, K. Kohse-Hoeinghaus. “Inferring Fuel-Rich Toluene Flame Chemistry from Photo-Ionization MBMS Analysis and Modeling” 2009 AIChE National Meeting, Nashville, TN, Nov. 2009
15. N. Labbe and P. Westmoreland. “Reaction Pathways in Hypergolic MMH/RFNA Combustion” Eastern States Section of the Combustion Institute Fall Technical Meeting, College Park, MD, Oct. 2009
16. A. Lucassen, P. Oßwald, U. Struckmeier, N. Labbe, T. Kasper, K. Kohse-Hoeinghaus, N. Hansen, W. Li, P. Westmoreland, B, Yang, J. Wang, and T. Cool. “Molecular-beam Mass Spectrometry for Flame Structure Analysis of Nitrogen-Containing Model Substances with Various Structural Motifs,” 18th International Mass Spectrometry Conference, Bremen, Germany, Sept. 2009
17. B. Anderson, B. Luct, T. Pourpoint, S. Son, P. Westmoreland, and N. Labbe “Task 3.2 Reaction Kinetics Studies (Modeling and Experimental)” MURI Hypergolic Rocket Fuel Review Meeting, Purdue University, Aug. 2009
18. P. Westmoreland and N. Labbe. “Applying Computational Quantum Chemistry to Devise a Reaction Mechanism for Use of Morpholine, a Surrogate Biofuel,” FOMMS 2009, Blaine, WA, July 2009
19. W. Li, M. Law, N. Labbe, P. Westmoreland, T. Kasper, N. Hansen, J. Wang, T. Cool, and K. Kohse-Hoeinghaus. “Determining Oxidation and Growth Kinetics through Photoionization MBMS Analysis and Modeling of Cyclohexane Flames” 6th US National Combustion Meeting, Ann Harbor, MI, May 2009
20. N. Labbe and P. Westmoreland. “Morpholine Flame Modeling and Mechanism Development”, 27th Regional Meeting on Kinetics and Dynamics, UMass Amherst, Jan. 2009
21. P. Westmoreland, N. Labbe, W. Li, and A. Pereverzev. “Measuring and Predicting Reaction Kinetics for Clean Use of Biofuels”, *1st Annual TIMBR conference, UMass Amherst, Sept. 2008*
22. *N. Labbe, W. Li, P. Westmoreland, A. Lucassen, P. Obwald, U. Struckmeier, K. Kohse-Hoinghaus, T. Kasper, N. Hansen, T. Cool. “Development of a Combustion Mechanism for Morpholine”, 32nd International Symposium on Combustion, Montreal, Canada, Aug. 2008*
23. *N. Labbe, P. Westmoreland. “Determining the Kinetics of C3H2 and C3H3 Reactions Using Ab Initio Methods”*, 26th Regional Meeting on Kinetics and Dynamics, Albany, NY, Jan. 2008
24. *N. Labbe, J. Wilcox. “Ab Initio Studies of Cyclohexane Adsorption in Zeolites”, ICEE 2006, San Juan, Puerto Rico, July 2006*
25. *J. Caulkins, N.Labbe, C. Luth, P. Vallieres. “Using Computational Chemistry to Understand Effective Adsorption Strategies for Separating Contaminants from Water”, ASEE 2006,Worecester, MA, March 2006*
26. *B. Padak, N. Labbe, C. Callahan. “The Effective Use of Technology in a Graduate Molecular Modeling Class”*, ASEE *2006,Worecester, MA, March 2006*

Extracurricular activities:

- Big Brothers Big Sisters, Amherst, MA (2009-present)
- Chemical Engineering Graduate Society, UMass Amherst (Social Chair 2009-2010) (2008 – present)
- New Faculty Search Student Committee (2009-2010)
- Ballroom Dance Team, Worcester Polytechnic Institute (2005-2006)
- Student Alumni Society, Worcester Polytechnic Institute (2004-2006)
- Resident Assistant, Worcester Polytechnic Institute (2004-2006)
- Alpha Phi Omega – Omicron Iota Chapter, Worcester Polytechnic Institute, Fellowship Vice President (2004-2006)
- WPI Student Ambassador, Worcester Polytechnic Institute (2004-2005)