

## **William J. Rogers, PhD**

**Laboratory Director**

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**TEES Research Scientist**

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### **Education**

Ph.D. in Physical Chemistry, Ohio State University, Columbus, Ohio, 1976

B.A., College of Wooster, Wooster, Ohio, 1962

### **Professional Experience**

TEES Research Scientist, Chemical Eng. Dept., Texas A&M University, 2002

Laboratory Director, Mary Kay O'Connor Process Safety Center, 1999

Research Scientist, Mary Kay O'Connor Process Safety Center, 1999

Visiting Scientist, Institutet for Kemiteknik, Lyngby, Denmark, 1985

Asst. Res. Scientist, Chemical Eng. Dept., Texas A&M University, 1983

Eng. Res. Associate, Chemical Eng. Dept., Texas A&M University, 1979 - 1983

Research Associate, Ohio State University, 1977 - 1978

### **Professional Affiliation**

American Institute of Chemical Engineers

Decision Analysis Society

### **Research**

Estimations of thermophysical and thermochemical properties; assessment, measurements, and models of chemical reactivity; thermal behavior of chemical processes, measurements and correlations; applications of quantum chemistry and statistical mechanics in chemical engineering; design of apparatus and experiments to measure properties and chemical behavior; formation behavior and flammability of aerosols and dusts; liquid mixture flammability measurements and predictive models. System reliability, risk analysis, and decision making.

William Rogers has been a leader of experimental research and laboratories in the Chemical Engineering Department at TAMU and has guided graduate students on experimental research and laboratory safety practices since 1979. He was co-author of a new chapter on reactive chemicals and editor of an appendix on laboratory safety in the 3<sup>rd</sup> edition (2005) of the Frank Lees' *Loss Prevention in the Process Industries*.

## Peer-Reviewed Publications

1. Gerkin, R.E., W.J. Rogers, "Observation of Nonlinearity and Asymmetry in Energies of EPR Transitions of  $^{160}\text{Gd}^{3+}$  in  $\text{La}(\text{C}_2\text{H}_5\text{SO}_4)_3 \cdot 9\text{D}_2\text{O}$  at Low Magnetic Fields," *Chem. Phys. Letters*, 43(3), 1976, pp. 592-596.
2. Gerkin, R.E., W.J. Rogers, and W.J. Tourek, "High-Precision Electromagnetic Paramagnetic Resonance Study of  $\text{Gd}^{3+}$  in Single Crystals of the Lanthanide Ethyl Sulfate Nonahydrates near Room Temperature," *J. Chem. Phys.*, 66(9), 1977, pp. 4166-4171.
3. Gerkin, R.E. and W.J. Rogers, "EPR Spectroscopic Determination and Interpretation of g.f.v. of Gadolinium $^{3+}$  in Single Crystals of the Lanthanide Ethyl Sulfate Nonahydrates," *J. Chem. Phys.*, 68(2), 1978, pp. 504-512.
4. Gerkin, R.E. and W.J. Rogers, "A High-Precision Electromagnetic Paramagnetic Resonance Study of  $\text{Gd}^{3+}$  in Single Crystals of the Lanthanide Ethyl Sulfate Nonahydrates near Room Temperature," *J. Chem. Phys.*, 70(8), 1979, pp. 3764-3774.
5. Rogers, W.J., J.C. Holste, P.T. Eubank, and K.R. Hall, "Microwave Apparatus for Phase Transition Studies of Corrosive Fluids to 1.7 kbar and 588 K," *Rev. Sci. Instrum.*, 56(10), 1985, pp. 1907-1912.
6. Rogers, W.J., F. Fontalba, E.F. Capps, J.C. Holste, K.N. Marsh, and K.R. Hall, "Magnetic Circulating Pumps for use over wide ranges of Temperature and Pressure," *Rev. Sci. Instrum.*, 59(1), 1988, pp. 193-194.
7. Brugge, H.B., C.-A. Hwang, J.C. Holste, K. R. Hall, W.J. Rogers, W. Lemming, G.J. Esper, K. N. Marsh, and B.E. Gammon, "Experimental Cross Virial Coefficients for Binary Mixtures of Carbon Dioxide with Nitrogen, Methane and Ethane at 300 and 320 K," *Physica A*, 156(1), 1989, pp. 382-416.
8. Lau, W.R., C.-A. Hwang, H. B. Brugge, G. A. Iglesias-Silva, H. A. Duarte-Garza, W.J. Rogers, K.R. Hall, J.C. Holste, B.E. Gammon, and K.N. Marsh, "A Continuously Weighed Pycnometer for Measuring Fluid Properties," *J. Chem. Eng. Data*, 42(4), 1997, pp. 738-744.
9. Rogers, W.J., J.A. Bullin, R.R. Davison, R.E. Frazier, and K.N. Marsh, "FTIR Method for VLE Measurements of Acid Gas - Alkanolamine Systems," *AIChE J.*, 43, 1997, pp. 3223-3231.
10. Rogers, W.J., J.A. Bullin, and R.R. Davison, "FTIR Measurements of Acid-Gas-Methyldiethanolamine Systems," *AIChE J.*, 44(11), 1998, 2423-2430.

11. Cisneros, L.O., W.J. Rogers and M.S. Mannan, "Adiabatic Calorimetric Decomposition Studies of 50-wt% Hydroxylamine/Water," *Journal of Hazardous Materials*, vol. 82, no. 1, 2001, pp. 13-24.
12. Al-Qurashi, F., G. Sharma, W.J. Rogers, and M.S. Mannan, "Application of Relational Chemical Process Safety Databases for Lowering Mean Failure Rates," *Process Safety Progress*, vol. 20, no. 4, December 2001, pp. 280-285.
13. Sukmarg, P., K. Krishna, W.J. Rogers, K.D. Kihm, and M.S. Mannan, "Effect of Operating Conditions and Orifice Size on Formation and Behavior of Aerosols from Heat Transfer Fluids," *Journal of Loss Prevention in the Process Industries*, vol. 15, no. 1, January 2002, pp. 19-27.
14. Aldeeb, A.A., W.J. Rogers, and M.S. Mannan, "Theoretical and Experimental Methods for the Evaluation of Reactive Chemical Hazards," *Process Safety and Environmental Protection, Transactions of the Institute of Chemical Engineers: Part B*, vol. 80, May 2002, pp. 141-149.
15. Vidal, M., J.P. Wagner, W.J. Rogers, and M.S. Mannan, "Charge Generation During Filling of Insulated Tanks," *Process Safety Progress*, vol. 80, no.3, September 2002, pp. 181-184.
16. Aldeeb, A.A., W.J. Rogers, and M.S. Mannan, "Understanding the Role of Process Chemistry in Fires and Explosions," *Process Safety Progress*, vol. 21, no. 4, December 2002, pp. 323-328.
17. Cisneros, L.O., W.J. Rogers, and M.S. Mannan, "Effect of Air in the Thermal Decomposition of 50 wt.% Hydroxylamine/water," *Journal of Hazardous Materials*, vol. 95, no. 1-2, 2002, pp. 13-25.
18. Krishna, K., T.K. Kim, K.D. Kihm, W.J. Rogers, and M.S. Mannan, "Predictive Correlations for Leaking Heat Transfer Fluid Aerosols in Air," *Journal of Loss Prevention*, vol. 16, no. 1, January 2003, pp. 1-8.
19. Saraf, S.R., W.J. Rogers, and M.S. Mannan, "Prediction of Reactive Hazards Based on Molecular Structure," *Journal of Hazardous Materials*, vol. 98, no. 1-3, March 2003, pp. 15-29.
20. Saraf, S.R., W.J. Rogers, and M.S. Mannan, "Application of Transition State Theory for Thermal Stability Prediction," *Industrial and Engineering Chemistry Research*, 42, 2003, pp. 1341-1346.
21. Saraf, S.R., W.J. Rogers, M.S. Mannan, M.B. Hall, and L.M. Thomson, "Theoretical Thermochemistry: Ab initio Heat of Formation for Hydroxylamine," *Journal of Physical Chemistry, A*, vol. 107, no. 8, February 27, 2003, pp 1077-1081.

22. Gentile, M., W.J. Rogers, and M.S. Mannan, "Development of an Inherent Safety Index Based on Fuzzy Logic," *AIChE Journal*, vol. 49, no. 4, April 2003, pp. 959-968.
23. Mannan, M.S., W.J. Rogers, M. Gentile, and T.M. O'Connor, "Inherently Safer Design: Implementation Challenges Faced by New and Existing Facilities," *Hydrocarbon Processing*, vol. 82, no. 3, March 2003, pp. 59-61.
24. Cisneros, L.O., X. Wu, W.J. Rogers, M.S. Mannan, J. Park, and S. North, "Decomposition Products of 50 mass% Hydroxylamine/water Under Runaway Reaction Conditions," *Process Safety and Environmental Protection, Transactions of the Institute of Chemical Engineers*, vol. 81, part B, March 2003, pp. 121-124.
25. Aldeeb, A.A., W.J. Rogers, and M.S. Mannan, "New Method Estimates the Parameters for Evaluating Process Reactivity Hazards," *Oil & Gas Journal*, vol. 101, no. 24, June 23, 2003, pp. 66-70.
26. Mannan, M.S., W.J. Rogers, J.T. Baldwin, J.P. Gupta, Y. Wang, S.R. Saraf, and K. Krishna, "Hydroxylamine Production: Will a QRA Help You Decide," *Reliability Engineering and System Safety*, vol. 81, no. 2, August 2003, pp. 215-224.
27. Krishna, K., W.J. Rogers, and M.S. Mannan, "The Use of Aerosol Formation, Flammability, and Explosion Information for Heat Transfer Fluid Selection," *Journal of Hazardous Materials*, vol. 104, no. 1-3, November 2003, pp. 215-226.
28. Roberts, M.A., W.J. Rogers, M.S. Mannan, and S.W. Ostrowski, "Prevention and Suppression of Metal Packing Fires," *Journal of Hazardous Materials*, vol. 104, no. 1-3, November 2003, pp. 247-253.
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30. Cisneros, L.O., W.J. Rogers, M.S. Mannan, X. Li, and H. Koseki, "Effect of Iron Ion in the Thermal Decomposition of 50 mass% Hydroxylamine/water Solutions," *Journal of Chemical and Engineering Data*, vol. 48, no. 5, September 2003, pp. 1164-1169.
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33. Gentile, M., W.J. Rogers, and M.S. Mannan, "Development of a Fuzzy Logic-based Inherent Safety Index," *Process Safety and Environmental Protection, Transactions of the Institute of Chemical Engineers*: vol. 81, Part B, no. 6, November 2003, pp. 444-456.
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35. Castro-Gomez, Raul, W.J. Rogers, J.C. Holste, K.R. Hall, and G.A. Iglesias-Silva, "Experimental P-T-r and Enthalpy-Increment Measurements of an Equimolar Mixture of Trichlorofluoromethane (R-11) + Dichlorodifluoromethane (R-12)," *Journal of Chemical and Engineering Data* (2003), 48, no. 6, 2003, pp. 1432-1434.
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37. Iglesias-Silva, G. A., R. Castro-Gomez, W.J. Rogers, J.C. Holste, and K.R. Hall, "Experimental P-T-r and Enthalpy-Increment Measurements of an Equimolar Mixture of Trichlorofluoromethane (R-11) + Chlorotrifluoromethane (R-13)," *Journal of Chemical and Engineering Data* (2003), 48, no. 6, 2003, pp. 1440-1441.
38. Aldeeb, A.A., W.J. Rogers, and M.S. Mannan, "Evaluation of Styrene-Acrylonitrile Copolymerization Thermal Stability and Runaway Behavior," *Journal of Hazardous Materials*, vol. 104, no. 1-3, November 2003, pp. 269-282.
39. Krishna, K., W.J. Rogers, and M.S. Mannan, "The Use of Aerosol Formation, Flammability, and Explosion Information for Heat-Transfer Fluid Selection," *Journal of Hazardous Materials*, vol. 104, no. 1-3, 2003, pp. 215-226.
40. Vidal, M., W.J. Rogers, J.C. Holste, and M.S. Mannan, "A Review of Estimation Methods for Flash Points and Flammability Limits," *Process Safety Progress*, vol. 23, no. 1, 2004, pp. 47-55.
41. Cisneros, L.O., W.J. Rogers, and M.S. Mannan, "Comparison of the Thermal Decomposition Behavior for Members of the Hydroxylamine/water Family," *Thermochimica Acta*, vol. 414, no. 2, 2004, pp. 177-183.

42. Saraf, S.R., W.J. Rogers, and M.S. Mannan, "Challenges in Classification of Reactive Chemicals," *Chemical Engineering Progress*, vol. 100, no. 3, March 2004, pp. 34-37.
43. Krishna, K., W.J. Rogers, and M.S. Mannan, "Prediction of Aerosol Formation for Safe Utilization of Industrial Fluids," *Chemical Engineering Progress*, vol. 100, no. 7, July 2004, pp. 25-28.
44. Wei, C., W.J. Rogers, and M.S. Mannan, "Application of Screening Tools in the Prevention of Reactive Chemical Incidents," *J. of Loss Prevention*, vol. 17, no. 4, July 2004, pp. 261-269.
45. Saraf, S.R., W.J. Rogers, D.M. Ford, and M.S. Mannan, "Integrating Molecular Modeling and Process Safety Research," *Fluid Phase Equilibria*, vols. 222-223, July 2004, pp. 205-211.
46. Wei, C., S.R. Saraf, W.J. Rogers, and M.S. Mannan, "Thermal Runaway Reaction Hazards and Mechanisms of Hydroxylamine with Acid/base Contaminants," *Thermochimica Acta*, vol. 421, no. 1-2, November 2004, pp. 1-9.
47. Cisneros, L.O., W.J. Rogers, M.S. Mannan, "Adiabatic Calorimetric Decomposition Studies of 35 mass% Hydroxylamine Hydrochloride/water," *The Canadian Journal of Chemical Engineering*, vol. 82, no. 6, December 2004, pp. 1106-1111.
48. Aldeeb, A.A., W.J. Rogers, and M.S. Mannan "Evaluation of 1,3-Butadiene Dimerization and Secondary Reactions in the Presence and Absence of Oxygen," *Journal of Hazardous Materials*, vol. 115, no. 1-3, November 2004, pp. 51-56.
49. Liu, Y-S., V.M. Ugaz, W.J. Rogers, and M.S. Mannan, "Development of a Nanocalorimeter for Material Characterization," *Journal of Loss Prevention in the Process Industries*, vol. 18, no. 3, May 2005, pp. 139-144.
50. Vidal, M, W.J. Rogers, and M.S. Mannan, "Prediction of Minimum Flash Point Behavior for Binary Mixtures," *Trans IChemE, Part B, Process Safety and Environmental Protection*, May 2005, vol 83, no. B6, November 2005, pp. 1-9.
51. Wei, C., W.J. Rogers, and M.S. Mannan, "Detection of Autocatalytic Decomposition Behavior of Energetic Materials Using APTAC," *Journal of Thermal Analysis and Calorimetry*, vol. 83, no. 1, January 2006, pp. 125-130.
52. Badders, N.R., C. Wei, A.A. Aldeeb, W.J. Rogers, and M.S. Mannan, "Predicting the Impact Sensitivities of Energetic Materials Using Quantum Chemical Descriptors," *Journal of Energetic Materials*, vol. 24, no. 1, January-March 2006, pp. 17-33.

53. Vidal, M., W. Wong, W.J. Rogers and M.S. Mannan, "Evaluation of Lower Flammability Limits of Fuel–Air–Diluent Mixtures Using Calculated Adiabatic Flame Temperatures," *Journal of Hazardous Materials*, vol. 130, no. 1-2, March 2006, pp. 21-27.
54. Wei, C., W.J. Rogers, and M.S. Mannan, "Thermal Decomposition Hazard Evaluation of Hydroxylamine Nitrate," *Journal of Hazardous Materials*, vol. 130, no. 1-2, March 2006, pp.163-168.
55. Liu, Yen-Shan, W.J. Rogers, and M.S. Mannan, "Screening Reactive Chemical Hazards," *Chemical Engineering Progress*, vol. 102, no. 5, May 2006, pp. 41-47.
56. Liu, Yen-Shan, V.M. Ugaz, S.W. North, W.J. Rogers, and M.S. Mannan, "Development of a Miniature Calorimeter for Identification and Detection of Explosives and Other Energetic Compounds," *J. of Hazardous Materials*, vol. 142, 2007, pp. 662-668.
57. Wei, C., W.J. Rogers, and M.S. Mannan, "Understanding Reactive Hazards using Molecular Simulation: Mechanisms of Hydroxylamine Decomposition," *Chemical Engineering Communications*, vol. 194, no. 5, May 2007, pp. 579-585.
58. Wei, C., W.J. Rogers, and M.S. Mannan, "Layer of Protection Analysis for Reactive Chemical Risk Assessment," *Journal of Hazardous Materials*, vol. 159, no. 1, November 2008, pp. 19-24.
59. Dinh, L.T.T., W.J. Rogers, and M.S. Mannan, "Reactivity of Ethylene Oxide in Contact with Basic Contaminants," *Thermochimica Acta*, vol. 480, no. 1-2, December 2008, pp. 53-60.
60. Yun, G.W., W.J. Rogers, and M.S. Mannan, "Risk Assessment of an LNG Importation Terminal using Bayesian-LOPA Methodology," *Journal of Loss Prevention in the Process Industries*, vol. 22, no 1, January 2009, p. 91-96.
61. Liu, L., Y. Guo, W.J. Rogers, and M.S. Mannan, "Computational Fluid Dynamics Analysis on the Critical Behavior of Reactive Chemicals," *Journal of Loss Prevention in the Process Industries*, vol., 22, no. 2, March 2009, pp. 187-196.
62. Zhao, F., W.J. Rogers, and M.S. Mannan, "Experimental Measurement and Numerical Analysis of Binary Hydrocarbon Mixture Flammability Limits," *Transactions of the Institute of Chemical Engineers, Part B, Process Safety and Environmental Protection*, vol. 87, no. 2, March 2009, pp. 94-104.
63. Liu, L., C. Wei, Y. Guo, W.J. Rogers, and M.S. Mannan, "Hydroxylamine Nitrate Self-Catalytic Kinetics Study with Adiabatic Calorimetry," *Journal of Hazardous Materials*, vol. 162, no. 2-3, March 2009, pp. 1217-1222.

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65. Liu, L., M. Papadaki, E. Pontiki, P. Stathi, W.J. Rogers and M.S. Mannan, "Isothermal Decomposition of Hydroxylamine and Hydroxylamine Nitrate in Aqueous Solutions in the Temperature Range 80-160°C," *Journal of Hazardous Materials*, vol. 165, no. 1-3, June 2009, pp. 573-578.
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67. Wang, Q., W.J. Rogers and M.S. Mannan, "Thermal Risk Assessment and Rankings for Reaction Hazards in Process Safety," *Journal of Thermal Analysis and Calorimetry*, vol. 98, no. 1, October 2009, pp. 225-233.
68. Liu, Lijun; Guo, Yuyan; Rogers, William J.; Mannan, M. Sam, "Computational fluid dynamics analysis on the critical behavior of reactive chemicals," *Journal of Loss Prevention in the Process Industries* (2009), 22(2), pp.187-196.
69. Saenz, L., V.H. Carreto-Vazquez, L. Liu, W.J. Rogers, M.S. Mannan, M. Papadaki, "2-Methylpyridine-N-oxidation runaway studies," *Journal of Loss Prevention in the Process Industries*, vol. 22, no. 6, November 2009, pp. 839-843.
70. Carreto-Vázquez, V.H., I. Hernández, D., Ng, W.J. Rogers, and M.S. Mannan, "Inclusion of Pressure Hazards into NFPA-704 Instability Rating System," *Journal of Loss Prevention in the Process Industries*, vol. 23, no. 1, January 2010, pp. 30-38.
71. Zhao, Fuman; Rogers, William J.; Mannan, M. Sam, "Calculated flame temperature (CFT) modeling of fuel mixture lower flammability limits," *Journal of Hazardous Materials* (2010), 174(1-3), pp. 416-423.
72. Yang, X., W.J. Rogers and M.S. Mannan, "Uncertainty delimitation and reduction for improved mishap probability prediction: application to level control of distillation unit," vol. 23, no. 1, January 2010, pp. 149-156.
73. Pokoo-Aikins, G., A. Heath, R.A. Mentzer, M.S. Mannan, W.J. Rogers, and M. El-Halwagi, "A Multi-Criteria Approach To Screening Alternatives For Converting Sewage Sludge To Biodiesel," *Journal of Loss Prevention in the Process Industries*, 23, 2010, pp. 412-420.



## Technical Meeting Proceedings

1. Rogers, W.J., J.C. Holste, and K.R. Hall "Microwave Method for Measurement of Phase Boundaries," *Proceedings of the 1986 International Gas Research Conference (IGRC)*, Toronto, Canada, September 8-11, 1986.
2. Rogers, W.J., J.C. Holste, and K.R. Hall, "Microwave Technique for Phase Behavior Studies of Petroleum and Natural Gas Mixtures," *Proc. Soc. of Pet. Eng.*, Dallas, Texas, 1988.
3. Holste, J.C., K. R. Hall, and W.J. Rogers, "Cross Virial Coefficient Correlations for Binary Mixtures of Carbon Dioxide with Nitrogen, Methane and Ethane," *Proceedings of the 1989 International Gas Research Conference (IGRC)*, Tokyo, Japan, November 6-9, 1989.
4. Cisneros, L., W.J. Rogers, and M.S. Mannan, "Thermal Runaway Reaction Studies of Poly(ethylene glycol) and Poly(propylene glycol)," *Proceedings of the 2<sup>nd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 26-27, 1999, pp. 202-212.
5. Al-Qurashi, F., W.J. Rogers, and M.S. Mannan, "Analysis of the EPA RMP\*INFO Database," *Proceedings of the 3<sup>rd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 24-25, 2000, pp. 40-45.
6. Cisneros, L., W.J. Rogers, and M.S. Mannan, "Thermal Decomposition Study of Hydroxylamine," *Proceedings of the 3<sup>rd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 24-25, 2000, pp. 140-168.
7. Saraf, S., W.J. Rogers, and M.S. Mannan, "Application of Ab-Initio Principles for Prediction of Chemical Reactivity," *Proceedings of the 3<sup>rd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 24-25, 2000, pp. 199-207.
8. Zhou, Y., N. Kazantzis, H.H. West, W.J. Rogers, and M.S. Mannan, "Abnormal Situation Management: A Process Dynamics Approach," *Proceedings of the 3<sup>rd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 24-25, 2000, pp. 228-230.
9. Krishna, K., P. Sukmarg, K.D. Kihm, W.J. Rogers, and M.S. Mannan, "Droplet Size Distributions of Heat Transfer Fluid Aerosols in Air," *Proceedings of the 3<sup>rd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory*

- Compliance: Making Safety Second Nature*, College Station, Texas, October 24-25, 2000, pp. 392-407.
10. Gentile, M., W.J. Rogers, and M.S. Mannan, "Application of Fuzzy Logic for the Development of an Inherent Safety Index," *Proceedings of the 3<sup>rd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 24-25, 2000, pp. 469-486.
  11. Sposato, C.F., W.J. Rogers, and M.S. Mannan, "Effects of Obstacle Geometry on Jet Mixing for Releases of Silane," *Proceedings of the 3<sup>rd</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 24-25, 2000, pp. 500-533.
  12. Mannan, M.S., W.J. Rogers, A. Aldeeb, L. Cisneros, and S. Saraf, "Assessing the Potential Hazards of Reactive Chemicals," *Proceedings of the 29<sup>th</sup> North Atlantic Thermal Analysis Society Conference*, St. Louis, Missouri, September 24-26, 2001, pp. 443-448.
  13. Cisneros, L., W.J. Rogers, and M.S. Mannan, "Effect of Air in the Thermal Decomposition of 50 wt% Hydroxylamine/Water," *Proceedings of the 4<sup>th</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 30-31, 2001, pp. 233-253.
  14. Aldeeb, A.A., W.J. Rogers, and M.S. Mannan, "Theoretical and Experimental Techniques for the Evaluation of Reactive Chemical Hazards," *Proceedings of the 4<sup>th</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 30-31, 2001, pp. 268-284.
  15. Aldeeb, A.A., W.J. Rogers, and M.S. Mannan, "Understanding the Role of Process Chemistry in Fires and Explosions," *Proceedings of the 36<sup>th</sup> Annual Loss Prevention Symposium*, AIChE 2002 Spring National Meeting, New Orleans, Louisiana, March 10-14, 2002, pp. 211-221.
  16. Saraf, S., W.J. Rogers, and M.S. Mannan, "Of Computers, Chemistry, Chemical Engineering and Reactivity," *Proceedings of the 4<sup>th</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 30-31, 2001, pp. 308-320.
  17. Krishna, K., T-K. Kim, K.D. Kihm, W.J. Rogers, and M.S. Mannan, "Understanding the Formation of Heat Transfer Fluid Aerosols in Air," *Proceedings of the 4<sup>th</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond*

*Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 30-31, 2001, pp. 384-393.

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19. Zhou, Y., W.J. Rogers, and M.S. Mannan, "A Sensor Fault Detection Scheme Using a Semi-Independent Process Model," *Proceedings of the 4<sup>th</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 30-31, 2001, pp. 693-701.
20. Keren, N., W.J. Rogers, and M.S. Mannan, "Chemical Plant Safety Performance Measurements," *Proceedings of the 4<sup>th</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 30-31, 2001, pp. 717-721.
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22. Mannan, M.S., W.J. Rogers, and A. Aldeeb, "A Systematic Approach to Reactive Chemicals Analysis," *Proceedings of Hazards XVI, Institution of Chemical Engineers*, Manchester, United Kingdom, November 6-8, 2001, pp. 41-58.
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43. Wei, C., W.J. Rogers, and M.S. Mannan, "Thermal Decomposition Hazard Evaluation of Hydroxylamine Nitrate," *Proceedings of the 7<sup>th</sup> Annual Mary Kay O'Connor Process Safety Center Symposium – Beyond Regulatory Compliance: Making Safety Second Nature*, College Station, Texas, October 26-27, 2004, pp.

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48. Vidal, M., M.S. Mannan, and W.J. Rogers, "Prediction of Minimum Flash Point Behavior for Binary Mixtures," *Proceedings of the 39th Annual Loss Prevention Symposium*, Atlanta, Georgia, April 11–13, 2005, 89B/1 – 89B/21.
49. Qiao, Yuanhua, N. Keren, W.J. Rogers, and M.S. Mannan, "Quantitative Risk Analysis for Hazardous Materials Transportation," *AIChE Spring National Meeting, Conference Proceedings*, Atlanta, GA, United States, April 10-14, 2005
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58. Saenz, L.R., W.J. Rogers, M.S. Mannan, and M. Papadaki, "Approach for the Development of a More Efficient and Safer Process in the Pharmaceutical Industry," *Proceedings of the 43th Annual Loss Prevention Symposium*, Tampa, Florida, April 26- 30, 2009, pp. 1-14.
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## Major Reports

1. Bailey, D.M., G.J. Esper, W.J. Rogers, J.C. Holste, K.R. Hall, P.T. Eubank, and K.M. Marsh "Properties of Carbon Dioxide Mixtures with Nitrogen and with Methane," *GRI Research Report*, GRI RR-122, 1989.
2. Hall, K.R. and W.J. Rogers, "Relative Density Equation for Natural Gas," *GRI Annual Report*, Gas Research Institute, 1990.
3. Mannan, M.S., M.T. O'Connor, W.J. Rogers, and M. Gentile, "Challenges in Implementing Inherent Safety Principles in New and Existing Chemical Processes," White Paper, Mary Kay O'Connor Process Safety Center, College Station, Texas, August 2002.
4. Mannan, M.S. and W.J. Rogers, "Challenges of Regulating or Implementing a Reactive Chemicals Hazard Management Program," Comments provided to the United States Chemical Safety and Hazard Investigation Board, Reactive Chemicals Public Hearing, Houston, Texas, Mary Kay O'Connor Process Safety Center, College Station, Texas, September 17, 2002.
5. "Best Practices in Prevention and Suppression of Metal Packing Fires," Mary Kay O'Connor Process Safety Center, College Station, August 2003.
6. Mannan, M.S. and W.J. Rogers, "Prevent Dust Fires and Explosions," Comments provided to the United States Chemical Safety and Hazard Investigation Board, Dust Incidents Public Hearing, Washington, D.C., Mary Kay O'Connor Process Safety Center, College Station, Texas, June 22, 2005.

## Technical Meeting Presentations

1. "Microwave Apparatus to Determine Phase Behavior of Sour Gases," Mobil Research and Development, Westhollow, Houston, March 20, 1983.
2. "Hydrogen Cyanide Incident Information Database and Website," 2000 Hydrogen Cyanide Safety Seminar, March 30, 2000, Baltimore, MD (presented by M.S. Mannan).
3. "Development of an Inherent Safety Index Based on Fuzzy Logic," 2001 AIChE Annual Meeting, November 5-9, 2001, Reno, Nevada (presented by M. Gentile, graduate student).
4. "Thermal Decomposition Studies of Hydroxylamine Compounds," AIChE Annual Meeting, November 5-9, 2001, Reno, Nevada (presented by L.O. Cisneros, graduate student).



5. "Density Functional Investigation of Hydroxylamine Decomposition," 2001 AIChE Annual Meeting, November 5-9, 2001, Reno, Nevada (presented by S. Saraf, graduate student).
6. "Computational Chemistry and Molecular Simulation for Engineers: A Cooperative Effort across College Boundaries," 2001 AIChE Annual Meeting, November 5-9, 2001, Reno, Nevada (presented by D.M. Ford).
7. "Computational Methods for Determining the Heat of Formation of Hydroxylamine," Fundamental Research Group, National Institute of Fire and Disaster, Tokyo, Japan, January 30, 2002.
8. "Aerosol Flammability Research," Fundamental Research Group, National Institute of Fire and Disaster, Tokyo, Japan, January 30, 2002.
9. "Experimental Research and Modeling at the Mary Kay O'Connor Process Safety Center," Chemical Safety Research Group, National Institute of Industrial Safety, Tokyo, Japan, February 6, 2002.
10. "Charge Generation During Filling of Insulated Tanks," 36<sup>th</sup> Annual Loss Prevention Symposium, AIChE Meeting, March 10-14, 2002, New Orleans, Louisiana (presented by M. Vidal, graduate student).
11. "Understanding the Role of Process Chemistry in Fires and Explosions," 36<sup>th</sup> Annual Loss Prevention Symposium, AIChE Meeting, March 10-14, 2002, New Orleans, Louisiana (presented by A.A. Aldeeb, graduate student).
12. "Calorimetric Studies of Hydroxylamine and Related Compounds," 1<sup>st</sup> International Congress on the Process Industries, AchemAmerica 2002, March 18-20, 2002, Mexico City, Mexico (presented by L.O. Cisneros, graduate student).
13. "CISP Thermal Safety Software Development Program for Chemical Reactivity Assessment," DIERS users Group Meeting, October 1, 2002, Houston, Texas (presented by S.G. Coats (DuPont) and W.J. Rogers).
14. "Calorimetric Data Correlations Using Molecular Descriptors," paper presented at the 2002 AIChE Annual Meeting, November 4-8, 2002, Indianapolis, Indiana (presented by S.R. Saraf).
15. "Analyzing Reaction Pathways for Evaluation of Reactive Hazards," paper presented at the 2002 AIChE Annual Meeting, November 4-8, 2002, Indianapolis, Indiana (presented by A.A. Aldeeb, graduate student).

16. "Predicting Reaction Pathways: Reactivity Evaluation Approach," Fundamental Research Group, National Research Institute of Fire and Disaster, Tokyo, Japan, January 17, 2003 (presented by A.A. Aldeeb, graduate student).
17. "Measurement and Modeling of Liquid Flammability Limits," AIChE Spring 2003 Meeting, New Orleans, LA, March 31-April 3, 2003 (presented by W. Wong, graduate student).
18. "Challenges in Classification of Reactive Chemicals," AIChE Spring 2003 Meeting, New Orleans, LA, March 31-April 3, 2003.
19. "Challenges of Regulating or Implementing a Reactive Chemicals Hazard Management Program," AIChE Spring 2003 Meeting, New Orleans, LA, March 31-April 3, 2003.
20. "Research on Reactive Chemical Hazards at the Mary Kay O'Connor Process Safety Center," Texas Chemical Council 2003 Safety Seminar, Galveston, Texas, June 2-5, 2003 (presented by M.S. Mannan).
21. "Integrating Molecular Modeling and Process Safety," NIST Fifteenth Symposium on Thermophysical Properties, Boulder, CO, June 22-27, 2003 (presented by Professor James C. Holste).
22. "Current Research of the Mary Kay O'Connor Process Safety Center," Shell Chemical Co., Houston, TX, July 27, 2003).
23. "Adiabatic Calorimetric Analysis of Runaway Polymerization Reactions," AIChE 2003 Annual Meeting, San Francisco, November 16-21, 2003 (presented by Abdul Aldeeb, graduate student).
24. "Predicting Properties of Energetic Materials via Molecular Modeling," AIChE 2003 Annual Meeting, San Francisco, November 16-21, 2003 (presented by Sanjeev Saraf, graduate student).
25. "Thermal Stability of Inhibited 1,3-Butadiene in the Presence and Absence of Oxygen." AIChE 2003 Annual Meeting, San Francisco, November 16-21, 2003 (presented by Abdul Aldeeb, graduate student)
26. "Experimental and Computational Methods for Process Safety Research," 3<sup>rd</sup> NRIFD Symposium, Mitaka, Tokyo, Japan, March 10-12, 2004.
27. "Calorimetric Analysis and Kinetic Studies of the Hydroxylamine Family," AIChE Spring Meeting, New Orleans, April 25-29, 2004 (presented by Chunyang Wei, graduate student).

28. "A Systematic Approach to Reactive Chemical Analysis," 3<sup>rd</sup> Annual NaTex Meeting, Frontiers in materials Research: Applications of Thermal Analysis and Rheology, Dallas, Texas April 29-30, 2004 (presented by M.S. Mannan).
29. "Reactive Chemical Hazards Research," Texas Chemical Council 2004 Safety Seminar, Galveston, Texas, June 7-10, 2004.
30. "Dust Explosion Research," Texas Chemical Council 2004 Safety Seminar, Galveston, Texas, June 7-10, 2004.
31. "Hydroxylamine Decomposition Pathways in the Presence of Acid or Base," AIChE 2004 Annual Meeting, November 7-12, 2004, Austin, Texas (presented by Chunyang Wei, graduate student).
32. "Computational Tools to Predict Heat of Reaction and Activation Energy for Reactivity Hazards Evaluation," AIChE 2004 Annual Meeting, November 7-12, 2004, Austin, Texas (presented by Migvia Vidal, graduate student).
33. "Flash Points of Mixtures: Can Computational Chemistry Help you Decide?," AIChE 2004 Annual Meeting, November 7-12, 2004, Austin, Texas (presented by Migvia Vidal, graduate student).
34. "Experimental and Computational Methods for Process Safety Research," 11<sup>th</sup> National Engineering Congress, Maracaibo, Venezuela, November 8-12, 2004 (presented by M.S. Mannan).
35. "Experimental and Computational Methods for Process Safety Research," International Conference on the 20<sup>th</sup> Anniversary of the Bhopal Tragedy, Indian Institute of Technology, Kanpur, India, December 1-3, 2004 (presented by M.S. Mannan).
36. "Dust Explosion Research, 2" Texas Chemical Council 2005 Safety Seminar, Galveston, Texas, June 6-9, 2005 (presented by H.H. West).
37. "Use of Adiabatic Calorimetry and Aging Test for Safe Storage Study of Hydroxylamine Nitrate," paper presented at the AIChE 2007 Spring Meeting, April 22- 26, 2007, Houston, Texas (presented by L. Liu, graduate student).
38. "Development of a Miniature Calorimeter for Identification and Detection of Explosives and Other Energetic Compounds," paper presented at the AIChE 2007 Spring Meeting, April 22-26, 2007, Houston, Texas (presented by Y.-S. Liu, Assistant Professor, University of Louisiana at Lafayette).
39. "Optimum Route Selection for Hazardous Materials Transportation Incorporating Security and Cost-Effectiveness Considerations," paper presented at the AIChE 2007 Spring Meeting, April 22-26, 2007, Houston, Texas (presented by Y. Qiao, DNV Inc.).

40. "The Risk Assessment of Bayesian-LOPA Methodology for an LNG Importation Terminal," paper presented at the 2008 AIChE Spring National Meeting, 8th Topical Conference on Natural Gas Utilization, New Orleans, Louisiana, April 6-10, 2008 (presented by G. Yun, graduate student).
41. Medina, A.F., M.S. Mannan, H.H. West, W.J. Rogers, R.J. Solano and C. Aiello, "Initiation and Mechanism of Carbon Filter Fires," 18th International Congress of Chemical and Process Engineering, August 24-28, 2008, Prague, Czech Republic.
42. Qi, R., D. Ng, W.J. Rogers and M. S. Mannan, "LNG Vapor Dispersion Modeling with ANSYS CFX," 9th Topical Conference on Natural Gas Utilization, 2009 AIChE Spring National Meeting, Tampa, Florida, April 26-30, 2009.

## University Service

Mary Kay O'Connor Process Safety Center Steering Committee  
Mary Kay O'Connor Process Safety Center Technical Advisory Committee  
Engineering College Safety Committee  
Chemical Engineering Department Curriculum Development Committee  
University Summer Performance Series Board Member  
Department of Performance Studies, Friends of Chamber Music Board  
Gilbert and Thyra Plass Foundation Board President

## Professional Service

Prepared and helped to develop protocols for a hydrogen cyanide website and database of property and industrial information in collaboration with the hydrogen cyanide industrial community.

Co-developed and co-taught a two-day continuing education course for industrial personnel, "Reactive Chemical Hazards", sponsored by the Mary Kay O'Connor Process Safety Center, Houston, Texas, July 11-12, 2001, and November 21-22, 2002.

Co-developed and co-taught a one-day continuing education course for industrial personnel, "Identification of Reactive Chemical Hazards", sponsored by the Mary Kay O'Connor Process Safety Center, Galveston, Texas, June 3, 2003.

Co-developed and taught a two-day onsite continuing education course for industrial personnel, "Chemical Behavior and Reactive Chemical Hazard Case

Studies", sponsored by the Mary Kay O'Connor Process Safety Center, Batesville, Arkansas, May 17-18, 2004.

Arranged a session on Safety Culture at the AIChE, Process Plant Safety Symposium, Atlanta, Georgia, April 10-14, 2005.

Developed a course for juniors and seniors on risk analysis and a course for graduate students and selected seniors of quantitative risk analysis and decision making.

## **Biographical Information**

William Rogers has extensive experience in designing apparatus and methods for precision measurements of fluid properties over wide ranges of conditions. He also has co-designed or helped to develop various types of novel apparatus for corrosive and hazardous fluids. A microwave apparatus to detect phase regions of corrosive fluids at extreme conditions of pressure and temperature was successful for measurements of natural gas fluids at deep well conditions. Other apparatus include development of a FITR measurement method for gas treating research and a laser cell for natural gas conversion research.

He has been co-guiding graduate student research in thermodynamics, reactive chemicals, and chemical process safety. As Laboratory Director of the Mary Kay O'Connor Process Safety Center, he is responsible for experimental measurements, modeling, and computations to extend the use of experimental data. As a co-PI or senior investigator on numerous proposals, he helps to acquire support for the research programs. Also, he has been a principal or senior investigator in various proprietary research projects that were not reported in the open literature or at symposia.

With Sam Mannan, he developed and co-taught a continuing education course on reactive chemicals. Also, he teaches an introductory process safety course in the Chemical Engineering Department for senior engineering students. Together with David Ford and M. Sam Mannan, he has directed an initiative, supported by a 2001 grant from the Dreyfus Foundation, to develop and integrate a molecular approach in the chemical engineering curriculum. As part of this program in 2001 and 2003, he co-taught a course on molecular modeling and computational chemistry.

## **Representative Major Projects**

**Texas Higher Education Coordinating Board, Behavior of Heat Exchange Fluid Aerosols Leaking from Manufacturing Processes, 01/01/99 - 8/31/03**

**Laboratory Director:** The primary goal of this research is to study the formation and dispersion of aerosols that form because of escape of heat transfer fluids through leak structures in industry. This research involves a variety of heat exchange fluids and a non-intrusive laser method based on the Malvern Instrument Diffraction Particle Analyzer to measure droplet sizes, spatial distributions, and concentrations forming from nozzles of various shapes to simulate leaks in pipes and vessels. The goal is to improve industrial process safety and economic practices through an understanding of how aerosols can form and strategies for safe handling of leaking fluids.

**Ashland, Inc. and Pharmacia, Inc, Reactive Chemicals Analysis of Hydroxylamine Compounds, 01/01/01 - 12/31/01**

**Co-Principal Investigator:** This project involved the measurement of thermal stability and decomposition behavior of hydroxylamine and hydroxylamine compounds including hydroxylamine hydrochloride. Studied were the effects of inhibitors on the thermal stability and the effects of metal surfaces and added contaminants. Tests were performed in closed glass cells in the Automatic Pressure Tracking Adiabatic Calorimeter APTAC calorimeter. The thermal behavior information was required for safe storage, transport, handling, and use of hydroxylamine and hydroxylamine hydrochloride/water solutions at industrial sites.

**Process Safety Consortium, Computations and Modeling for Reactivity Predictions, 01/01/00 - 12/31/03**

**Co-Principal Investigator:** This research employs computational models, both quantum and classical, to estimate property values and to predict chemical reactivity. The work is currently focused on investigating homogeneous catalysis pathways for hydroxylamine decomposition using density functional theory. The heat of formation of hydroxylamine was calculated using a variety of models, including quantum together with isodesmic reactions. To test the theoretical calculations, thermal decomposition of systems are measured using an Automated Pressure Tracking Adiabatic Calorimeter (APTAC) and Reactive System Screening Tool (RSST) calorimeters.

**Process Safety Consortium, Systematic Approach for Assessment of Chemical Reactive Hazards, 01/01/00 - 12/31/04**

**Co-Principal Investigator:** This research is developing a systematic approach for evaluating reactive chemicals to determine potential hazards. This approach employs a combination of theoretical and experimental methods that include both screening and advanced levels of analysis. Understanding the reaction stoichiometry, thermodynamics, and kinetics is of critical importance for reactivity assessment and safer process design.

Various reactive systems of industrial interest will be analyzed to develop and test this approach to chemical reactivity metrics.

**Dreyfus Foundation, Engineering Application of Molecular Modeling and Computational Chemistry, 06/01/01 - 06/01/05**

**Co-Principal Investigator:** The purpose of this initiative is to help integrate a microscopic approach with the traditional macroscopic approach in the chemical engineering curriculum to increase the knowledge and competency of engineering students in the use of molecular-level computational tools. The main focus is a new graduate course wherein computational chemistry and molecular modeling tools are applied to solve engineering problems related to material properties, chemical reactivity, and chemical process safety. To help achieve this integration, the ideas and tools presented in the new course will be employed also in other engineering courses.

**Hydrogen Cyanide Consortium and Dupont, Hydrogen Cyanide Incident Database and Website, 07/03/01 (established)**

**Co-Principal Investigator:** This project involves assembling, transferring, archiving the combined incident knowledge of participating hydrogen cyanide companies. The information is continually evaluated, updated, and made available at three levels of access on the hydrogen cyanide website and provides a forum for exchange of safety information for operations involving hydrogen cyanide chemicals and equipment.

**Dow Chemical Co. and Eastman Kodak Co., Structure based Predictions of Chemical Reactivity, 09/24/01 - 09/24/07**

**Co-Principal Investigator:** In collaboration with Dow Chemical and Eastman Kodak, a Quantitative Structure Property Relationships (QSPR) model is used to correlate onset temperatures and heats of decomposition, experimentally measured in differential scanning calorimeters, using molecular properties for a variety of important industrial chemicals. Also, activation energies will be predicted using correlations of heats of reaction and molecular properties. These correlations will help to extend available experimental data to predict potential reactivity hazards.

**Texas Higher Education Coordinating Board, Flammability of Liquid Mixtures, 01/01/02 - 12/31/04**

**Co-Principal Investigator:** This research is a combined theoretical and experimental study that will develop calculation and software tools for predicting flash points and flammability limits for liquid mixtures and test those tools using experimental data. Systems will be tested both on a standard flash point tester used in industry and with a flammability apparatus that will be designed and constructed for this research. The

established standard methods for determining flash points are known to be inaccurate and they generally apply only to pressures and oxygen concentrations near atmospheric. Therefore, test methods will be developed for the wide ranges of pressures, temperatures, and oxygen levels encountered in industrial manufacturing processes.

**Solutia, Inc., Flammability Studies on Heat Transfer Fluid Aerosol Sprays, 03/01/02 - 02/28/03**

**Co-Principal Investigator:** Continued research on aerosols formed by leaking heat transfer fluids involves the study of flame speeds and flammable limits of aerosols with mono-disperse drop sizes. A predictive model to relate characteristic flammability limits to aerosol drop size, volume concentration and ignition energy will be developed to estimate and reduce explosion hazards of heat transfer fluid aerosols and guide their selection and use in industry.

**Frank Lees Loss Prevention in the Process Industries, 3<sup>rd</sup> Edition, 04/01/02 - 12/31/03**

**Co-author of a new chapter on reactive chemicals and editor of an appendix on laboratories:** The Mary Kay O'Connor Process Safety Center is editing the entire 3<sup>rd</sup> edition of this classic, three-volume reference on chemical process safety.

**International Science and Technology Center, Methods for Evaluating Hazardous Chemical Reactivity, 05/01/02 - 04/30/04**

**Co-Principal Investigator:** This project involves collaboration in chemical reactivity research and process hazard evaluation with *Cheminform St Petersburg*, Russia (CISP), with support from the International Science and Technology Center (ISTC). This collaboration will combine the Mary Kay O'Connor Process Safety research initiatives in reactivity hazard assessment and thermal reactivity measurements with the experience in thermal research and reactive modeling software of CISP. A goal of the proposed collaboration is to incorporate the CISP methods with the Center Reactive Chemical Hazards Assessment method, which reduces the complexity of the overall system to the most probable reactions and mechanisms and reduces the amount of required experimental analyses. A second goal of this collaboration is to analyze reactive systems and processes involved with industrial fires and explosions to test the effectiveness of this systematic approach and its applicability by scientists and industrial personnel. Information from the experimental testing and analyses will be used by CISP to refine the models and to develop software tools for use by industrial personnel for reactivity hazard assessments and to design inherently safer processes.



**National Institute of Fire and Disaster (NIFD), Japan**

**Co-Principal Investigator:** This project involves collaborations with NIFD for chemical reactivity measurements and hazard assessments of energetic chemicals, such as organic peroxides, under wide ranges of conditions and sample sizes. This project includes exchange of students and researches and sharing of reactivity and application information.

**National Institute of Industrial Safety (NIIS), Chemical Safety Research Group, Japan**

**Co-Principal Investigator:** This project involves collaborations with NIIS to develop models for prediction of hazards to property, personnel, and environment from accidental releases or explosions followed by releases. This research includes two-phase releases, computational studies and modeling of reactive chemicals, analysis of aerosol explosion hazards, database analysis, and failure rate metrics.