CURRICULUM VITAE

1 Name, Position, Department

C. Franklin Goldsmith
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School of Engineering, Brown University
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2 Education

B.A, **University of North Carolina–Chapel Hill**, Philosophy, 1999
B.S, **North Carolina State University**, Applied Mathematics, 2003
B.S, **North Carolina State University**, Chemical Engineering, 2003
Ph.D., **Massachusetts Institute of Technology**, Chemical Engineering, 2010
Dissertation: "Predicting the Combustion Properties of Hydrocarbon Fuel Mixtures"

3 Professional Appointments

- *Associate Professor*, **Brown University**, January 2021–present.
- *Assistant Professor*, **Brown University**, January 2014–2021.
- *Argonne Director's Fellow*, **Argonne National Laboratory**, October 2012–December 2013. Advisors: Stephen J. Klippenstein and Robert S. Tranter
- *Alexander von Humboldt Postdoctoral Fellow*, **The Fritz-Haber Institute of the Max Planck Society**, September 2010–August 2012. Advisor: Raimund Horn
- *Research Assistant*, **Massachussetts Institute of Technology**, September 2004–June 2010. Advisor: William H. Green
- *Contract Engineer*, **BD Technologies**, Summer 2003.

4 Completed Publications

4.1 Refereed Journal Articles

[1] Blöndal†, K.; Sargsyan, K.; Bross, D.H.; Ruscic, B.; and Goldsmith*, C.F. Adsorbate partition functions via phase space integration: Quantifying the effect of translational anharmonicity on thermodynamic properties. *The Journal of Physical Chemistry C*, (in press):–, 2021.

[2] Danilack†, A.D.; Mulvihill, C.R.; Klippenstein, S.J.; and Goldsmith*, C.F. Diastereomers and low-temperature oxidation. *The Journal of Physical Chemistry A*, (in press):–, 2021.

[3] Fuller, M.E.; Morsch, P.; Preußker, M.; Goldsmith, C.F.; and Heufer*, K.A. The impact of NO_x addition on the ignition behaviour of n-pentane. *React. Chem. Eng.*, pp. –, 2021.

[4] Kreitz†, B.; Sargsyan, K.; Blöndal†, K.; Mazeau, E.J.; West, R.H.; Wehinger, G.D.; Turek, T.; and Goldsmith*, C.F. Quantifying the impact of parametric uncertainty on automatic mechanism generation for co2 hydrogenation on ni(111). *JACS Au*, (in press):–, 2021.

[5] Rose, C.; Medford, A.J.; Goldsmith, C.F.; Vegge, T.; Weitz, J.S.; and Peterson*, A.A. Heterogeneity in susceptibility dictates the order of epidemic models. *Journal of Theoretical Biology*, 528:110839, 2021.

[6] Yin[†,*], G.; Goldsmith[*], C.F.; Chen[†], X.; Hu, E.; and Huang, Z. Rate coefficients for 1,2-dimethyl-allyl + HO_2 and the implications for 2-methyl-2-butene combustion. *Combustion and Flame*, 230:111433, 2021.

[7] Mazeau, E.J.; Satpute, P.; Blöndal[†], K.; Goldsmith[*], C.F.; and West[*], R.H. Automated mechanism generation using linear scaling relationships and sensitivity analyses applied to catalytic partial oxidation of methane. *ACS Catalysis*, 11(12):7114–7125, 2021.

[8] Liu, M.; Grinberg Dana, A.; Johnson, M.S.; Goldman, M.J.; Jocher, A.; Payne, A.M.; Grambow, C.A.; Han, K.; Yee, N.W.; Mazeau, E.J.; Blöndal[†], K.; West, R.H.; Goldsmith, C.F.; and Green[*], W.H. Reaction mechanism generator v3.0: Advances in automatic mechanism generation. *Journal of Chemical Information and Modeling*, 61(6):2686–2696, 2021.

[9] Miller[*], J.A.; Sivaramakrishnan, R.; Tao, Y.; Goldsmith, C.F.; Burke, M.P.; Jasper, A.W.; Hansen, N.; Labbe, N.J.; Glarborg, P.; and Zádor, J. Combustion chemistry in the twenty-first century developing theory-informed chemical kinetics models. *Progress in Energy and Combustion Science*, 83:100886, 2021.

[10] Kreitz[*,†], B.; Wehinger, G.D.; Goldsmith, C.F.; and Turek, T. Microkinetic modeling of the CO_2 desorption from supported multi-faceted Ni catalysts. *Journal of Physical Chemistry C*, 2020 (under review).

[11] Vaddypally, S.; Kiselev[‡], V.G.; Byrne, A.N.; Goldsmith, C.F.; and Zdilla[*], M.J. Transition-metal-mediated, reversible double-cyclization of cyanuric triazide to an asymmetric bitetrazolate coupled to cleavage of the six-membered aromatic ring. *Chemical Science*, 12:2268–2275, 2021.

[12] Fuller, C.; Sinrud, J.; Schwind[‡], R.; Klassen, M.; Goldsmith[*], C.F.; and Walker[*], R. A continuous flow liquid propellant strand burner for high pressure monopropellant and bipropellant combustion studies. *Review of Scientific Instruments*, 2020 (in press).

[13] Danilack[†], A.A. and Goldsmith[*], C.F. A statistical model for the product energy distribution in reactions leading to prompt dissociation. *Proceedings of the Combustion Institute*, 38(1):507–514, 2021.

[14] Danilack[†], A.A.; Klippenstein, S.J.; Georgievskii, Y.; and Goldsmith[*], C.F. Low-temperature oxidation of diethyl ether: Reactions of hot radicals across coupled potential energy surfaces. *Proceedings of the Combustion Institute*, 38(1):671–679, 2021.

[15] Sikes, T.; Burdett, K.B.; Speth, R.L.; Goldsmith, C.F.; Sivaramakrishnan, R.; and Tranter[*], R.S. Ring opening in cycloheptane and dissociation of 1-heptene at high temperatures. *Proceedings of the Combustion Institute*, 38(1):929–937, 2021.

[16] Almodovar[‡], C.A. and Goldsmith[*], C.F. Laser schlieren study of the thermal decomposition of 2-ethylhexyl-nitrate. *Proceedings of the Combustion Institute*, 38(1):997–1005, 2021.

[17] Gorn, M.V.; Gritsan, N.P.; Goldsmith, C.F.; and Kiselev[*,‡], V.G. Thermal stability of bis-tetrazole and bis-triazole derivatives with long catenated nitrogen chains: Quantitative insights from high-level quantum chemical calculations. *The Journal of Physical Chemistry A*, 124(38):7665–7677, 2020.

[18] Chen[†], X. and Goldsmith[*], C.F. Accelerating variational transition state theory via artificial neural networks. *The Journal of Physical Chemistry A*, 124(5):1038–1046, 2020.

[19] Kiselev[‡], V. and Goldsmith[*], C.F. Accurate thermochemistry of novel energetic fused tricyclic 1,2,3,4-tetrazine nitro derivatives from local coupled cluster methods. *The Journal of Physical Chemistry A*, 123(45):9818–9827, 2019.

[20] Blöndal[†], K.; Jelic, J.; Mazeau, E.; Studt, F.; West, Richard, H.; and Goldsmith[*], C.F. Computer-generated kinetics for coupled heterogeneous/homogeneous systems: A case study in catalytic combustion of methane on platinum. *Industrial & Engineering Chemistry Research*, 58(38):17682–17691, 2019.

[21] Fuller[†], M.E. and Goldsmith[*], C.F. Shock tube laser schlieren study of the pyrolysis of isopropyl nitrate. *The Journal of Physical Chemistry A*, 123(28):5866–5876, 2019.

[22] Kiselev[‡], V. and Goldsmith[*], C.F. Accurate prediction of bond dissociation energies and barrier heights for high-energy caged nitro and nitroamino compounds using a coupled cluster theory. *The Journal of Physical Chemistry A*, 123(23):4883–4890, 2019.

[23] Fuller[†], M.E.; Skowron[†], M.; Tranter, R.S.; and Goldsmith[*], C.F. A modular, multi-diagnostic, automated shock tube for gas-phase chemistry. *Review of Scientific Instruments*, 90(6):064104, 2019.

[24] Chen[†], X.; Fuller[†], M.E.; and Goldsmith[*], C.F. Decomposition kinetics for HONO and HNO_2. *Reaction Chemistry and Engineering*, 4:323–333, 2019.

[25] Sivaramakrishnan[*], R.; Goldsmith, C.F.; Peukert, S.; and Michael, J.V. Direct measurements of channel specific rate constants in OH + C_3H_8. *Proceedings of the Combustion Institute*, 37:231–238, 2019.

[26] Randazzo, J.B.; Fuller[†], M.E.; Goldsmith, C.F.; and Tranter[*], R.S. Thermal dissociation of alkyl nitrites and recombination of alkyl radicals. *Proceedings of the Combustion Institute*, 37:703–710, 2019.

[27] Fuller[†], M.E.; West, R.H.; and Goldsmith[*], C.F. A computational investigation into the combustion byproducts of a liquid monopropellant. *Proceedings of the Combustion Institute*, 37:5671–5677, 2019.

[28] Fuller[†], M.E. and Goldsmith[*], C.F. On the relative importance of HONO versus HNO_2 in low-temperature combustion. *Proceedings of the Combustion Institute*, 37:695–702, 2019.

[29] Danilack[†], A.A. and Goldsmith[*], C.F. A computational investigation into the kinetics of NO + CH_2CCH and its effect on NO reduction. *Proceedings of the Combustion Institute*, 37:687–694, 2019.

[30] Chen[†], X. and Goldsmith[*], C.F. Predictive kinetics for the thermal decomposition of RDX. *Proceedings of the Combustion Institute*, 37:3167–3173, 2019.

[31] Kiselev[*,‡], V.; Muravyev, N.; Monogarov, K.; Gribanov, P.; Asachenko, A.; Fomenkov, I.; Goldsmith[*], C.F.; Pivkina, A.; and Gritsan, N. Toward reliable characterization of energetic materials: Interplay of theory and thermal analysis in the study of thermal stability of tetranitroacetimidic acid (TNAA). *Physical Chemistry Chemical Physics*, 20:29285–29298, 2018.

[32] West[*], R.H. and Goldsmith, C.F. The impact of roaming radicals on the combustion properties of transportation fuels. *Combustion and Flame*, 194:387–395, 2018.

[33] Middaugh, J.E.; Buras, Z.J.; Matrat, M.; Chu, T.C.; Kim, Y.S.; Alecu, I.M.; Vasiliou, A.K.; Goldsmith, C.F.; and Green[*], W.H. A combined photoionization time-of-flight mass spectrometry and laser absorption spectrometry flash photolysis apparatus for simultaneous determination of reaction rates and product branching. *Review of Scientific Instruments*, 89(7):074102, 2018.

[34] Tranter*, R.S.; Lynch, P.T.; Randazzo, J.B.; Lockhart, J.P.A.; Chen†, X.; and Goldsmith, C.F. High temperature pyrolysis of 2-methyl furan. *Physical Chemistry Chemical Physics*, 20:10826–10837, 2018.

[35] Chen†, X. and Goldsmith*, C.F. A theoretical and computational analysis of the methyl-vinyl + O_2 reaction and its effects on propene combustion. *The Journal of Physical Chemistry A*, 121(48):9173–9184, 2017.

[36] Lockhart, J.P.A.; Goldsmith, C.F.; Randazzo, J.B.; and Tranter*, R.S. An experimental and theoretical study of the thermal decomposition of C_4H_6 isomers. *Journal of Physical Chemistry A*, 121(20):3827–3850, 2017.

[37] Goldsmith*, C.F. and West, R.H. Automatic generation of microkinetic mechanisms in heterogeneous catalysis. *Journal of Physical Chemistry C*, 121(18):9970–9981, 2017.

[38] Zhou, C.W.; Simme, J.M.; Somers, K.P.; Goldsmith, C.F.; and Curran*, H.J. Chemical kinetics of hydrogen atom abstraction from allylic sites by $^3O_2$: Implications for combustion modelling and simulation. *Journal of Physical Chemistry A*, 121(9):1890–1899, 2017.

[39] Gimenez-Lopez, J.; Rasmussen, C.T.; Hashemi, H.; Alzueta, M.U.; Gao, Y.; Marshall, P.; Goldsmith, C.F.; and Glarborg*, P. Experimental and kinetic modeling study of C_2H_2 oxidation at high pressure. *International Journal of Chemical Kinetics*, 48(11):724–738, 2016.

[40] Chai‡, J. and Goldsmith*, C.F. Rate coefficients for fuel+NO_2: Predictive kinetics for HONO and HNO_2 formation. *Proceedings of the Combustion Institute*, 36:617–626, 2016.

[41] Labbe, N.J.; Sivaramakrishnan*, R.; Goldsmith, C.F.; Georgievskii, Y.; Miller, J.A.; and Klippenstein, S.J. Ramifications of including non-equilibrium effects for HCO in flame chemistry. *Proceedings of the Combustion Institute*, 36:525–532, 2016.

[42] Miller*, J.A.; Klippenstein, S.J.; Robertson, S.H.; Pilling, M.J.; Shannon, R.; Zador, J.; Jasper, A.W.; Goldsmith, C.F.; and Burke, M.P. Comment on "when rate constants are not enough". *Journal of Physical Chemistry A*, 120:306–312, 2016.

[43] Labbe, N.J.; Sivaramakrishnan*, R.; Goldsmith, C.F.; Georgievskii, Y.; Miller, J.A.; and Klippenstein, S.J. Weakly bound free radicals in combustion: "prompt" dissociation of formyl radicals and its effect on laminar flame speeds. *Journal of Physical Chemistry Letters*, 7(1):85–9, 2016.

[44] Merchant, S.S.; Goldsmith, C.F.; Vandeputte, A.G.; Burke, M.P.; Klippenstein, S.J.; and Green*, W.H. Understanding low-temperature first-stage ignition delay: Propane. *Combustion and Flame*, 162(10):3658–3673, 2015.

[45] Goldsmith*, C.F.; Harding, L.B.; Georgievskii, Y.; Miller, J.A.; and Klippenstein, S.J. Temperature and pressure-dependent rate coefficients for the reaction of vinyl radical with molecular oxygen. *The Journal of Physical Chemistry A*, 119(28):7766–7779, 2015.

[46] Burke*, M.P.; Goldsmith, C.F.; Klippenstein, S.J.; Welz, O.; Huang, H.; Antonov, I.O.; Savee, J.D.; Osborn, D.L.; ZÃ¡dor, J.; Taatjes, C.A.; and Sheps, L. Multiscale informatics for low-temperature propane oxidation: Further complexities in studies of complex reactions. *The Journal of Physical Chemistry A*, 119(28):7095–7115, 2015.

[47] Welz*, O.; Burke, M.P.; Antonov, I.O.; Goldsmith, C.F.; Savee, J.D.; Osborn, D.L.; Taatjes, C.A.; Klippenstein, S.J.; and Sheps*, L. New insights into low-temperature oxidation of propane from synchrotron photoionization mass spectrometry and multiscale informatics modeling. *The Journal of Physical Chemistry A*, (28):119, 2015.

[48] Goldsmith, C.F.; Burke, M.P.; Georgievskii, Y.; and Klippenstein*, S.J. Effect of non-thermal product energy distributions on ketohydroperoxide decomposition kinetics. *Proceedings of the Combustion Institute*, 35(1):283–290, 2015.

[49] Burke*, M.P.; Goldsmith, C.F.; Georgievskii, Y.; and Klippenstein, S.J. Towards a quantitative understanding of the role of non-Boltzmann reactant distributions in low temperature oxidation. *Proceedings of the Combustion Institute*, 35(1):205–213, 2015.

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[51] Schwarz, H.; Geske, M.; Goldsmith, C.F.; Schloegl, R.; and Horn*, R. Fuel-rich methane oxidation in a high-pressure flow reactor studied by optical-fiber laser-induced fluorescence, multi-species sampling profile measurements and detailed kinetic simulations. *Combustion and Flame*, 161(7):1688–1700, 2014.

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[53] Korup, O.; Goldsmith, C.F.; Weinberg, G.; Geske, M.; Kandemir, T.; Schloegl, R.; and Horn*, R. Catalytic partial oxidation of methane on platinum investigated by spatial reactor profiles, spatially resolved spectroscopy, and microkinetic modeling. *Journal of Catalysis*, 297:1–16, 2013.

[54] Goldsmith, C.F.; Magoon, G.R.; and Green*, W.H. Database of Small Molecule Thermochemistry for Combustion. *Journal of Physical Chemistry A*, 116(36):9033–9057, 2012.

[55] Goldsmith, C.F.; Tomlin, A.S.; and Klippenstein*, S.J. Uncertainty propagation in the derivation of phenomenological rate coefficients from theory: A case study of n-propyl radical oxidation. *Proceedings of the Combustion Institute*, 34(1):177–185, 2013.

[56] Goldsmith, C.F. Estimating the Thermochemistry of Adsorbates Based Upon Gas-Phase Properties. *Topics in Catalysis*, 55(5-6):366–375, 2012.

[57] Goldsmith, C.F.; Green, W.H.; and Klippenstein*, S.J. Role of O_2 + QOOH in Low-Temperature Ignition of Propane. 1. Temperature and Pressure Dependent Rate Coefficients. *Journal of Physical Chemistry A*, 116(13):3325–3346, 2012.

[58] Allen, J.W.; Goldsmith, C.F.; and Green*, W.H. Automatic estimation of pressure-dependent rate coefficients. *Physical Chemistry Chemical Physics*, 14(3):1131–1155, 2012.

[59] Korup, O.; Mavlyankariev, S.; Geske, M.; Goldsmith, C.F.; and Horn*, R. Measurement and analysis of spatial reactor profiles in high temperature catalysis research. *Chemical Engineering and Processing*, 50(10, SI):998–1009, 2011.

[60] Goldsmith, C.F.; Klippenstein, S.J.; and Green*, W.H. Theoretical rate coefficients for allyl + HO_2 and allyloxy decomposition. *Proceedings of the Combustion Institute*, 33(1):273–282, 2011.

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[64] Goldsmith, C.F.; Ismail, H.; Abel, P.R.; and Green, W.H. Pressure and temperature dependence of the reaction of vinyl radical with alkenes II: Measured rates and predicted product distributions for vinyl plus propene. *Proceedings of the Combustion Institute*, 32:139–148, 2009.

[65] Ismail, H.; Goldsmith, C.F.; Abel, P.R.; Howe, P.T.; Fahr, A.; Halpern, J.B.; Jusinski, L.E.; Georgievskii, Y.; Taatjes, C.A.; and Green, W.H. Pressure and temperature dependence of the reaction of vinyl radical with Ethylene. *Journal of Physical Chemistry A*, 111(29):6843–6851, 2007.

[66] Wen, J.Z.; Goldsmith, C.F.; Ashcraft, R.W.; and Green*, W.H. Detailed kinetic modeling of iron nanoparticle synthesis from the decomposition of $Fe(CO)_5$. *Journal of Physical Chemistry C*, 111(15):5677–5688, 2007.

5 Service

5.1 To the School of Engineering / Brown University

- Concentration Advisor, Chemical Engineering, 2020–present
- Graduate Representative, Chemical & Environmental Engineering, 2014–2020
- First-Year Advisor, 2014–present

6 Academic Honors, Fellowships, Honorary Societies

- Argonne Director's Fellow, Argonne National Laboratory, 2012–2013.
- Alexander von Humboldt Postdoctoral Research Fellow, 2010–2012.
- National Science Foundation, Graduate Research Fellowship, 2007–2009.
- Department of Defense, National Defense Science and Engineering Graduate Fellowship, 2004–2007.
- Fulbright Scholar, Mathematics, 2003-2004.

6.1 Research Theses & Independent Studies

PhD theses completed.

- Chen, Xi. (Chemistry) "The Application of Variational Transition State Theory in Combustion Related Reactions". Successfully defended 19.September.2019.
- Fuller, Mark E. (School of Engineering, Chemical Engineering Group) "Design and Construction of a Shock Tube Facility for Investigations of Nitrogenated Fuel Additives". Successfully defended 01.May.2019.
- Danilack, Aaron D. (School of Engineering, Chemical Engineering Group) "Master Equation Methods in the Low-Temperature Oxidation of Oxygenated Fuels". Successfully defended on 16.July.2021

PhD theses supervised. All are in progress, titles are placeholders.

- Bae, Jongyoon. (School of Engineering, Chemical Engineering Group) "(TBD)". Beginning 5$^{\text{rd}}$ year of graduate study.
- Blöndal, Katrín. (School of Engineering, Chemical Engineering Group) "(TBD)". Beginning 5$^{\text{rd}}$ year of graduate study.
- Guzman, Eduardo. (School of Engineering, Chemical Engineering Group) "(TBD)". Beginning 3$^{\text{cd}}$ year of graduate study.
- Kim, Youbin. (School of Engineering, Chemical Engineering Group) "(TBD)". Beginning 2$^{\text{cd}}$ year of graduate study.
- Sharma, Siddha. (School of Engineering, Chemical Engineering Group) "(TBD)". Beginning 2$^{\text{cd}}$ year of graduate study.

Masters theses supervised, in progress.

- Caralp, Hervé. (School of Engineering, Chemical Engineering Group) "(TBD)'.

Masters theses supervised, completed.

- Tierney, Eric. (School of Engineering, Chemical Engineering Group) "Predictive kinetics for the combustion of Otto Fuel II". May, 2016.

Undergraduate honors theses supervised, completed.

- Nozik, Danna. (Chemical Engineering) "*in situ* detection of NO_2 in a shock tube". May, 2016.
- Rosenthal, Aaron. (Mechanical Engineering) "Design of a diaphragm less, high-repetition rate shock tube". May, 2016.
- James, Solon. (Chemical Engineering) "TBD'. April, 2021.

6.2 Academic Advising

- Postdoctoral advisor for 4 postdocs:
  - Dr. Christopher Almodovar: 2019.08.01 -
  - Dr. Mostafa Abedi: 2019.11.01 -
  - Dr. Rachel Schwind: 2020.02.01 -
- prior postdocs:
  - Dr. Avik Mahata: 2019.09.01 - 2021.02.01
  - Dr. Vitaly Kiselev: 2018.02.01 - 2019.10.15
  - Dr. Malte Döntgen: 2018.05.01 - 2019.06.01
  - Dr. Alireza Khorshidi: 2018.05.01 - 2018.11.01
  - Dr. Jiajue Chai: 2014.04.01 - 2016.03.31
- PhD advisor for five students, named above.
- Chemical Engineering Concentration Advisor, approximately 15 B.S. students.
- First-year advisor, approximately 6 students per year.
- Second-year advisor, approximately 7 students per year.
- Host for visiting scholars:
  - Bjarne Kreitz, Clausthal University, 2019 – 2020
  - Geyuan Yin, Jiaotong University, 2018 – 2020
  - Gregor Wehinger, Technical University of Berlin, July–Sept 2015
- External opponent for the PhD defense of Pierre Bhoorasingh, Northeastern University (R. West, advisor), June, 2016
- External opponent for the PhD defense of Gregor Wehinger, Technical University of Berlin (M. Kraume, advisor), July, 2016

- External opponent for the PhD defense of Bjarne Kreitz, Clausthal University (T. Turek, advisor), 2021