

## **Jonathan P. Mathews, Ph.D.**

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### **Professional Preparation**

The Nottingham Trent University, UK Applied Chemistry B.Sc. (Hons), 1991  
The Pennsylvania State University, Fuel Science Ph.D., 1998

### **Appointments**

April 2018 – Current Energy Engineering Undergraduate Program Chair  
July 2016 – Current Professor of Energy & Mineral Engineering, The Pennsylvania State University (tenured)  
July 2013 – June 2016 Associate Professor of Energy & Mineral Engineering, The Pennsylvania State University (tenured)  
July 2008 – June 2013 Assistant Professor of Energy & Mineral Engineering, The Pennsylvania State University (tenure track)  
July 2000 – June 2008 Assistant Professor of Energy & Geo-Environmental Engineering, The Pennsylvania State University  
June 1998 – June 2000, Research Associate, The Energy Institute & The Energy & Geo-Environmental Engineering Department, The Pennsylvania State University

### **Summary**

A coal scientist, ~80 peer-reviewed journal articles, 2 book chapters, 85 conference papers, graduated 5 Ph.D. and 7 M.S. students.

### **Graduate Advisors**

Alan W. Scaroni (retired), Pennsylvania State University & Patrick Hatcher (currently at Old Dominion).

### **Publications**

#### *Peer-reviewed journal articles*

1. Du, Y.; Wang, C.; Xin, H.; Mathews, J. P., Competitive or additive behavior for H<sub>2</sub>O and CO<sub>2</sub> gasification of coal char? Exploration via simplistic atomistic simulation. *Carbon* **2019**, 141, 226-237.
2. Zhong, Q.; Mao, Q.; Zhang, L.; Xiang, J.; Xiao, J.; Mathews, J. P., Structural features of Qingdao petroleum coke from HRTEM lattice fringes: Distributions of length, orientation, stacking, curvature, and a large-scale image-guided 3D atomistic representation. *Carbon* **2018**, 129, 790-802.
3. Zhong, Q.; Mao, Q.; Xiao, J.; van Duin, A.; Mathews, J. P., ReaxFF simulations of petroleum coke sulfur removal mechanisms during pyrolysis and combustion *Combustion and Flame* **2018**, 198, 146-157.
4. Zhong, Q.; Mao, Q.; Xiao, J.; van Duin, A.; Mathews, J. P., Sulfur removal from petroleum coke during high-temperature pyrolysis. analysis from TG-MS data and ReaxFF simulations. *Journal of Analytical and Applied Pyrolysis* **2018**, 132, 134-142.

5. Wang, C.; Huddle, T.; Huang, C.-H.; Zhu, W.; Vander Wal, R. L.; Lester, E.; Mathews, J. P., Improved quantification of curvature in high-resolution transmission electron microscopy lattice fringe micrographs of soots. *Carbon* **2017**, *117*, 174-181.
6. Song, Y.; Jiang, B.; Mathews, J. P.; Yan, G.; Li, F., Structural transformations and hydrocarbon generation of low-rank coal (vitrinite) during slow heating pyrolysis. *Fuel Processing Technology* **2017**, *167*, 535-544.
7. Mathews, J. P.; Campbell, Q. P.; Xu, H.; Halleck, P., Application of X-ray computed tomography to the study of coal *Fuel* **2017**, *209*, 10-24.
8. Coetzee, G. H.; Sakurovs, R.; Neomagus, H. W. J. P.; Everson, R.; Mathews, J. P.; Bunt, J. R., Particle size influence on the pore development of nanopores in coal gasification chars: from micron to millimeter particles. *Carbon* **2017**, *112*, 37-46.
9. Abrahamson, J. P.; Singh, M.; Mathews, J. P.; Vander Wal, R. L., Pulsed laser annealing of carbon black. *Carbon* **2017**, *124*, (Supplement C), 380-390.
10. Zhao, J.; Xu, H.; Tang, D.; Mathews, J. P.; Li, S.; Tao, S., A comparative evaluation of coal specific surface area by CO<sub>2</sub> and N<sub>2</sub> adsorption and its influence on CH<sub>4</sub> adsorption capacity at different pore sizes. *Fuel* **2016**, *183*, 420-431.
11. Zhao, J.; Xu, H.; Tang, D.; Mathews, J. P.; Li, S.; Tao, S., Coal seam porosity and fracture heterogeneity of macrolithotypes in the Hancheng Block, eastern margin, Ordos Basin, China. *International Journal of Coal Geology* **2016**, *159*, 18-29.
12. Xu, H.; Tang, D.; Mathews, J. P.; Zhao, J.; Li, B.; Tao, S.; Li, S., Evaluation of coal macrolithotypes distribution by geophysical logging data in the Hancheng Block, Eastern Margin, Ordos Basin, China. *International Journal of Coal Geology* **2016**, *165*, 265-277.
13. Xin, H.; Wang, C.; Louw, E.; Wang, D.; Mathews, J. P., Atomistic simulation of coal char isothermal oxy-fuel combustion: char reactivity and behavior. *Fuel* **2016**, *182*, 935-943.
14. Wang, C.; Huddle, T.; Lester, E. H.; Mathews, J. P., Quantifying curvature in HRTEM lattice fringe micrographs of coals. *Energy and Fuels* **2016**, *30*, 2694-2704.
15. Louw, E.; Mitchell, G. D.; Winans, R. E.; Mathews, J. P., Constitution of drop-tube generated coal chars from vitrinite-rich and inertinite-rich south African coals. *Energy & Fuels* **2016**, *30*, 112-120.
16. Huang, Y.; Cannon, F. S.; Guo, J.; Watson, J. K.; Mathews, J. P., Atomistic modeling insight into the structure of lignite-based activated carbon, and behavior of benzene sorption. *RSC Advances* **2016**, *6*, 56623-37.
17. Wang, C.; Watson, J. K.; Louw, E.; Mathews, J. P., A construction strategy for atomistic models of coal chars capturing stacking diversity and pore size distribution. *Energy Fuels* **2015**, *29*, 4814-4826.
18. Roberts, M. J.; Everson, R. C.; Neomagus, H. W. J. P.; Van Niekerk, D.; Mathews, J. P.; Branken, D. J., Influence of maceral composition on the structure, properties and behavior of chars derived from South African coals. *Fuel* **2015**, *142*, 9-20.
19. Roberts, M. J.; Everson, R. C.; Domazetis, G.; Neomagus, H. W. J. P.; Jones, J. M.; Van Sittert, C. G. C. E.; Okolo, G. N.; Niekerk, D. V.; Mathews, J. P., Density functional

- theory molecular modelling and experimental particle kinetics for CO<sub>2</sub>-char gasification. *Carbon* **2015**, 93, (0), 295-314.
20. Roberts, M. A.; Everson, R. C.; Neomagus, H. W. J. P.; Van Niekerk, D.; Okolo, G. N.; Mathews, J. P., The characterisation of slow-heated inertinite- and vitrinite-rich coals from the South African coalfields. *Fuel* **2015**, 158, 591-601.
  21. Okolo, G. N.; Neomagus, H. W. J. P.; Everson, R. C.; Roberts, M. J.; Bunt, J. R.; Sakurovs, R.; Mathews, J. P., Chemical-structural properties of South African bituminous coals: Insights from wide angle XRD-carbon fraction analysis, ATR-FTIR, solid state <sup>13</sup>C NMR, and HRTEM techniques. *Fuel* **2015**, 158, 779-792.
  22. Mathews, J. P.; Burgess-Clifford, C.; Painter, P. C., The interactions of Illinois No. 6 bituminous coal with solvents: a review of solvent swelling and extraction literature. *Energy Fuels* **2015**, 29, 1279-1294.
  23. Kumar, H.; Elsworth, D.; Mathews, J. P.; Marone, C., Permeability evolution in sorbing media: analogies between organic-rich shale and coal. *Geofluids* **2015**, 133, 695-704.
  24. Kumar, H.; Elsworth, D.; Mathews, J. P., Permeability evolution of propped artificial fractures in coals on injection of CO<sub>2</sub>. *Journal of Petroleum Science and Engineering* **2015**, 133, 695-704.
  25. Huang, Y.; Cannon, F. S.; Watson, J. K.; Reznik, B.; Mathews, J. P., Activated carbon efficient atomistic model construction that depicts experimentally-determined characteristics. *Carbon* **2015**, 83, 1-14.
  26. Coetzee, S.; Neomagus, H. W. J. P.; Bunt, J. R.; Mathews, J. P.; Strydom, C. A.; Schobert, H. H., Reduction of caking propensity in large (mm sized) South African coal particles with potassium carbonate impregnation to expand fixed and fluidised bed gasification feedstock suitability. *Energy & Fuels* **2015**, 29, (7), 4255-4263.
  27. Coetzee, G. H.; Sakurovs, R.; Neomagus, H. W. J. P.; Morpeth, L.; Everson, R.; Mathews, J. P.; Bunt, J. R., Pore development during gasification of South African inertinite-rich chars evaluated using small angle X-ray scattering. *Carbon* **2015**, 95, 250-260.
  28. Tselev, A.; Ivanov, I. N.; Lavrik, N. V.; Belianinov, A.; Jesse, S.; Mathews, J. P.; Mitchell, G. D.; Kalinin, S. V., Mapping internal structure of coal by confocal micro-Raman spectroscopy and scanning microwave microscopy. *Fuel* **2014**, 126, (15), 32-37.
  29. Mathews, J. P.; Krishnamoorthy, V.; Louw, E.; Tchapda, A. H. N.; Castro-Marcano, F.; Karri, V.; Alexis, D. A.; Mitchell, G. D., A review of correlations of coal properties with elemental composition. *Fuel Processing Technology* **2014**, 121, 104-113.
  30. Kumar, H.; Elsworth, D.; Mathews, J. P.; Liu, J.; Pone, D., Effect of CO<sub>2</sub> injection on heterogeneously permeable coalbed reservoirs. *Fuel* **2014**, 135, 509-521.
  31. Collins, L.; Tselev, A.; Jesse, S.; Okatan, M. B.; Proksch, R.; Mathews, J. P.; Mitchell, G. D.; Rodriguez, B. J.; Kalinin, S. V.; Ivanov, I. N., Breaking the limits of structural and mechanical imaging of the heterogeneous structure of coal macerals. *Nanotechnology* **2014**, 25, (43), 435402.

32. Castro-Marcano, F.; Russo, M. F.; van Duin, A. C. T.; Mathews, J. P., Pyrolysis of a large-scale molecular model of Illinois No. 6 coal using the ReaxFF reactive force field. *Journal of Analytical and Applied Pyrolysis* **2014**, 109, 79-89.
33. Cai, Y.; Liu, D.; Mathews, J. P.; Pan, Z.; Elsworth, D.; Yao, Y.; Li, J.; Guo, X., Permeability evolution in fractured coal - combining triaxial confinement with X-ray computed tomography, acoustic emission and ultrasonic techniques. *International Journal of Coal Geology* **2014**, 122, 91-104.
34. Binner, E.; Lester, E.; Kingman, S.; Dodds, C.; Robinson, J.; Wu, T.; Wardle, P.; Mathews, J. P., A review of microwave coal processing. *Journal of Microwave Power and Electromagnetic Energy* **2014**, 48, (1), 35-60.
35. Mathews, J. P.; Miller, B. G.; Song, C.; Schobert, H. H.; Botha, F.; Finkelman, R. B., The ebb and flow of U.S. coal research 1970-2010 with a focus on academic institutions. *Fuel* **2013**, 105, 1-12.
36. Hattingh, B. B.; Everson, R. C.; Neomagus, H. W. J. P.; Bunt, J. R.; Van Niekerk, D.; Jordaan, J. H. L.; Mathews, J. P., Elucidation of the structural and molecular properties of typical South African coals. *Energy and Fuels* **2013**, 27, 3161-3172.
37. Alvarez, Y. E.; Moreno, B. M.; Klein, M. T.; Watson, J. K.; Castro-Marcano, F.; Mathews, J. P., A novel simplification approach for large-scale structural models of coal: 3D molecules to 2D lattices. 3. Reactive lattice simulations. *Energy and Fuels* **2013**, 27, 2915-2922.
38. Tolliver, R. L.; Mathews, J. P., Reviews of science for science librarians: coal science and technology research 1970-2010. *Science & Technology Libraries* **2012**, 31, 146-163.
39. Pulati, N.; Sobkowiak, M.; Mathews, J. P.; Painter, P., Low temperature treatment of Illinois No. 6 coal in ionic liquids. *Energy & Fuels* **2012**, 26, 3548-3552.
40. Pou, J. O.; Alvarez, Y. E.; Watson, J. K.; Pisupati, S.; Mathews, J. P., Co-primary thermolysis molecular modeling simulation of lignin and subbituminous coal via a reactive coarse-grained simplification. *Journal of Analytical and Applied Pyrolysis* **2012**, 95, 101-111.
41. Mathews, J. P.; Sharma, A., The structural alignment of coals and the analogous case of Argonne Upper Freeport *Fuel* **2012**, 95, 19-24.
42. Mathews, J. P.; Chaffee, A., The molecular representations of coal — a review. *Fuel* **2012**, 96, 1-14.
43. Kumar, H.; Elsworth, D.; Mathews, J. P.; Lui, J.; Pone, D., Optimizing enhanced coalbed methane recovery for unhindered production and CO<sub>2</sub> injectivity. *International Journal of Greenhouse Gas Control* **2012**, 11, 86-97.
44. Castro-Marcano, F.; Winans, R. E.; Chupas, P.; Chapman, K.; Calo, J. M.; Watson, J. K.; Mathews, J. P., Fine structure evaluation of the pair distribution function with molecular models of the Argonne Premium coals. *Energy & Fuels* **2012**, 26, 4336-4345.
45. Castro-Marcano, F.; Lobodin, V. V.; Rodgers, R. P.; McKenna, A. M.; Marshall, A. G.; Mathews, J. P., A molecular model for the Illinois no. 6 Argonne Premium coal: moving towards capturing the continuum structure. *Fuel* **2012**, 95, 35-49.
46. Castro-Marcano, F.; Kamat, A. M.; Russo, M. F.; van Duin, A.; Mathews, J. P., Combustion of an Illinois No. 6 coal char simulated using an atomistic char

- representation and the ReaxFF reactive force field. *Combustion and Flame* **2012**, 159, 1272-1285.
47. Alvarez, Y. E.; Watson, J. K.; Pou, J. O.; Mathews, J. P., A novel simplification approach for large-scale structural models of coal: 3D molecules to 2D lattices. 2. Visualization capabilities. *Energy & Fuels* **2012**, 26, 4946-4952.
  48. Alvarez, Y. E.; Watson, J. K.; Mathews, J. P., A novel simplification approach for large-scale structural models of coal: 3D molecules to 2D lattices. 1. Lattice creation. *Energy & Fuels* **2012**, 26, 4938-4945.
  49. Van Niekerk, D.; Mathews, J. P., Molecular dynamics simulation of coal-solvent interactions in Permian-aged South African coals. *Fuel Processing Technology* **2011**, 92, (4), 729-734.
  50. Van Niekerk, D.; Castro-Marcano, F.; Colina, C. M.; Mathews, J. P., Solvent swelling extent of Permian aged vitrinite- and inertinite-rich coals: experiments and modeling using perturbed-chain statistical associating fluid theory (PC-SAFT). *Energy & Fuels* **2011**, 25, (6), 2559-2564.
  51. Mathews, J. P.; van Duin, A.; Chaffee, A., The utility of coal molecular models. *Fuel Processing Technology* **2011**, 92, (4), 718-728.
  52. Mathews, J. P.; Pone, J. D. N.; Mitchell, G. D.; Halleck, P., High-resolution X-ray computed tomography observations of the thermal drying of lump-sized subbituminous coal. *Fuel Processing Technology* **2011**, 92, (1), 58-64.
  53. Kumar, H.; Lester, E.; Kingman, S.; Avila, C.; Jones, A.; Robinson, J.; Halleck, P. M.; Mathews, J. P., Inducing fractures and increasing cleat apertures in bituminous coal under isostatic stress via application of microwave energy. *International Journal of Coal Geology* **2011**, 88, (1), 75-82.
  54. Fernandez-Alos, V.; Watson, J. K.; vander Wal, R.; Mathews, J. P., Soot and char molecular representations generated directly from HRTEM lattice fringe images using Fringe3D. *Combustion and Flame* **2011**, 158, (9), 1807-1813.
  55. Castro-Marcano, F.; Mathews, J. P., Constitution of Illinois No. 6 Argonne Premium coal: a review. *Energy & Fuels* **2011**, 25, (3), 845-853.
  56. Van Niekerk, D.; Mitchell, G. D.; Mathews, J. P., Petrographic and reflectance analysis of solvent-swelled and solvent-extracted South African vitrinite-rich and inertinite-rich coals. *International Journal of Coal Geology* **2010**, 81, (1), 45-52.
  57. Van Niekerk, D.; Mathews, J. P., Simulation of solvent extraction of South African vitrinite-rich and inertinite-rich coals. *Energy & Fuels* **2010**, 24, (12), 6393-6399.
  58. Van Niekerk, D.; Mathews, J. P., Molecular representations of vitrinite-rich and inertinite-rich Permian aged South African coals. *Fuel* **2010**, 89, (1), 73-82.
  59. Van Niekerk, D.; Halleck, P.; Mathews, J. P., Solvent swelling behavior of Permian-aged South African vitrinite-rich and inertinite-rich coals. *Fuel* **2010**, 89, (1), 19-25.
  60. Pone, J. D. N.; Halleck, P. M.; Mathews, J. P., 3D characterization of strains in coal induced by compression, carbon dioxide sorption, and desorption at in situ stress conditions. *International Journal of Coal Geology* **2010**, 82, (3-4), 262-268.
  61. Painter, P.; Pulati, N.; Cetiner, R.; Sobkowiak, M.; Mitchell, G.; Mathews, J., Dissolution and dispersion of coal in ionic liquids. *Energy & Fuels* **2010**, 24, (3), 1848-1853.

62. Painter, P.; Cetiner, R.; Pulati, N.; Sobkowiak, M.; Mathews, J. P., The dispersion of liquefaction catalysts in coal in ionic liquids. *Energy & Fuels* **2010**, *24*, (5), 3086-3092.
63. Mathews, J. P.; Ferdandez-Alos, V.; Jones, D. A.; Schobert, H. H., Determining the molecular weight distribution of Pocahontas No. 3 low-volatile bituminous coal utilizing HRTEM and laser desorption ionization mass spectra data. *Fuel* **2010**, *89*, (7), 1461-1469.
64. Tambach, T. J.; Mathews, J. P.; van Bergen, F., Molecular exchange of CH<sub>4</sub> and CO<sub>2</sub> in coal: enhanced coalbed methane on a nanoscale. *Energy & Fuels* **2009**, *23*, (10), 4845-4847.
65. Sarunac, N.; Ness, M.; Bullinger, C.; Mathews, J. P.; Halleck, P., A novel fluidized bed drying and density segregation process for upgrading low-rank coals. *International Journal of Coal Preparation and Utilization* **2009**, *29*, (6), 317-332.
66. Pone, J. D. N.; Hile, M.; Halleck, P. M.; Mathews, J. P., Three-dimensional carbon dioxide-induced strain distribution within a confined bituminous coal. *International Journal of Coal Geology* **2009**, *77*, (1-2), 103-108.
67. Pone, J. D. N.; Halleck, P. M.; Mathews, J. P., Sorption capacity and sorption kinetic measurements of CO<sub>2</sub> and CH<sub>4</sub> in confined and unconfined bituminous coal. *Energy & Fuels* **2009**, *23*, (9), 4688-4695.
68. Narkiewicz, M. R.; Mathews, J. P., Visual representations of carbon dioxide adsorption in a low-volatile bituminous coal molecular model. *Energy & Fuels* **2009**, *23*, (10), 5326-5246.
69. Hsu, Y.-C.; Ching, Y.-H.; Mathews, J. P.; Carr-Chellman, A., Undergraduate students' self-regulated learning experience in a web-based learning environment. *Quarterly Review of Distance Education* **2009**, *10*, (2), 109-121.
70. Van Niekerk, D.; Pugmire, R. J.; Solum, M. S.; Painter, P.; Mathews, J. P., Structural characterization of vitrinite-rich and interinite-rich Permian aged South African coals. *International Journal of Coal Geology* **2008**, *76*, 290-300.
71. Narkiewicz, M. R.; Mathews, J. P., Improved low-volatile bituminous coal representation: incorporating the molecular weight distribution. *Energy & Fuels* **2008**, *22*, (5), 3104-3111.
72. Mathews, J. P.; Eser, S.; Hatcher, P. G.; Scaroni, A. W., The shape of pulverized bituminous vitrinite coal particles. *KONA Powder and Particle* **2007**, *25*, 145-152.
73. Painter, P. C.; Sobkowiak, M.; Mathews, J. P.; Scaroni, A., Concerning the nature of coal solutions and suspensions. *Energy & Fuels* **2004**, *18*, (4), 1104-1107.
74. Groenzin, H.; Mullins, O. C.; Eser, S.; Mathews, J. P.; Yang, M. G.; Jones, A. D., Molecular size of asphaltene solubility fractions. *Energy & Fuels* **2003**, *17*, (2), 498-503.
75. Mathews, J. P.; Hatcher, P. G.; Scaroni, A. W., Proposed model structures for Upper Freeport and Lewiston-Stockton vitrinites. *Energy & Fuels* **2001**, *15*, (4), 863-873.
76. Acharya, M.; Strano, M. S.; Mathews, J. P.; Billinge, J. L.; Petkov, V.; Subramoney, S.; Foley, H. C., Simulation of nanoporous carbons: a chemically constrained structure. *Philosophical Magazine B-Physics of Condensed Matter Statistical Mechanics Electronic Optical and Magnetic Properties* **1999**, *79*, (10), 1499-1518.

77. Mathews, J. P.; Hatcher, P. G.; Scaroni, A. W., Particle size dependency of volatile matter: Is there a non-maceral related effect? *Fuel* **1997**, 76, (4), 359-362.
78. Faulon, J.-L.; Mathews, J. P.; Carlson, G. A.; Hatcher, P. G., Correlation between micropore and fractal dimension of bituminous coal based on computer generated models. *Energy & Fuels* **1994**, 8, (2), 408-415.

#### *Book Chapters*

2. Rempel, J.; Halverson, J.; Burket, C.; Strano, M. S.; Mathews, J. P.; Foley, H. C., Structural Modeling of Nanoporous Carbon: A Review of Approaches to Simulating an Aperiodic and Non-Equilibrium Solid. In *From Semiconductors to Proteins: Beyond the Average Structure, a Volume in the Fundamental Materials Research Series*, Thorpe, M. W.; Billinge, S. J., Eds. Kluwer, New York: 2001.
1. Hatcher, P. G.; Faulon, J.-L.; Clifford, D. J.; Mathews, J. P., A Three-dimensional Structural model for Humic Acids from Oxidized soil. In *Humic Substances in the Global Environment and Implications on Human Health*, Senesi, N.; Miano, T. M., Eds. Elsevier Science B. V.: 1994; pp 133-138.

#### *Conference Papers (technical, not peer reviewed)*

74. Zhu, W.; Wang, C.; Vander Wal, R.; Mathews, J. P., A 2D fingerprinting approach for structural visualization of complex 3D soot atomistic representations. In *The World Conference on Carbon*, State College, PA, 2016; pp 1-3.
73. Xin, H.; Huang, C.-H.; Mathews, J. P., An exploration of char reactivity capturing temperature effects within a simplistic but large-scale atomistic simulation. In *The World Conference on Carbon*, State College, PA, 2016; pp 1-3.
72. Wang, C.; T., H.; Huang, C.-H.; Vander Wal, R. L.; Lester, E.; Mathews, J. P., Improved curvature analysis for HRTEM lattice fringes applied to soot. In *The World Conference on Carbon*, State College, PA, 2016; pp 1-4.
71. Thanasattayaviboon, B.; Mathews, J. P., Porosity and morphology transformations of Pittsburgh no. 8 coal char in CO<sub>2</sub> gasification under pore diffusion limitation. In *The World Conference on Carbon*, State College, PA, 2016; pp 1-4.
70. Huang, Y.; Cannon, F. S.; Gao, J.; Watson, J. K.; Mathews, J. P., Atomistic modeling insight into the structure of lignite-based activated carbon, and behavior of benzene sorption. In *The World Conference on Carbon*, State College, PA, 2016.
69. Xin, H. H.; Wang, C.; Wang, D.; Mathews, J. P., Examination of changing char reactivity with isothermal oxy-fuel combustion by a simplified atomistic simulation. In *International Pittsburgh Coal Conference*, Pittsburgh, USA, 2015; pp 1-7.
68. Xin, H. H.; Wang, C.; Wang, D.; Mathews, J. P., Simplified atomistic simulation of coal char oxy-combustion: sensitivity analysis for reaction distance and factors influencing oxygen penetration. In *International Conference on Coal Science and Technology*, Melbourne, Australia, 2015; pp 1-4.
67. Xin, H.; Wang, C.; Louw, E.; Watson, J. K.; Mathews, J. P. In *Coal char atomistic exploration of oxy-combustion reactivity*, 8th International Conference on Coal Combustion, Beijing, China, 2015; Beijing, China, 2015; pp 1-3.
66. Mathews, J. P.; Huddle, T.; Wang, C.; Lester, E., Quantifying curvature in coal HRTEM lattice fringe micrographs. In *International Conference on Coal Science and Technology*, Melbourne, Australia, 2015.

65. Mathews, J. P. In *Plenary Lecture and paper: The structure and behavior of coals and chars via atomistic simulations of pyrolysis and combustion*, 8th International Conference on Coal Combustion, Beijing, China, 2015; Beijing, China, 2015; pp 1-5.
64. Winans, R. E.; Seifert, S.; Calo, M. J.; Mathews, J. P.; Gilbert, K.; Wang, J.; Lock, D., Characterization of coal porosity and gas-solid interfaces by SAXS. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013; pp 889-895.
63. Roberts, M. J.; Everson, R. C.; Neomagus, H. W. J. P.; Van Sitter, C. G. C. E.; Van Niekerk, D.; Mathews, J. P., The molecular structure of selected South African coal-chars to elucidate fundamental principles of the reaction between char and carbon dioxide. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013; pp 91-103.
62. Ramachandran, V.; Castro-Marcano, F.; Van Niekerk, D.; Ferdandez-Alos, V.; Alvares Rojas, Y. E.; Pou, J. O.; Watson, J. K.; Mathews, J. P., Construction, structural evaluation, and exploring chemical transformations of coal molecular models using scripting. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013; pp 1015-1026.
61. Mitchell, G. D.; Mathews, J. P., Penn State's Coal Repository: Penn State and Argonne Premium Coal Sample Bank & Database. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013; pp 1122-1132.
60. Mathews, J. P.; Ramachandran, V.; Castro-Marcano, F.; Van Duin, A. C. T.; Anderson, K. B., Exploring oxidative hydrolysis dissolution (OHD) reaction chemistry of Illinois no. 6 coal with molecular modeling approaches. In *Clearwater Clean Coal Conference*, Clearwater, FL, 2013; Vol. 1, pp 936-945.
59. Louw, E.; Watson, J. K.; Mathews, J. P., Evaluating combustion reactivity of large-scale molecular coal char models with control over structural features. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013; pp 569-576.
58. Louw, E.; Watson, J. K.; Mathews, J. P., An alternate construction approach for large-scale atomistic representations of carbon with controls over structural diversity and orientation. In *Annual World Conference on Carbon*, Rio De Janeiro, Brazil, 2013; pp 1-2.
57. Kumar, H.; Elsworth, D.; Mathews, J. P., Evaluation of the role of coal softening on permeability for a sand propped fracture. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013; pp 1485-1491.
56. Campbell, Q. P.; Viljoen, J.; le Roux, M.; Mathews, J. P., Following coal processes using micro focus X-ray computed tomography. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013; pp 881-888.
55. Mathews, J. P.; Winans, R. E.; Rodgers, R.; Sharma, A., Advances in coal analysis and simulation 1989-2012. In *International Pittsburgh Coal Conference*, Pittsburgh, PA, USA, 2012; pp 1-11.
54. Mathews, J. P.; Song, C.; Finkelman R., B.; Yue, W., Chinese coal-in-title journal articles in Chinese and English. In *International Pittsburgh Coal Conference*, Pittsburgh, PA, USA, 2012; pp 1-15.
53. Kumar, H.; Elsworth, D.; Mathews, J. P.; Liu, J.; Pone, D., The dynamic permeability of propped and non-propped artificial fracture in granite and bituminous coal with



- changes in effective stress. In *International Pittsburgh Coal Conference*, Pittsburgh, PA, USA, 2012; pp 1-9.
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- molecular "slice" models of the Argonne Premium coals. In *International Pittsburgh Coal Conference*, Pittsburgh, PA, 2011.
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25. Van Niekerk, D.; Mathews, J. P., Solvent swelling of similar rank South African vitrinite-rich and inertinite-rich coals: swelling extent and maceral influences. In *International Conference on Coal Science and Technology*, The University of Nottingham, England, 28-31 August, 2007.
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4. Mathews, J. P.; Hatcher, P. G.; Scaroni, A. W., Influence of chemical structure on the fluidity of rapidly heated bituminous vitrinites. In *Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem.*, San Francisco, April 13-17, 1997; Vol. 42, pp 214-217.
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11. Pisupati, S.; Mathews, J. P. In *Differences in teaching and learning outcomes in face-to-face, online, and hybrid modes of energy conservation course*, American Society for Engineering Education Annual Conference, Pittsburgh, PA, 2008; Pittsburgh, PA, 2008.
10. Mathews, J. P.; Wherley, M.; Spielvogel, E. In *Reaching the masses, web enabled redesign of "Energy & the Environment" general education class*, Prepr. Pap.-Am. Chem. Soc., Div. Pet. Chem., New Orleans, LA, 2008; New Orleans, LA, 2008.
9. Eser, S.; Mathews, J. P.; Bridger, J. C. In *Integrating general education courses in natural science and social science using a common thread, for example Pennsylvania coal*, Prepr. Pap.-Am. Chem. Soc., Div. Pet. Chem., New Orleans, LA, 2008; New Orleans, LA, 2008.
8. Mathews, J. P.; DiBiase, D. In *Institutional Perspective on Online Education at Penn State*, International Conference on Education and Information Systems, Technologies and applications: EISTA '06, Orlando, FL, 2006; Howell, P. R., Ed. Orlando, FL, 2006; pp 29-32.
7. Howell, P. R.; Mathews, J. P.; Pisupati, S.; Babb, D.; Locklin, R. H. In *Designing on-line general education, natural science courses, in the College of Earth and Mineral Sciences (EMS), at the Pennsylvania State University*, The 4th International Conference on Education and Information Systems, Technologies and Applications: EISTA '06, Orlando, Florida, July 20-23, 2006; Orlando, Florida, July 20-23, 2006; pp 12-17.
6. Morales, D. R.; Mathews, J. P. In *Success in online learning: Does faculty intercession via e-mail message alter student procrastination behavior and enhance learning?*, American Society for Engineering Education Annual Conference, June 12-15, Portland, OR, 2005; Portland, OR, 2005.
5. Mathews, J. P.; Wiesner, A.; Pisupati, S. V. In *What online quizzing can tell us about our students*, American Society for Engineering Education Annual Conference, June 12-15, Portland, OR, 2005; Portland, OR, 2005.
4. Pisupati, S.; Mathews, J. P.; DiBiase, D.; Scaroni, A. W., An assessment of active and project based learning in energy conservation education for non-technical students. In *Proceedings of the 2004 ASEE Annual Conference & Exposition*, 2004.
3. Mathews, J. P.; Haughton, N. A.; DiBiase, D.; Pisupati, S. In *For an online course encompassing "traditional students": How, where, and when students work and engage with the course material*, Frontiers in Education Conference, Savannah, Georgia, 2004; Savannah, Georgia, 2004; pp 1-5.
2. Pisupati, S.; Mathews, J. P.; Scaroni, A. W. In *Energy conservation education for non-engineering students and effectiveness of active learning components*, American Society for Engineering Education Annual Conference, Nashville, TN, 2003; Nashville, TN, 2003.
1. Mathews, J. P.; Spielvogel, E.; Wherley, M.; DiBiase, D.; Pisupati, S. In *Online teaching of "Energy & the Environment"*, American Society for Engineering Education Annual Conference, Nashville, TN, 2003; Nashville, TN, 2003.

#### *Ph.D Thesis Supervised*

5. Kumar, H. Poromechanical response of naturally fractured sorbing media. Ph.D. thesis, The Pennsylvania State University, 2014.\*
4. Louw, E. Structure and combustion reactivity of inertinite-rich and vitrinite-rich South African coal chars: quantification of the structural factors contributing to reactivity differences. Ph.D., The Pennsylvania State University, 2013.

3. Castro-Marcano, F. Improved generation of large-scale atomistic representations and pyrolysis/combustion simulations of Illinois coal and char using the ReaxFF reactive force field. The Pennsylvania State University, 2012.
  2. Pone, J. D. N. Carbon dioxide sequestration in coal: characterization of matrix deformation, sorption capacity and dynamic permeability at in-situ stress conditions. Ph.D., The Pennsylvania State University, 2009.\*
  1. Van Niekerk, D. Structural elucidation, molecular representation and solvent interactions of vitrinite-rich and inertinite-rich South African coals. The Pennsylvania State University, 2008.
- \* co-advised student

#### *MS Thesis Supervised*

7. Thanasattayaviboon, B. Porosity, morphology, and structural transformation of bituminous coal char conversion under pore diffusion limitation: A comparison of CO<sub>2</sub> gasification conversion and burnout in oxy-fuel combustion. The Pennsylvania State University, 2016.
6. Pool, S. A preliminary natural gas resource assessment of the Marcellus Shale for West Virginia using basic geologic data and GIS. Masters of Geographic Information Systems, The Pennsylvania State University, 2013.
5. Cetiner, R. Fragmentation of coal and improved dispersion of liquefaction catalysts using ionic liquids. The Pennsylvania State University, 2011.
4. Alvarez, Y. E. Development of a reactive coarse-graining approach for the utility enhancement of complex large-scale molecular models of coal. The Pennsylvania State University, State College, PA, 2011.
3. Kumar, H. Inducing fractures and cleat aperture enhancement in bituminous coal via the application of microwave energy applied under hydrostatic stress conditions. MS thesis, The Pennsylvania State University, 2010.
2. Hile, M. CO<sub>2</sub> sorption by Pittsburgh-seam coal subjected to confining pressure. MS thesis, The Pennsylvania State University, University Park, 2006.
1. Narkiewicz, M. R. Carbon dioxide sequestration in low-volatile bituminous coal molecular representations. MS, The Pennsylvania State University, 2005.

#### **Awards**

American Chemical Society Fellow, inducted 2016  
 Outstanding Service, Energy and Fuels Technical Division, American Chemical Society 2016  
 Honorable mention for Best Paper Pittsburgh Coal Conf. 2012  
 2011 Best Poster (supervising Enette Louw), and honorable mention Best Paper (supervising Fidel Castro-Marcano) International Pittsburgh Coal Conference, Pittsburgh  
 EMS Energy Institute Research Productivity Award (2010)  
 Wilson Award for Outstanding Teaching (2006)  
 Best Papers within the ECCD symposium co-author (ASEE-2004)  
 Best Overall use of ANGEL Prize (ANGEL DAY II – 2004)  
 John A. Dutton e-Education Fellowship (2003, 2004, & 2006, 2007)  
 Mitchell Award for Innovative Teaching (2001)  
 Recipient 1999 award for Employee Dedication (Energy Institute)  
 Recipient 1998 C. C. Wright Award, (Excellence in Graduate Studies)

Twice (1994 & 1996) the recipient of the annual Outstanding Service Award for the Energy & Fuels Research Center

### **Plenary, Keynotes, and Invited Presentations**

Mathews, J. P., **Invited Keynote**: Large-scale atomistic evaluations of coal char reactivity in oxygen: Following porosity and pore size development. In *IST International Workshop on Oxy-fuel Combustion*, Montabaur, Germany, 2015

Xin, H.; Wang, C.; Louw, E.; Watson, J. K.; Mathews, J. P. *Coal char atomistic exploration of oxy-combustion reactivity*, **Invited Plenary** at the 8th International Conference on Coal Combustion, Beijing, China, 2015; Beijing, China, 2015

Mathews, J. P., **Invited presentation**: Coal Structure and Behaviors a Mixture of Approaches. In *Pennsylvania Coal Ash Research Group*, Penn State, 2015

Mathews, J. P., **Invited presentation**: "Meaningful Student Feedback". *eConversations*, Dutton Education Institute, the Pennsylvania State University 2014,

Mathews, J. P., **Invited presentation**: "Quantifying, incorporating, and using structural diversity within coal". *Canadian Centre for Clean Coal/Carbon and Mineral Processing Technologies*, University of Alberta, Canada 2014

Mathews, J. P., **Invited presentation**: Coal structure molecular models and their utility. In *Thermochemical Conversion Workshop*, University of Delaware, 2013.

Mathews, J. P., **Invited presentation**: Advancing the creation of large-scale coal and coal-char atomistic representations. In *EMS Energy Institute Energy Exchange*, The Pennsylvania State University, PA, USA, 2013

Mathews, J. P., **Plenary**: One hundred things you did not know about coal. In *International Conference on Coal Science & Technology*, The Pennsylvania State University, PA, USA, 2013. (note self-invited when speaker was unable to attend).

Mathews, J. P., **Invited presentation**: The Walker Memorial: Coal research benefits from carbon science: repaying the favor with transferable coal/char molecular modeling advances In *Annual World Conference on Carbon*, Rio de Janeiro, Brazil, 2013

Tuana, N., (Moderator), Becker, C.; Maruszewski, S.; Mathews, J. P.; Monahan, R.; Moser, P.; Richard, T., **Roundtable discussion**: Penn State's Energy Future. *Berg Auditorium, Life Sciences, University Park*, 2009, Sponsored by Rock Ethics, Office of Physical Plant, and PSIEE.

Richards, T.; Santavavicca, D.; Mathews, J. P.; Grimes, C., **Briefing of Congressional Aids**: CO<sub>2</sub> can it fuel a nation? *Capital Building Complex, Longworth building, Washington D.C.* **2009**.

Mathews, J. P.; van Duin, A.; Chaffee, A., **Keynote**: The utility of coal molecular models. In *International Conference on Coal Science & Technology*, Cape Town, South Africa, 2009

Mathews, J. P., **Invited presentation:** Coal past and future. *Shennango Campus, Honors Society 2009*.

Mathews, J. P., **Invited presentation:** Carbon dioxide sequestration in coal: molecular modeling and X-ray computed tomography observations. *Colorado School of Mines, Golden, CO 2009*.

Mathews, J. P., **Presentation at Sponsor Meeting:** Microwave-induced fractures in coal. *Research Partnership for a Secure Energy for America, Golden, CO 2009*.

Mathews, J. P., **Invited presentation:** 50 things you didn't know about coal. *Westmoreland Museum of American Art, Greensburg, PA 2009*.

Mathews, J. P., **Invited presentation:** Application of high-resolution X-ray computed tomography to coal. *Coal Research Group, North-West University: Potchefstroom, 2009*.

Mathews, J. P., **Invited presentation:** Coal molecular modeling, moving forward with large-scale modeling. *Gordon Conference on Hydrocarbon Resources 2009*, Ventura, California.

Mathews, J. P., **Invited presentation:** The legacy of coal and its art. *Sponsored by EMS museum and Art Gallery and The Centre County Historical Society 2009*, Match Factory Place, Bellefonte, PA



## Past Funding

Title	Sponsor	Start	Finish	Value	Role
University/NETL Student Partnership	University of Pittsburgh	2001	2004	\$140,000	co-PI
Use of Molecular Modeling to Determine the Interaction and Competition of Gases Within Coal for Carbon Dioxide Sequestration	Duquesne University	2001	2002	\$28,908	PI
Use of Molecular Modeling to Determine the Interaction and Competition of Gases Within Coal for Carbon Dioxide Sequestration	Duquesne University	2002	2006	\$100,000	PI
MOA supporting Visiting Scientist and Grad Student Research and Training	SASOL	2005	2009	\$95,535	PI
Supporting FOR Visiting Scientist and Grad Student Research and Training	SASOL	2005	2010	\$101,062	PI
Scanning and Imaging Analysis Services	Great River Energy	2006	2007	\$11,826	PI
Coal-Solvent Interactions Under Non-cracking Conditions	Chevron	2008	2010	\$974,112	Associate
Coal Drying	Chevron	2008	2009	\$63,979	PI
Coal Collection, Preparation & Storage	Chevron	2008	2008	\$48,600	PI
Coal Model Representation Creation & Use	Chevron	2008	2010	378,771	PI
Coal Characterization	Chevron	2008	2009	\$104,835	PI
Enhancing Coalbed Methane Extraction with Microwave Induced Fractures	RPSEA	2008	2010	\$50,699	PI
Development and Validation of a Char-Slag Interaction Model for Entrained Coal	Industrial	2010	2010	\$48,902	co-PI
Large-Scale Coal Model Generation and Pyrolysis/Liquefaction Simulations	Southern Illinois University, Carbondale	2010	2011	\$160,000	PI
Modeling CO <sub>2</sub> Sequestration in CBM Reservoirs	ConocoPhillips	2010	2011	\$175,724	co-PI
Literature Survey Assessing the State of Coal Chemistry R&D in 2010	Southern Illinois University, Carbondale	2010	2012	\$60,000	PI
ARRA: Geothermal Energy Technologies Education Through Research	AIDI Analytics LLC	2010	2013	\$50,000	PI
ARRA: Geothermal Energy Technologies Education Through Research	AIDI Analytics LLC	2010	2013	\$20,541	PI
Hybrid Reactive Lattice/ReaxFF Evaluation of OHD Process for Illinois Coal	Southern Illinois University, Carbondale	2012	2013	\$125,000	PI
Retaining and Expanding Illinois No. 6 Coals in the Penn State & Argonne Premium Coal Sample Bank and Database	Southern Illinois University, Carbondale	2014	2015	\$24,707	co-PI

Note departmental funding is also obtained via summer teaching. Sasol awards did not include tuition or student stipends that were paid directly from Sasol.

### **Reviewer**

Energy & Fuels, Fuel, International Journal of Coal Geology, Fuel Processing Technology, Journal of Applied and Analytical Pyrolysis, Carbon, Chemical Engineering Science, Molecular Physics, and others. Currently review ~25 articles per year.

### **Professional Societies and Service Positions**

Member of the Guest Editor team for two special issues of Fuel  
Advisory Board Energy & Fuels, American Chemical Society journal, (2016-current)  
Chair 2013 International Conference on Coal Science and Technology (held at the Penn State Conference Center)  
The U.S. representative on the International Organizing Committee of the International Coal Science and Technology Conference (2011-current)  
Chair (co-chair) Division of Energy and Fuels, 2012 American Chemical Society  
Chair for Fuel Chemistry, 2012 American Chemical Society  
Member of the Divisions of Petroleum, Chemical Education, & Fuel Chemistry (Petroleum and Fuel is now merged into the division of Energy and Fuels) American Chemical Society  
Membership for Fuel Chemistry, Pre-print Subscriptions 2011 American Chemical Society  
Member of the American Society of Engineering Educators  
External Reviewer for Engineering Evaluation, University of the North West, South Africa 2012  
External thesis reviewer for Universities in South Africa (multiple) and Australia (several).

### **University Service**

Faculty Senate (2018-current)  
Conflict of Interest Committee member (2016-current)  
Penn State Representative to the Coal Utilization Research Council (2015-current)  
Graduate Fellowships and Awards Committee (2014-2017)

### **College Service**

Member Ad-Hoc Committee on the Status of Female Faculty (2016)  
Member Associate Dean Search Committee (2016)  
Chair of the EMS Museum Advising Committee (2008-2012)  
Secretary EMS Museum Advising Committee (2005-2008)  
Chair of the Fixed-Term & Research Advisory Committee (2007-2008)  
Member (2006-2007)  
AESEDA Strategic Planning Committee. (2008)  
EMS Energy & EESI Institutes Promotion Committee. (2009-2012) as the tenure-line member  
College Computing Committee (2004)  
Co-chair Coal Research Thrust for the EMS Energy Institute

### **Department Service**

Energy Engineering Undergraduate Program Chair (2018-current)  
Interim Graduate Program Officer Energy and Geo-Environmental Engineering (2007-2008).  
Chair Fuel Science Awards  
Organizer Given Lecture Series  
Lead ABET Assessment for Energy Engineering

### **Courses Taught**

EGEE 101 Energy & the Environment (online, hybrid, and face-to-face)  
EGEE 411W\* Energy science and Engineering Laboratory Course (writing intensive course)  
FSc 410 Fuel Technology Lab  
FSc 401 Introduction to Fuel Technology  
ENNEC 484 Energy Economics\*  
EGEE 410 & 411 Social Legacy of Pennsylvania Coal & the Technological Legacy of Pennsylvania Coal\*  
EGEE 580 Design Engineering\*,  
EGEE 102 Energy Conservation\*,  
EGEE 597a Coal Structure & Behavior.  
EGEE 401 Energy in a Changing World  
EGEE Petrol Processing\*  
EGEE 431 Chemistry of Fuels\*  
EM SC 580 CAUSE (2003) Industrial Revolution to Industrial Ecology\*  
EM SC 580 CAUSE (2013) The Energy New Deal Down Under\*  
EM SC 580 CAUSE (2015) Sustainable Energy in Scandinavia: one Region, Many Choices\*  
EM SC 100s Earth and Mineral Sciences First-Year Seminar\* (regular semester and LEAP summer version: combined with Energy and the Environment).

\* Team-taught classes.

### **Short Courses to Industry and Academia**

These are typically ~5 lectures.

Tata Steel, India, 2015

Tsinghua University, China, 2015

North West University, Potchefstroom Campus, South Africa, 2013

Sasol, South Africa 2005