

Reviews

9367

A Review of Numerical Modeling and Experimental Analysis of Combustion in Moving Grate Biomass Combustors
Mohammad Hosseini Rahdar,* Fuzhan Nasiri, and Bruno Lee
DOI: 10.1021/acs.energyfuels.9b02073

9403

Effects of Carbon Dioxide on Laminar Burning Speed and Flame Instability of Methane/Air and Propane/Air Mixtures: A Literature Review
Ziyu Wang,* Sai C. Yelishala, Guangying Yu, Hameed Metghalchi, and Yiannis A. Levendis
DOI: 10.1021/acs.energyfuels.9b02346

Articles

Fossil Fuels

9419

Protonated Nitrogen Structure in ¹⁵N-Labeled Model Coal Investigated by Solid-State ¹H–¹⁵N Double-CP NMR Experiments under Ultrafast Magic-Angle Spinning
Keiko Okushita,* Yuki Hata, Yoshikazu Sugimoto, Takafumi Takahashi, and Koji Kanehashi
DOI: 10.1021/acs.energyfuels.9b00910

9429

Effect of Ethyl Octanoate and Ethyl Oleate on the Properties of Gasoline Fuel Mixture
Suzara Rayanne de Castro Sena,* Eduardo Lins de Barros Neto,* and Camila Gambini Pereira*
DOI: 10.1021/acs.energyfuels.9b01282

9437

Catalytic Effect of Metal Chloride Additives on the Volatile Gas Release Characteristics for High-Temperature Lignite Pyrolysis
Zhihua Wang, Jiaxin Tan, Yong He,* Ye Yuan, Longlong Liu, Yanqun Zhu, and Kefa Cen
DOI: 10.1021/acs.energyfuels.9b01342

9446

Wetting of Mineral Surfaces by Fatty-Acid-Laden Oil and Brine: Carbonate Effect at Elevated Temperature
Martin E. J. Haagh, Nathalie Schilderink, Frieder Mugele, and Michel H. G. Duits*
DOI: 10.1021/acs.energyfuels.9b01351

- 9457 **Measurements of Hydrate Formation Behavior in Shut-In and Restart Conditions**
Celina Kakitani, Daniela C. Marques, Moisés A. Marcelino Neto, Adriana Teixeira, Leandro S. Valim, Rigoberto E. M. Morales,* and Amadeu K. Sum*
DOI: 10.1021/acs.energyfuels.9b01395
- 9466 **Experimental Investigation and Thermodynamic Modeling of Wax Precipitation in Crude Oil Using the Multi-Solid Model and PC-SAFT EOS**
Hamed Heidariyan, Mohammadreza Ehsani, Taraneh Jafari Behbahani,* and Mohsen Mohammadi
DOI: 10.1021/acs.energyfuels.9b01445
- 9480 **Efficient Ring-opening Reaction of Tetralin over Nanosized ZSM-5 Zeolite: Effect of SiO₂/Al₂O₃ Ratio and Reaction Condition**
Peipei Miao, Kang Li, Jiangtao Fan, Naiwen Xu, Xiaolin Zhu, and Chunyi Li*
DOI: 10.1021/acs.energyfuels.9b01491
- 9491 **Organic Matter Type, Maturity, Depositional Environmental Characteristics, and Liquid Hydrocarbon Potential of Late Carboniferous Kozlu Bituminous Coal and Coaly Shale Beds (Zonguldak-Amasra Basin, NW Anatolia, Turkey): An Application of Biomarker Geochemistry**
R. Kara-Gulbay,* G. Yaylali-Abanuz, S. Korkmaz, M. S. Erdoğan, F. Hoş-Çebi, S. Çevik, and E. Ağırman-Aktürk
DOI: 10.1021/acs.energyfuels.9b01528
- 9510 **Mechanistic Model To Predict Hydrate Deposition under Stratified Flow Conditions**
Sriram Ravichandran and Nagu Daraboina*
DOI: 10.1021/acs.energyfuels.9b01624
- 9520 **Correlations of the Elemental Compositions of Primary Coal Tar and Char**
Andrew P. Richards, Colson Johnson, and Thomas H. Fletcher*
DOI: 10.1021/acs.energyfuels.9b01627
- 9538 **Asphaltene and Maltene Adsorption into Graphene**
Estrella Rogel,* Michael E. Moir, Matthew Hurt, Toni Miao, and Eddy Lee
DOI: 10.1021/acs.energyfuels.9b01681
- 9546 **Thermal Cracking of Oil under Water Pressure up to 900 Bar at High Thermal Maturities: 2. Insight from Light Hydrocarbon Generation and Carbon Isotope Fractionation**
Lijuan Xie, Yongge Sun,* Clement N. Uguna, Youchuan Li, Colin E. Snape, and Will Meredith
DOI: 10.1021/acs.energyfuels.9b01697
- 9559 **Theoretical Study of Structural and Spatial Properties of Kerogen**
Qing Wang,* Shuo Pan, Jingru Bai, Mingshu Chi, Da Cui, Zhichao Wang, Qi Liu, and Fang Xu
DOI: 10.1021/acs.energyfuels.9b01730
- 9570 **Effect of Asphaltenes on the Structure and Surface Properties of Wax Crystals in Waxy Oils**
Huiyong Xue, Jinjun Zhang,* Shanpeng Han, Mengran Sun, Xiaohan Yan, and Hongying Li
DOI: 10.1021/acs.energyfuels.9b01825
- 9585 **Synthesis of Magnetic Graphene Oxide (MGO) and Auxiliary Microwaves To Enhance Oil Recovery**
Zhengxiao Xu, Zhaomin Li,* Aiwen Jing, Fanyu Meng, Faqiang Dang, and Teng Lu*
DOI: 10.1021/acs.energyfuels.9b01841
- 9596 **Effects of Aging on Asphaltene Deposit Composition Using Ultrahigh-Resolution Magnetic Resonance Mass Spectrometry**
Estrella Rogel,* Matthias Witt, and Michael E. Moir
DOI: 10.1021/acs.energyfuels.9b01864
- 9604 **Experimental Investigation of the Rheology and Crystal Morphology of Model Waxy Oils under Gelling Conditions**
Thiago O. Marinho, Márcia C. K. De Oliveira, and Márcio Nele*
DOI: 10.1021/acs.energyfuels.9b01972
- 9619 **Impact of Composition on Pore Structure Properties in Shale: Implications for Micro-/Mesopore Volume and Surface Area Prediction**
Yujie Yuan,* Reza Rezaee, Emad A. Al-Khdheawi, Si-Yu Hu, Michael Verrall, Jie Zou, and Kouqi Liu
DOI: 10.1021/acs.energyfuels.9b02232
- 9629 **Experimental Evaluation of Carbon Dots Stabilized Foam for Enhanced Oil Recovery**
Sivabalan Sakthivel, Abdulauf Adebayo, and Mazen Yousef Kanj*
DOI: 10.1021/acs.energyfuels.9b02235
- 9644 **Coupling Smart Seawater Flooding and CO₂ Flooding for Sandstone Reservoirs: Smart Seawater Alternating CO₂ Flooding (SMSW-AGF)**
Hasan N. Al-Saedi, Yifu Long,* Ralph E. Flori, and Baojun Bai
DOI: 10.1021/acs.energyfuels.9b02289
- 9654 **Synergistic Effect of Hydrogen Transfer Ability on the Co-carbonization of Different FCC Slurry Oil Fractions**
Cunhui Lin, Li Wang, Shikui Wu, Ruijin Zhou, Xingye Zeng, Zhanjun Zhang, and Linhai Duan*
DOI: 10.1021/acs.energyfuels.9b02271
- 9661 **Study of Cu–Ni–Ca Composite Catalysts in Catalytic Hydrogasification of Char**
Hao Sun, Feng Zhang, Jicheng Bi, Xuan Qu, Shuai Yan, Jinhui Zhang, and Jianshu Zhang*
DOI: 10.1021/acs.energyfuels.9b02279

9671 **5** DOI: 10.1021/acs.energyfuels.9b02288
Effect of the NiO/SiO₂ Nanoparticles-Assisted Ultrasound Cavitation Process on the Rheological Properties of Heavy Crude Oil: Steady State Rheometry and Oscillatory Tests
Daniel Montés, Esteban A. Taborda, Mario Minalé,* Farid B. Cortés, and Camillo A. Franco*

9681 DOI: 10.1021/acs.energyfuels.9b02317
Effect of Na₂O in Ash Composition on Petroleum Coke Ash Fusibility
Jiazhou Li, Jiansheng Zhang,* Jiantao Zhao, and Yitian Fang

9690 **5** DOI: 10.1021/acs.energyfuels.9b02349
Green Fuel Desulfurization with β -Cyclodextrin Aqueous Solution for Thiophenic Sulfides by Molecular Inclusion
Zunbin Duan, He Bian, Zhijian Gao, Lijun Zhu, and Daohong Xia*

9702 DOI: 10.1021/acs.energyfuels.9b02389
Experimental Study on the Impact of Thermal Maturity on Shale Microstructures Using Hydrous Pyrolysis
Kouqi Liu,* Mehdi Ostadhassan,* Paul C. Hackley, Thomas Genzlis, Jie Zou, Yujie Yuan, Humberto Carvajal-Ortiz, Reza Rezaee, and Bailey Bubach

9720 DOI: 10.1021/acs.energyfuels.9b02419
Laboratory Evaluation of a Low pH and Low Polymer Concentration Zirconium-CMHGP Gel System for Hydraulic Fracturing
Kaiyu Zhang,* Guodong Zhang, Zhuojing Li, and Jirui Hou*

9736 **5** DOI: 10.1021/acs.energyfuels.9b02425
Heavy Oil Viscosity Reduction Performance of Novel Water-Soluble Terpolymers
Juan Li, Yigang Liu, Qixia Wang, Yugui Han, Minggang Wang, and Yebang Tan*

9747 DOI: 10.1021/acs.energyfuels.9b02491
Experimental Study on the Relationship between Carbonate Reservoir Quality Index and Dynamic Parameters of Chemical Solutions for Oil Recovery Practice
Xianmin Zhou* and Muhammad Shahzad Kamal

9759 **5** DOI: 10.1021/acs.energyfuels.9b02518
Nanoscale Molecular Fractionation of Organic Matter within Unconventional Petroleum Source Beds
Aaron M. Jubb,* Paul C. Hackley, Javin J. Hatcherian, Jing Qu, and Timothy O. Nesheim

9767 **5** DOI: 10.1021/acs.energyfuels.9b02543
Influence of Wax Precipitation on the Impedance Spectroscopy of Waxy Oils
Chaohui Chen, Jinjun Zhang,* Chenbo Ma, Huaqing Liang, Meiyi Qing, Yiwei Xie, Qian Huang, Shanpeng Han, and Hongying Li

9779 **5** DOI: 10.1021/acs.energyfuels.9b02605
Catalogue of Plausible Molecular Models for the Molecular Dynamics of Asphaltenes and Resins Obtained from Quantitative Molecular Representation
Jason C. Law, Thomas F. Headen, Guadalupe Jiménez-Serratos, Edo S. Boek, Juan Murgich, and Erich A. Müller*

9796 **5** DOI: 10.1021/acs.energyfuels.9b02938
Preparation and Characterization of Single-Component Poly- α -olefin Oil Base Stocks
Su Q. Dong, Pu K. Mi,* Sheng Xu, Jun Zhang, and Rui D. Zhao

Biofuels and Biomass

9805 **5** DOI: 10.1021/acs.energyfuels.9b00672
Characteristics of Biomass Devolatilization and in Situ Char Gasification Tested by the Non-Isothermal Method
Xi Zeng,* Kaito Kahara, Yasuaki Ueki, Ryo Yoshiie, Guangwen Xu, and Ichiro Naruse

9818 DOI: 10.1021/acs.energyfuels.9b01564
Modeling Study of the Entrained Flow Gasification of Ethylene Glycol, a Surrogate Fuel for a Pyrolysis Oil
Niranjan Fernando,* Marina Braun-Unkhoff, and Uwe Riedel

9828 **5** DOI: 10.1021/acs.energyfuels.9b01604
Effect of Oxygenated Functional Groups in Essential Oils on Diesel Engine Performance, Emissions, and Combustion Characteristics
S. M. Ashrafur Rahman,* T. M. I. Mahila, Arslan Ahmad, M. N. Nabi, M. Jafari, A. Dowell, M. A. Islam, A. J. Marchese, J. Tryner, P. R. Brooks, T. A. Bodisco, Svetlana Stevanovic, T. Rainey, Z. D. Ristovski, and R. J. Brown

9835 DOI: 10.1021/acs.energyfuels.9b01662
Dynamic Study of Butanol and Water Adsorption onto Oat Hull: Experimental and Simulated Breakthrough Curves
Qian Huang, Catherine Hui Niu,* and Ajay Kumar Dalai

9843 DOI: 10.1021/acs.energyfuels.9b01650
Food and Market Waste—A Pathway to Sustainable Fuels and Waste Valorization
Miloud Ouadi, Muhammad Asif Bashir, Lais Galileu Speranza, Hessaam Jahangiri,* and Andreas Hornung

9851 **5** DOI: 10.1021/acs.energyfuels.9b01760
Reactivity and Physicochemical Properties of the Soot Produced in the Pyrolysis of 2,5-Dimethylfuran and 2-Methylfuran
Katuska Alexandrino,* Ángela Millera, Rafael Bilbao, and María U. Alzueta*

9859 DOI: 10.1021/acs.energyfuels.9b01778
Online Measurement of Sub-ppm, Total Sulfur in Biogas by Chemiluminescence
Adelaide S. Calbry-Murzyka,* Julian Indlekofer, Jörg Schneebeli, and Serge M. A. Biollaz

- 9870 **5** DOI: 10.1021/acs.energyfuels.9b01846
Effect of Aging in Nitrogen and Air on the Properties of Biocrude Produced by Hydrothermal Liquefaction of *Spirulina*
Yingxian Wang, Yuanhui Zhang, and Zhidan Liu*
- 9879 **5** DOI: 10.1021/acs.energyfuels.9b01979
Production of Organic Compounds through Catalyzed Hydrothermal Carbonization of Woody Biomass
Amin Ghaziaskar,* Glenn A. McKee,* Alexis Mackintosh, Edward P. C. Lai, and Onita D. Basu
- 9886 Esterification, Distillation, and Chemical Characterization of Bio-Oil and Its Fractions
Maria J. Suota, Edesio L. Simonatto,* Dilamara R. Scharf, Henry F. Meier, and Vinicyus R. Wiggers
- 9895 A New Microcomputed-Tomography-Based Approach for Visualizing Microstructure Changes of Corn Stalk Pretreated with Dilute Sulfuric Acid
Ruyue Xie, Ying Zhu, Junbao Li, Xinlei Wang, and Lujia Han*
- 9904 Molecular Structure and Formation Mechanism of Hydrochar from Hydrothermal Carbonization of Carbohydrates
Ning Shi,* Qiyang Liu, Xiong He, Gui Wang, Ni Chen, Jiayu Peng, and Longlong Ma
- 9916 Prediction of Hydrothermal Carbonization with Respect to the Biomass Components and Severity Factor
Mohammad Heidari, Omid Norouzi, Shakirudeen Salaudeen, Bishnu Acharya, and Animesh Dutta*
- 9925 **5** DOI: 10.1021/acs.energyfuels.9b02303
Free Glycerol Sensing in Biodiesel: Automatic System Based on Sequential Enzymatic Reactions Using a Fit-for-Purpose Chemiluminescence Detection Chamber
Nicolás A. Narro, Matías Insausti, Claudia E. Domini, and Marcos Grünhut*
- 9934 **5** DOI: 10.1021/acs.energyfuels.9b02341
Lignin Characterization and Catalytic Pyrolysis for Phenol-Rich Oil with TiO₂-Based Catalysts
Zhiqiao Dong, Haijing Yang,* Peiao Chen, Zihao Liu, Yingquan Chen, Lei Wang, Xianhua Wang, and Hanping Chen
- 9942 Gasification of Crude Glycerol after Salt Removal
Ana Almeida, Rosa Piñao,* Albina Ribeiro, Elisa Ramalho, and Carlos Pinho
- 9949 **5** DOI: 10.1021/acs.energyfuels.9b02557
Camphorane as a Renewable Diesel Blendstock Produced by Cyclodimerization of Myrcene
Orion Staples, Juan H. Leal, Patrick A. Cherry, Charles S. McEnally, Lisa D. Pfefferle, Troy A. Semelsberger, Andrew D. Sutton, and Cameron M. Moore*
- 9956 Decarboxylation of Oleic Acid over Ordered Mesoporous Pt/SAPO-11
Meiqiu Hu, Hong Yuan,* and Wei Liu
- 9965 Microscale Analyses of Mineral Particles in Sugar Cane Bagasse and Straw Shed Light on How Debris Can Be Incorporated into Biomass
Djanira R. Negrão, Liu Y. Ling, Ricardo O. Bordonal, and Carlos Driemeier*
- 9974 Characteristics of Gas-Liquid-Solid Products in Corn Straw Gasification: Effect of the Char-Tar-H₂O Interaction
Hongliang Sun, Dongdong Feng,* Yijun Zhao, Dawei Guo, Yan Ma, Heping Tan, and Shaozeng Sun
- 9985 **5** DOI: 10.1021/acs.energyfuels.9b02863
Comparative Study on the Dehydration of Biomass-Derived Disaccharides and Polysaccharides to 5-Hydroxymethylfurfural
Yuan Zhao, Kaifeng Lu, Hao Xu, Yang Qu, Lingjun Zhu, and Shurong Wang*
- Environmental and Carbon Dioxide Issues**
- 9996 **5** DOI: 10.1021/acs.energyfuels.9b01118
Effects of the Inert Materials on the Stability of Ca-Based CO₂ Sorbents and the Synergy with Cement Manufacture
Xu He, Guozhao Ji, Tan Liu, and Ming Zhao*
- 10004 NO Removal from Flue Gas by Using Chlorine Dioxide Solution
Shujun Sun, Suxia Ma,* Bingchuan Yang, Rongji Cui, and Jie Wang
- 10011 **5** DOI: 10.1021/acs.energyfuels.9b01829
Aminoalkyl-Functionalized Pyridines as High Cyclic Capacity CO₂ Absorbents
Sigvart Evjen, Oda Siebke Løge, Anne Fiksdahl, and Hanna K. Knudtilla*
- 10016 Leaching Behavior of Heavy Metals from the Coal Gangue under the Impact of Site Ordovician Limestone Karst Water from Closed Shandong Coal Mines, North China
Dongjing Xu,* Longqing Shi,* Xingyue Qu, Jinjin Tian, Ke Wang, and Jie Liu

10029 **5** DOI: 10.1021/acs.energyfuels.9b01975
Development of SO₂ Phase Change Absorption: Viscosity Change and Component Distribution Rules
Shengchao Xu, Wenbo Zhao,* Muiyuan Chai, Tian Si, Yuan Chen, and Qingming Jia*

10039 **5** DOI: 10.1021/acs.energyfuels.9b01918
Pore-Scale CO₂ Displacement Simulation Based on the Three Fluid Phase Lattice Boltzmann Method
Mingming Tang,* Hongbin Zhan,* Shuangfang Lu, Huifang Ma, and Hongkun Tan

10056 DOI: 10.1021/acs.energyfuels.9b02092
Study on Preparation of an Oil Sludge-Based Carbon Material and Its Adsorption of CO₂: Effect of the Blending Ratio of Oil Sludge Pyrolysis Char to KOH and Urea
Zhiqiang Gong, Fanzhi Meng, Zhenbo Wang,* Peiwen Fang, Xiaoyu Li, Lei Liu, and Haoteng Zhang

10066 DOI: 10.1021/acs.energyfuels.9b02187
Speciation and Risk Assessment of Heavy Metals in Municipal Solid Waste Incineration Fly Ash during Thermal Processing
Kaixing Zhao, Yuyan Hu, Yunzhen Wang, Dezhen Chen, and Yuheng Feng*

10078 DOI: 10.1021/acs.energyfuels.9b02342
Simultaneous Removal of NO and SO₂ via an Integrated System of Nonthermal Plasma Combined with Catalytic Oxidation and Wet Electrostatic Precipitator
Shaoping Cui, Zhong Zhong, Yujie Liao, Liqiang Qi, and Dong Fu*

10090 **5** DOI: 10.1021/acs.energyfuels.9b02659
Aqueous Potassium Lysinate for CO₂ Capture: Evaluating at Desorber Conditions
Chenxu Li, Yue Zhao, and Shufeng Shen*

Efficiency and Sustainability

10099 **5** DOI: 10.1021/acs.energyfuels.9b01328
Insight into the Compositions of the Soluble/Insoluble Portions from the Acid/Base Extraction of Five Fractions Distilled from a High-Temperature Coal Tar
Zhi-Hao Ma, Xian-Yong Wei,* Guang-Hui Liu, Zhong-Qiu Liu, Fang-Jing Liu, and Zhi-Min Zong

10108 DOI: 10.1021/acs.energyfuels.9b01542
Modified Hyperbranched Polyethylenimine as a Novel Demulsifier for Oil-in-Water Emulsions
Houkai Teng, Cuiting Chen, Shu Yan, Dengfeng Ye, and Lifeng Zhang*

10115 DOI: 10.1021/acs.energyfuels.9b01761
Enhanced Recovery from Gas Condensate Reservoirs through Renewable Energy Sources
Saad Alafnan,* Murtada Aljawad, Fahad Alismail, and Abdulaziz Almejied

10123 **5** DOI: 10.1021/acs.energyfuels.9b01809
Inducing *In Situ* Hydrothermal Carbonization of Glucose To Synthesize Carbon–MIL–101 Hybrid Composites for Improved Hydrogen Uptake
Dharmendra K. Panchariya, E. Anil Kumar, and Sanjay K. Singh*

Catalysis and Kinetics

10133 DOI: 10.1021/acs.energyfuels.9b01935
Evaluation of Kinetic Inhibition of Methane Hydrate Formation by a Copolymer of *N*-Vinylcaprolactam with 1-Vinylimidazole
Zhen Long, ZhiLin Lu, Qihang Ding, Xuebing Zhou, Jiao Lei, and Deqing Liang*

10143 DOI: 10.1021/acs.energyfuels.9b02228
Molecular-Level Kinetic Modeling of a Real Vacuum Gas Oil Hydroprocessing Refinery System
Pratyush Agarwal, Mayuresh Sahasrabudhe, Sumit Khandalkar, Chandra Saravanan, and Michael T. Klein*

10159 DOI: 10.1021/acs.energyfuels.9b02335
Platinum–Copper Bimetallic-Modified Nanoprism Mordenite for Carbonylation of Dimethyl Ether
Haibing Sheng, Hongfang Ma, Weixin Qian, Nina Fei, Haitao Zhang,* and Weiyong Ying

10167 DOI: 10.1021/acs.energyfuels.9b02394
Kinetics of Thermal Decomposition of Tar in the Presence of Air and Nitrogen Gas
Olaekan S. Alade, M. Mahmoud,* D. A. Al Shehri,* Saheed A. Ganiyu, Ayman Al-Nakhli, and Mohammed Bataweel

10176 **5** DOI: 10.1021/acs.energyfuels.9b02454
Conversion of Isobutanol to Olefins and Aromatics over HZSM-5-Based Catalysts: Tuning of Product Selectivity
Zhen-Yi Du,* Bin-Bin Zhang, Ting-Sheng Chen, Yuli Betancur, and Wen-Ying Li*

Combustion

10185 **5** DOI: 10.1021/acs.energyfuels.9b01423
Chemical Ignition Characteristics of Ethanol Blending with Primary Reference Fuels
Eshan Singh,* Efstathios-Al. Tingas, Dimitris Goussis, Hong G. Im, and S. Mani Sarathy*

10197 **5** DOI: 10.1021/acs.energyfuels.9b01575
Shock Tube and Kinetic Study on the Effects of CO₂ on Dimethyl Ether Autoignition at High Pressures
Neda Djordjevic,* Mike Rekus, Johann Vinkeloe, and Lisa Zander

10209 **5** DOI: 10.1021/acs.energyfuels.9b01781
Kinetic Study of Long-Term T23 Tube Corrosion upon Low-Rank Coal Ash Deposition under Oxy-Fuel Combustion Conditions
Iman Ja'baz, Facun Jiao, Xiaojiang Wu, Yoshihiko Ninomiya, Dunxi Yu, and Lian Zhang*

10218 DOI: 10.1021/acs.energyfuels.9b01955
Study on the Physicochemical Properties and Spray and Combustion Characteristics of 1-Butanol/Diesel Fuel Blends in a Constant-Volume Combustion Chamber
 Xiaoqing Zhang, Tie Li,* Ruli Tian He, and Run Chen*

10228 DOI: 10.1021/acs.energyfuels.9b02027
Atomistic Simulation of Coal Char Oxy-Fuel Combustion: Quantifying the Influences of CO₂ to Char Reactivity
 Yongbo Du, Chang'an Wang, Haihui Xin, Defu Che, and Jonathan P. Mathews*

10237 DOI: 10.1021/acs.energyfuels.9b02179
Influence of Sewage Sludge on Ash Fusion during Combustion of Maize Straw
 Hongpeng Liu,* Shiqiang Zhang, Shiyu Feng, Jiyong Liu, Guangrui Liu, Baizhong Sun, Deyong Che, and Qing Wang

10247 DOI: 10.1021/acs.energyfuels.9b02201
Characteristics of Fine Particulate Matter and Polycyclic Aromatic Hydrocarbons Emitted from Coal Combustion Processes
 Chia Ming Lu, Nguyen Duy Dat, Chian Kou Lien, Kai Hsien Chi, and Moo Been Chang*

10255 DOI: 10.1021/acs.energyfuels.9b02284
A Theoretical Multiscale Approach to Study the Initial Steps Involved in the Chemical Reactivity of Soot Precursors
 Michel Keller, Theodoros de Bruin,* Mickaël Matrat, André Nicolle, and Laurent Catoire

10267 DOI: 10.1021/acs.energyfuels.9b02340
Numerical Investigation into Effects of Fuel Physical Properties on GCI Engine Performance and Emissions
 Jihad Bedra,* Abdullah Zubail, and Jaeheon Sim

10282 DOI: 10.1021/acs.energyfuels.9b02347
Ignition and Combustion Characteristics of Heptane-Based Nanofluid Fuel Droplets
 Weikang Han, Baoxin Dai, Jianzhong Liu, Yunlan Sun,* Baozhong Zhu,* and Xuedong Liu

10290 DOI: 10.1021/acs.energyfuels.9b02458
Development of a Data-Derived Sooting Index Including Oxygen-Containing Fuel Components
 Peter C. St. John,* Seonah Kim, and Robert L. McCormick

10297 DOI: 10.1021/acs.energyfuels.9b02479
Preparing Coal Water Slurry from BDO Tar to Achieve Resource Utilization: Combustion Process of BDO Tar-Coal Water Slurry
 Lirui Mao, Hanxu Li,* Yuanchun Zhang, and Chengli Wu

10307 DOI: 10.1021/acs.energyfuels.9b02514
Catalytic Effects on the Nonisothermal Oxidation of Solid Fuels by Oxygen: An Experimental Study
 A. Nyombi,* M. R. Williams, and R. Wessling

10317 DOI: 10.1021/acs.energyfuels.9b02563
Experiment and Kinetics Studies on Ash Fusion Characteristics of Biomass/Coal Mixtures during Combustion
 Yuan Lv, Yangqing Niu,* Yang Liang, Siqu Liu, Denghui Wang, and Shien Hui

Fuel Cells

10324 DOI: 10.1021/acs.energyfuels.9b01939
Evaluations of Concepts for the Integration of Fuel Cells in Liquid Organic Hydrogen Carrier Systems
 Karsten Müller,* Simon Thiele, and Peter Wasserscheid

Batteries and Energy Storage

10331 DOI: 10.1021/acs.energyfuels.9b01450
Mixtures of Ammonia and Organic Solvents as Alternative Fuel for Internal Combustion Engines
 M. C. Rehbein, C. Meier, P. Elits,* and S. Scholl

Process Engineering

10343 DOI: 10.1021/acs.energyfuels.9b01253
Effects of Operating Parameters on Solids Flux in a High-Density/-Flux Circulating Fluidized Bed Riser Reactor
 Xin Su, Chengxiu Wang,* Xingying Lan, and Jinsen Gao*

10356 DOI: 10.1021/acs.energyfuels.9b01463
Zr-Induced Thermostable Polymeric Nanospheres with Double-Cross-Linked Architectures for Oil Recovery
 Zhiyong Wang, Meiqin Lin,* Yuqi Xiang, Tianxiao Zeng, Zhaoxia Dong, Juan Zhang, and Zihao Yang

10365 DOI: 10.1021/acs.energyfuels.9b02182
Effect of Thiophenes on High-Temperature Corrosion by Sulfidation and Naphthenic Acids
 Peng Jin, Winston Robbins, and Gheorghe Bota*

10372 DOI: 10.1021/acs.energyfuels.9b02250
Generating Data-Driven Models from Molecular-Level Kinetic Models: A Kinetic Model Speedup Strategy
 Pratyush Agarwal and Michael T. Klein*

10380 DOI: 10.1021/acs.energyfuels.9b02463
Poly(ethylene glycol) Diacid-Based Deep Eutectic Solvent with Excellent Denitrogenation Performance and Distinctive Extractive Behavior
 Shuang Zhu, Jiaolai Xu, Hanlin Cheng, Jiajun Gao,* Xingmao Jiang, Chunxi Li, and Weimin Yang

10218 DOI: 10.1021/acs.energyfuels.9b01955
Study on the Physicochemical Properties and Spray and Combustion Characteristics of 1-Butanol/Diesel Fuel Blends in a Constant-Volume Combustion Chamber
 Xiaoqing Zhang, Tie Li,* Ruli Tian He, and Run Chen*

10228 DOI: 10.1021/acs.energyfuels.9b02027
Atomistic Simulation of Coal Char Oxy-Fuel Combustion: Quantifying the Influences of CO₂ to Char Reactivity
 Yongbo Du, Chang'an Wang, Haihui Xin, Defu Che, and Jonathan P. Mathews*

10237 DOI: 10.1021/acs.energyfuels.9b02179
Influence of Sewage Sludge on Ash Fusion during Combustion of Maize Straw
 Hongpeng Liu,* Shiqiang Zhang, Shiyu Feng, Jiyong Liu, Guangrui Liu, Baizhong Sun, Deyong Che, and Qing Wang

10247 DOI: 10.1021/acs.energyfuels.9b02201
Characteristics of Fine Particulate Matter and Polycyclic Aromatic Hydrocarbons Emitted from Coal Combustion Processes
 Chia Ming Lu, Nguyen Duy Dat, Chian Kou Lien, Kai Hsien Chi, and Moo Been Chang*

10255 DOI: 10.1021/acs.energyfuels.9b02284
A Theoretical Multiscale Approach to Study the Initial Steps Involved in the Chemical Reactivity of Soot Precursors
 Michel Keller, Theodoros de Bruin,* Mickaël Matrat, André Nicolle, and Laurent Catoire

10267 DOI: 10.1021/acs.energyfuels.9b02340
Numerical Investigation into Effects of Fuel Physical Properties on GCI Engine Performance and Emissions
 Jihad Bedra,* Abdullah Zubail, and Jaeheon Sim

10282 DOI: 10.1021/acs.energyfuels.9b02347
Ignition and Combustion Characteristics of Heptane-Based Nanofluid Fuel Droplets
 Weikang Han, Baoxin Dai, Jianzhong Liu, Yunlan Sun,* Baozhong Zhu,* and Xuedong Liu

10290 DOI: 10.1021/acs.energyfuels.9b02458
Development of a Data-Derived Sooting Index Including Oxygen-Containing Fuel Components
 Peter C. St. John,* Seonah Kim, and Robert L. McCormick

10297 DOI: 10.1021/acs.energyfuels.9b02479
Preparing Coal Water Slurry from BDO Tar to Achieve Resource Utilization: Combustion Process of BDO Tar-Coal Water Slurry
 Lirui Mao, Hanxu Li,* Yuanchun Zhang, and Chengli Wu

Additions and Corrections

10389

Correction to Minimized Skeletal Mechanism for Methyl Butanoate Oxidation and Its Application to the Prediction of C_3-C_4 Products in Nonpremixed Flames: A Base Model of Biodiesel Fuels
Kuang C. Lin,* Hairong Tao,* Fan-Hsu Kao, and Chuang-Te Chiu

DOI: 10.1021/acs.energyfuels.9b02792

10390

Correction to Does the Cloud Point Temperature of a Polymer Correlate with Its Kinetic Hydrate Inhibitor Performance?
Erik Gisle Dirdal and Malcolm A. Kelland*

DOI: 10.1021/acs.energyfuels.9b03286

A Review of Numerical Modeling and Experimental Analysis of Combustion in Moving Grate Biomass Combustors

Mohammad Hosseini Rahdar,*[†] Fuzhan Nasiri,[†] and Bruno Lee[†]

[†]Department of Building, Civil & Environmental Engineering, Concordia University, Montreal, Quebec H3G 1M8, Canada

ABSTRACT: This Review covers the current state-of-the-art literature dealing with numerical modeling and experimental analysis of moving grate biomass combustors. The greatest attention is paid to the modeling of the thermochemical conversion in the fuel bed. Changes in the fuel characteristics are also tracked during the combustion. Such a review can facilitate understanding a more robust model from viewpoints of thermal performance, chemical and physical properties, pollutant emissions, and combustion stability. Different modeling approaches for the moving grate biomass furnaces are introduced, with a focus on the independent fuel bed modeling. Stepwise biomass fuel degradation inside the bed and corresponding individual mathematical models are described, followed by overbed combustion modeling. Numerical methods for the conservation equations of the combustion model are classified, and a general iterative solution algorithm is delivered. Various NO_x formation mechanisms from the fuel-bed efflux and the combustion of hot zone gases are detailed, followed by the particle matter originating from inorganic materials. Air-staging, the flue gas recirculation mechanism, and restriction of the maximum flame temperature can significantly reduce the NO_x concentration in the flue gases. Industrial biomass combustion systems are addressed in terms of different grate technologies, and a general laboratory-scale biomass reactor is portrayed. For future work, according to the gaps found in the literature, it is recommended that, considering the intensive inhomogeneity of the biomass fuels, the effects of the fuel uncertainties should be considered in the bed modeling. Furthermore, deep investigation of the infrared images captured from biomass combustion can provide a comprehensive tool for the combustion system analysis. More recommendations are given in the conclusion of this Review.

1. INTRODUCTION

Today, there is no doubt that it is vital to take advantage of renewable energies instead of fossil fuels to support future global energy needs along with preserving the Earth from environmental threats. Among all kinds of renewable energy resources, biomass in different forms (solid, liquid, or gas) is the only one that includes a fixed carbon element which can be substituted for fossil fuels in combustion systems.¹ One reason for the prevalence of biomass combustors versus fossil fuel combustion systems is the reduced pollutant emissions from biomass combustion. It is recalled that the carbon released is as much as has been absorbed by the sourcing plants.^{2,3} The latter is a satisfying reason for conducting more research on the scope of biomass conversion which can considerably drive combustion systems toward a sustainable energy supply. Nevertheless, thermochemical conversion of biomass in contrast with traditional fossil fuels deals with a lot of ambiguous processes, e.g., char combustion.^{4,5} In spite of extensive development in the biofuels industry, the direct combustion of the biomass particles is still the most frequently used technology due to the high biofuels process cost.^{6–10} Grate firing technology is of interest to burn biomass due to its lower sensitivity to feed composition and size, which shows the wonderful capabilities of this technology.^{11–13} Likewise, grate firing biomass combustors are increasingly considered as district heating systems because they are available from small-scale to large-scale.

Although various biomass fuel conversion technologies are already running in different industries worldwide, they are not accounted for as fully mature technologies due to deficient performance such as combustion efficiency, contaminant emission, and combustion stability. The literature includes

multitudes of articles in which biomass fuel combustion has been discussed and investigated to various extents. However, there are few review papers, in terms of biomass combustion modeling, covering the whole conversion process in the bed along with the overbed gas combustion.^{14–17} Some papers have investigated different biomass feedstocks as fuel. For instance, combustion of municipal solid waste (MSW) and coal was compared on the basis of fuel features, the technology of combustion, pollutants, and ash disposal.¹⁸ In other studies, combustion of sewage¹⁹ and combustion of herbaceous residuals²⁰ were investigated comprehensively. Research works by Demirbas^{3,21,22} examined the combustion behavior of different biomass fuels together with the issues associated with employing them inside the combustion systems. However, modeling of the particle thermal conversion was ignored in their works. The growing market interest in biomass fuels, due to the policies set on fossil fuels consumption together with emission restrictions, forces designers to increasingly work on optimizing the biomass combustors using different sorts of particles such as chips, pellets, logs, etc.

Generally, there are two methods to optimize the biomass combustors, including experimental works and mathematical modeling. The experimental method is expensive and impossible in some aspects, while computational fluid dynamics (CFD) modeling is less expensive and more time-effective, but it still needs experimental results for validation.²³ The objective of

Received: June 26, 2019

Revised: September 5, 2019

Published: September 9, 2019

