

David Simakov, Ph.D.

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Email: dsimakov@uwaterloo.ca**Education**

Ph.D., Chemical Engineering, Technion – Israel Institute of Technology, Haifa, Israel	2010
M.Sc., Chemical Engineering, Technion – Israel Institute of Technology, Haifa, Israel	2004
Diploma, Biology & Chemistry, Pacific National University, Russia	1998

Professional Experience

Assistant Professor, Chemical Engineering, University of Waterloo	2015 – present
Senior Postdoctoral Associate, Chemical Engineering, MIT	2013 – 2015
Postdoctoral Researcher, Earth & Planetary Sciences, Harvard University	2011 – 2013
Postdoctoral Research Fellow, Chemical Engineering, Technion	2010 – 2011
Chemical Engineer, Celleria Inc., Caesarea Industrial Park, Israel	2008 – 2010

Awards & Honors

Honourary Symposium Lecture in Recognition of Sieghard E. Wanke for Outstanding Contributions in Chemical Reaction Engineering, 67th Canadian Chemical Engineering Conference	2017
Batsheva Seminar Scholarship, The Batsheva de Rothschild Fund	2007
Levi Eshkol Scholarship, Israel Ministry of Science	2006 – 2007

Memberships:

Canadian Society for Chemical Engineers, American Institute of Chemical Engineers

Research Interests: Thermocatalytic Conversion of CO₂, Renewable Synthetic Fuels, Heterogeneous Catalysis, Advanced Reactor Design, Nonlinear Chemical and Biochemical Dynamics

Teaching Interests: Chemical and Biochemical Reaction Engineering, Transport Phenomena, Heterogeneous Catalysis, Energy Conversion, Renewable Energy

Research Funding:

Waterloo-Technion Cooperation Program (\$60,000)	2019
Qualitrol Company (\$82,000)	2018-2019
Ontario Centers for Excellence Voucher for Innovation & Productivity (\$25,000)	2017
Canada Foundation for Innovation John Evans Leadership Fund (\$124,000)	2017
Natural Sciences and Engineering Research Council of Canada (NSERC)	
<i>NSERC Engage</i> (\$50,000)	2019
<i>NSERC Research Tools & Instruments</i> (\$141,000)	2017-2019
<i>NSERC Discovery Grant</i> (\$174,000)	2016-2021
Cisco Systems Smart Grid Research Fund (\$52,000)	2015-2016

Professional Service:

▪ Conference Programming Committee Member and Session Chair:

Canadian Chemical Engineering Conference	2017, 2018
International Conference on Chemical Reactors (CHEMREACTOR)	2016, 2018
International Conference on Catalysis for Renewable Sources: Fuel, Energy, Chemicals	2019

▪ Journal Reviewer:

Royal Society of Chemistry: RSC Advances, Reaction Chemistry & Engineering, Dalton Transactions

American Chemical Society: Industrial & Engineering Chemistry Research, ACS Sustainable Chemistry & Engineering

Elsevier: Chemical Engineering Journal, Chemical Engineering Science, Applied Energy, International Journal of Hydrogen Energy, Applied Catalysis A: General, Catalysis Communications, Energy Conversion & Management, Chemical Engineering & Processing - Process Intensification, Thermal Science and Engineering Progress, Journal of CO₂ Utilization, Renewable & Sustainable Energy Reviews

Wiley: The Canadian Journal of Chemical Engineering, AIChE Journal, Energy Technology, ChemistrySelect

De Gruyter: Reviews in Chemical Engineering

▪ Scientific Proposal Reviewer:

Canada Foundation for Innovation John Evans Leadership Fund (CFI JELF)

Natural Sciences & Engineering Research Council Discovery Grant (NSERC DG)

Natural Sciences & Engineering Research Council Collaborative Research & Development (CRD)

Journal Publications

- 29) García-Selfa, D., Muñuzuri, A.P., Pérez-Mercader, J. & Simakov, D.S.A. Resonant behavior in a periodically forced non-isothermal Oregonator. *J. Phys. Chem. A* 123(38), 8083-8088 (2019).
- 28) Currie, R., Mottaghi-Tabar, S., Zhuang, Y. & Simakov, D.S.A. Design of an air-cooled Sabatier reactor for thermocatalytic hydrogenation of CO₂: Experimental proof-of-concept and model-based feasibility analysis. *Ind. Eng. Chem. Res.* 58(29), 12899-13420 (2019).
- 27) Currie, R., Fowler, M.W. & Simakov, D.S.A. Catalytic membrane reactor for CO₂ hydrogenation using renewable streams: Model-based feasibility analysis. *Chem. Eng. J.* 372, 1240-1252 (2019).
- 26) Belinskaya, N., Altynov, A., Bogdanov, I., Popok, E., Kirgina, M. & Simakov, D.S.A. Production of gasoline using stable gas condensate and Zeoforming process products as blending components. *Energy Fuels* 33, 4202-4210 (2019).
- 25) Tathod, A.P., Hayek, N., Shpasser, D., Simakov, D.S.A. & Gazit, O.M. Mediating interaction strength between nickel and zirconia using a mixed oxide nanosheets interlayer for methane dry reforming. *Appl. Catal. B: Environ.* 249, 106-115 (2019).

- 24) Zhuang, Y., Currie, R., McAuley, K.B. & Simakov, D.S.A. Highly-selective CO₂ conversion via reverse water gas shift reaction over the 0.5wt% Ru-promoted Cu/ZnO/Al₂O₃ catalyst. ***Appl. Catal. A: Gen.*** 575, 74-86 (2019).
- 23) Dosi, M., Lau, I., Zhuang, Y., Simakov, D.S.A., Fowler, M.W. & Pope, M.A. Ultrasensitive electrochemical methane sensors based on solid polymer electrolyte-infused laser-induced graphene. ***ACS Appl. Mater. Interfaces*** 11(6), 6166-6173 (2019).
- 22) Currie, R., Nikolic, D., Petkovska, M. & Simakov, D.S.A. CO₂ conversion enhancement in a periodically operated Sabatier reactor: Nonlinear frequency response analysis and simulation-based study. ***Isr. J. Chem.*** 58, 1-15 (2018).
- 21) Simakov, D.S.A. & Román-Leshkov, Y. Highly efficient methane reforming over a low-loading Ru/ γ -Al₂O₃ catalyst in a Pd-Ag membrane reactor. ***AIChE J.*** 64(8), 3101-3108 (2018).
- 20) Walker, S.B., Sun, D., Kidon, D., Siddiqui, A., Kuner, A., Fowler, M. & Simakov, D.S.A. Upgrading biogas produced at dairy farms into renewable natural gas by methanation. ***Int. J. Energy Res.*** 1-15 (2018).
- 19) Sun, D., Khan, F.M. & Simakov, D.S.A. Heat removal and catalyst deactivation in a Sabatier reactor for chemical fixation of CO₂: Simulation-based analysis. ***Chem. Eng. J.*** 329, 165-177 (2017).
- 18) Sun, D. & Simakov, D.S.A. Thermal management of a Sabatier reactor for CO₂ conversion into CH₄: simulation-based analysis. ***J. CO₂ Util.*** 21, 368-382 (2017).
- 17) Said, S.A.M., Waseeuddin, M. & Simakov, D.S.A. A review on solar reforming systems. ***Renew. Sust. Energy Rev.*** 59, 149-159 (2016).
- 16) Said, S.A.M., Simakov, D.S.A., Waseeuddin, M. & Román-Leshkov, Y. Solar molten salt heated membrane reformer for natural gas upgrading and hydrogen generation: A CFD model. ***Sol. Energy*** 124, 163-176 (2016).
- 15) Simakov, D.S.A., Luo H.Y. & Román-Leshkov, Y. Ultra-low loading Ru/ γ -Al₂O₃: a highly active and stable catalyst for low temperature solar thermal reforming of methane. ***Appl. Catal. B: Environ.*** 169, 540-549 (2015).
- 14) Said S.A.M., Simakov D.S.A., Mokheimer E.M.A., Habib M.A., Ahmed, S., Waseeuddin M. & Román-Leshkov Y. Computational fluid dynamics study of hydrogen generation by low temperature methane reforming in a membrane reactor. ***Int. J. Hydrogen Energy*** 40, 3158-3169 (2015).
- 13) Simakov, D.S.A., Wright, M.M., Ahmed, S., Mokheimer E.M.A. & Román-Leshkov, Y. Solar thermal reforming of natural gas: a review on chemistry, catalysis and system design. ***Catal. Sci. Technol.*** 5, 1991-2016 (2015).
- 12) Simakov, D.S.A. & Pérez-Mercader, J. Effect of noise correlation on noise-induced oscillation frequency in the photosensitive Belousov-Zhabotinsky reaction in a continuous stirred tank reactor. ***J. Phys. Chem. A*** 117, 13999-14005 (2013).
- 11) Simakov, D.S.A. & Pérez-Mercader, J. Noise induced oscillations and coherence resonance in a generic model of the nonisothermal chemical oscillator. ***Sci. Rep.*** 3, 2404 (2013).

- 10) Cheung, L.S., Simakov, D.S.A., Fuchs, A., Pyrowolakis, G. & Shvartsman, S.Y. Dynamic model for the coordination of two enhancers of *broad* by EGFR signaling. *PNAS* 110, 17939-17944 (2013).
- 9) Simakov, D.S.A. & Pismen, L.M. Discrete model of periodic pattern formation through a combined autocrine-juxtacrine cell signaling. *Phys. Biol.* 10, 046001 (2013).
- 8) Simakov, D.S.A., Cheung L.S., Pismen, L.M. & Shvartsman, S.Y. EGFR-dependent patterning of *Drosophila* eggshell appendages. *Development* 139, 2814-2820 (2012).
- 7) Pismen, L.M. & Simakov, D.S.A. Genesis of two-dimensional patterns in cross-gradient fields. *Phys. Rev. E* 84, 061917 (2011).
- 6) Simakov, D.S.A. & Sheintuch, M. Model-based optimization of hydrogen generation by methane steam reforming in autothermal packed-bed membrane reformer. *AIChE J.* 57, 525-541 (2011).
- 5) Simakov, D.S.A. & Sheintuch, M. Experimental optimization of an autonomous scaled-down methane membrane reformer for hydrogen generation. *Ind. Eng. Chem. Res.* 49, 1123-1129 (2010).
- 4) Simakov, D.S.A. & Sheintuch, M. Demonstration of a scaled-down autothermal membrane methane reformer for hydrogen generation. *Int. J. Hydrogen Energy* 34, 8866-8876 (2009).
- 3) Simakov, D.S.A. & Sheintuch, M. Design of a thermally-balanced membrane reformer for hydrogen production. *AIChE J.* 54, 2735-2750 (2008).
- 2) Simakov, D.S.A. & Tsur, Y. Preparation of core-shell Ti-Nb oxide nanocrystals. *J. Nanopart. Res.* 10, 77-85 (2008).
- 1) Simakov, S.A. & Tsur, Y. Surface stabilization of nanosized titanium oxide: improving the colloidal stability and the sintering morphology. *J. Nanopart. Res.* 9, 403-417 (2007).

Books & Book Chapters

- 2) Simakov, D.S.A. *Renewable Synthetic Fuels and Chemicals from Carbon Dioxide* (Springer 2017).
- 1) Sheintuch, M. & Simakov, D.S.A. Alkanes dehydrogenation. In *Membrane Reactors for Hydrogen Production Processes* (Springer-Verlag London Ltd 2011).

Patents

- 3) Simakov, D.S.A. & Sheintuch, M. Hydrogen production by an autothermal heat exchanger packed-bed membrane gas reformer. **US Patent 9,359,201 B2** (2016).
- 2) Gottesfeld S., Dekel D. & Simakov, D.S. Catalyst coated membrane and catalyst film/layer for alkaline membrane fuel cells and methods of making same. **US Patent 8,304,368** (2012).
- 1) Gottesfeld S., Dekel D., Gottesfeld Z. & Simakov, D.S. Alkaline membrane fuel cells and apparatus and methods for supplying water thereto. **US Patent 8,257,872** (2012).

Invited Talks

- 5) Simakov, D.S.A. Making fuels from CO₂: Reverse water gas shift and Sabatier reaction, *University of Calgary*, November 19, 2018, Calgary, AB, Canada
- 4) Simakov, D.S.A. Thermocatalytic conversion of CO₂ into renewable synthetic fuels, *Technion – Israel Institute of Technology*, May 30, 2018, Haifa, Israel
- 3) Simakov, D.S.A. Carbon Capture and Utilization (CCU): Conversion pathways and techno-economic challenges, *Waterloo Institute for Sustainable Energy*, March 27, 2018, Waterloo, ON, Canada
- 2) Simakov, D.S.A. Thermocatalytic conversion of CO₂ into renewable synthetic fuels, *Henan Normal University*, October 13, 2017, Xinxian, Henan, China
- 1) Simakov, D.S.A. Making fuels from carbon dioxide: Design of a Sabatier reactor for CO₂ conversion into renewable natural gas, *Royal Military College of Canada*, March 01, 2017, Kingston, ON, Canada

Selected Conference Presentations (2015-2019)

- Guanjie, S., Yu, Y., Zhuang, Y. & Simakov, D.S.A. "High surface area transition metal carbides synthesized via reverse microemulsion method as high performance catalysts for thermocatalytic CO₂ conversion", **26th North American Catalysis Society Meeting**, June 2019, Chicago, IL, USA
- Guanjie, S., Mottaghi-Tabar, S., Ricardez Sandoval, L. & Simakov, D.S.A. "Reverse water gas shift reaction over high surface area γ -Al₂O₃ supported Mo₂C synthesized by reverse microemulsion method", **26th North American Catalysis Society Meeting**, June 2019, Chicago, IL, USA
- Guanjie, S., Zhuang, Y. & Simakov, D.S.A. "The effect of Ru promotion on the Cu/ZnO/Al₂O₃ catalytic performance in reverse water gas shift reaction", **26th North American Catalysis Society Meeting**, June 2019, Chicago, IL, USA
- Mottaghi-Tabar, S., Currie, R., Zhuang, Y. & Simakov, D.S.A. "The feasibility of the thermocatalytic conversion of CO₂ into Synthetic Natural Gas (SNG)", **12th Natural Gas Conversion Symposium**, June 2019, San Antonio, TX, USA
- Zhuang, Y., Mottaghi-Tabar, S., & Simakov, D.S.A. "Direct conversion of biogas into synthetic natural gas (SNG) over the 0.1-0.5wt% Ru/Al₂O₃ catalyst", **12th Natural Gas Conversion Symposium**, June 2019, San Antonio, TX, USA
- Simakov, D.S.A. "Techno-economic assessment of the Power-to-Gas system for Renewable Natural Gas production via biogas upgrading", **Value of Biogas East**, March 2019, Toronto, ON, Canada
- Currie, R., Mottaghi-Tabar, S., Zhuang, Y. & Simakov, D.S.A. "Design of an actively-cooled Sabatier reactor for thermocatalytic hydrogenation of CO₂: Model-based feasibility analysis and experimental proof-of-concept", **4th North American Symposium on Chemical Reaction Engineering**, March 2019, Houston, TX, USA

- Currie, R., Nikolic, D., Petkovska, M. & Simakov, D.S.A. "CO₂ conversion enhancement in a periodically operated Sabatier reactor: Nonlinear Frequency Response analysis and simulation-based study", **XXII International Conference on Chemical Reactors**, November **2018**, Ghent, Belgium
- Mottaghi-Tabar, S. & Simakov, D.S.A. "Techno-economic assessment of Power-to-Gas for synthetic natural gas production", **68th Canadian Chemical Engineering Conference**, October **2018**, Toronto, ON, Canada
- Simakov, D.S.A. "Thermocatalytic conversion of CO₂ into renewable synthetic fuels: catalysis and reactor design", **5th International School-Conference on Catalysis for Young Scientists**, May **2018**, Moscow, Russian Federation
- Zhuang, Y. & Simakov, D.S.A. "The effect of Ru promotion on the Cu/ZnO/Al₂O₃ catalytic performance in reverse water gas shift reaction", **25th Canadian Symposium on Catalysis**, May **2018**, Saskatoon, SK, Canada
- Zhuang, Y., Khan, F.M. & Simakov, D.S.A. "Supported transition metal carbides as catalysts for CO₂ conversion to syngas via reverse water gas shift reaction", **AIChE Annual Meeting**, November **2017**, Minneapolis, MN, USA
- Simakov, D.S.A. "Making Fuels from CO₂: Thermocatalytic conversion of CO₂ into renewable synthetic fuels", **67th Canadian Chemical Engineering Conference**, October **2017**, Edmonton, AB, Canada
- Currie, R., Khan, F.M., Zhuang, Y. & Simakov, D.S.A. "Design of a Sabatier reactor for CO₂ conversion into renewable natural gas: Heat removal and catalyst deactivation", **25th North American Catalysis Society Meeting**, June **2017**, Denver, CO, USA
- Currie, R. & Simakov, D.S.A. "Catalytic membrane reactor for CO₂ conversion into Renewable Natural Gas", **100th Canadian Chemistry Conference and Exhibition**, May **2017**, Toronto, ON, Canada
- Sun, D. & Simakov, D.S.A. "Design of a Sabatier Reactor for CO₂ Conversion into Synthetic Methane", **AIChE Annual Meeting**, November **2016**, San Francisco, CA, USA
- Sun, D. & Simakov, D.S.A. "Catalyst Coking in a Packed Bed Sabatier Reactor: Simulation-based Study", **66th Canadian Chemical Engineering Conference**, October **2016**, Quebec City, QC, Canada
- Sun, D. & Simakov, D.S.A. "Thermal management of a Sabatier reactor for chemical fixation of CO₂: simulation-based analysis and optimization", **XXII International Conference on Chemical Reactors**, September **2016**, London, UK
- Sun, D. & Simakov, D.S.A. "Thermo-catalytic conversion of CO₂ to CH₄ in a molten salt-cooled packed-bed reactor: simulation-based analysis", **24th Canadian Symposium on Catalysis**, May **2016**, Ottawa, ON, Canada
- Simakov, D.S.A. & Román-Leshkov Y. "Highly efficient methane reforming over the 0.15wt% Ru/γ-Al₂O₃ catalyst in the 5µm Pd-Ag film membrane reformer", **AIChE Annual Meeting**, November **2015**, Salt Lake City, UT, USA