Jonggeol Na

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RESEARCH INTERESTS

1. Autonomous design of non-intuitive process systems through artificial intelligence and robotics.
2. Multi-scale dynamic assessment of non-traditional processes for circular economy.

EMPLOYMENT

Assistant Professor (Mar. 2020 –)

Ewha Womans University, Seoul, Republic of Korea

Postdoctoral Research Fellow (Jul. 2019 – Feb. 2020)

Carnegie Mellon University, Pittsburgh, PA USA
- Principal Investigator: Professor Nikolaos V. Sahinidis

Postdoctoral Research Fellow (Mar. 2018 – Jun. 2019)

Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea
- Principal Investigator: Dr. Ung Lee

VISITING POSITION

Visiting Student (Aug. 2017 – Dec. 2017)

Massachusetts Institute of Technology (MIT), Cambridge, MA, USA
- Host Adviser: Professor Richard D. Braatz

EDUCATION

Ph.D. in Chemical and Biological Engineering (Mar. 2013 – Feb. 2018)

Seoul National University, Seoul, Republic of Korea
- Ph.D. Adviser: Professor Won Bo Lee
- Ph.D. Thesis on *Computational science approach for design and optimization of sustainable process and its industrial applications*

B.S. in Chemical and Biological Engineering with honors (*Cum Laude*) (Mar. 2009 – Feb. 2013)

Seoul National University, Seoul, Republic of Korea
- *Minor* Economics
- Senior Thesis Adviser: Professor Chonghun Han
- Senior Thesis on *Quantitative analysis of heat exchanger network synthesis for applying theoretical networks to the real industry*

Secondary Education in Science (Mar. 2006 – Feb. 2009)

Korea Science Academy of KAIST, Busan, Republic of Korea

AWARDS, FELLOWSHIPS, AND HONORS

Computers & Chemical Engineering (CACE) Best Paper Award, AIChE (2022)
Ewha Outstanding Research Grant (1st place), Ewha Womans University (2022)
AIChE Travel Award, Hanwha-Chemical&Total (2019)
DAELIM Graduate Research Award, DAELIM (2014)
KIChE Best Poster Presentation Award, KIChE (2014)
Korea Process Simulation Olympiad Invensys Award, KIChE (2012)
Doosan Heavy Industry Green Energy Project (1st place), Doosan Heavy Industry (2012)
Presidential Science Scholarship, National Research Foundation (Mar. 2009 – Feb. 2013)

Journal articles (refereed)

†Equally contributed, *Corresponding author

1. Lee, S.†, Choi, W.†, Kim, J. H., Park, S., Hwang, Y. J. *, **Na, J.*** (2023). Techno-economic analysis and life-cycle assessment of the electrochemical conversion process with captured CO_2 in amine-based solvent, *Energy & Environmental Science*, under review.

2. Kim, H.†, Choi, H.†, Kang, D.†, Lee, W. B. *, **Na, J.*** (2023). Materials Discovery with Extreme Properties via AI-Driven Combinatorial Chemistry, submitted.

3. Kang, D.†, Kang, D.†, Hwangbo, S., Niaz, H., Lee, W.B., Liu, J., **Na, J.*** (2023). Optimal Planning of Hybrid Energy Storage Systems using Curtailed Renewable Energy through Deep Reinforcement Learning. *Energy,* under review (2nd round).

4. Mok, D. H.†, Shin, D.†, **Na, J.***, Back, S.* (2023). Chemically Inspired Convolutional Neural Network using Electronic Structure Representation. *Journal of Materials Chemistry A,* accepted.

5. Akhtar, M. S., Khan, H., Liu, J. J.*, & **Na, J.** (2023). Green hydrogen and sustainable development–A social LCA perspective highlighting social hotspots and geopolitical implications of the future hydrogen economy. *Journal of Cleaner Production*, 395, 136438.

6. Jang, K., Hong, S., Kim, M., Moon, I.*, **Na, J.*** (2023). Explainable Artificial Intelligence for Fault Diagnosis of Industrial Processes. *IEEE Transactions on Industrial Informatics*, *Early Access.*.

7. Cho, S.†, Kim, M.†, Lee, J., Han, A., **Na, J.***, & Moon I.* (2023). Multi-objective Optimization of Explosive Waste Treatment Process Considering Environment and Process Cost via Bayesian Active Learning. *Engineering Applications of Artificial Intelligence, 117,* 105463.

8. Choi, W.†, Choi, Y.†, Choi, E., Yun, H., Jung, W., Lee, W. H., Oh, H.-S., Won, D.H., **Na, J.***, & Hwang, Y. J.* (2022). Microenvironments of Cu catalysts in zero-gap membrane electrode assembly for efficient CO_2 electrolysis to C_{2+} products. *Journal of Materials Chemistry A*, 10, 10363.
[Highlights on Front Cover Article]

9. Choi, W.†, Park, S.†, Jung, W.†, Won, D. H., **Na, J.***, & Hwang, Y. J.* (2022). Origin of Hydrogen Incorporated into Ethylene during Electrochemical CO_2 Reduction in Membrane Electrode Assembly. *ACS Energy Letters*, 7, 939-945.
[Highlights on Front Cover Article]

10. Seo, S. K., Yoon, Y. G., Lee, J. S., **Na, J.***, & Lee, C. J.* (2022). Deep Neural Network-based Optimization Framework for Safety Evacuation Route during Toxic Gas Leak Incidents. *Reliability Engineering & System Safety*, *218*, 108102.

11. Choi, S., Jung, I., Kim, H., **Na, J.***, & Lee, J. M.* (2022). Physics-informed deep learning for data-driven solutions of computational fluid dynamics. *Korean Journal of Chemical Engineering, 39*, 515-528.

12. Kim, M., Cho, S., Jang, K., Hong, S., **Na, J.***, Moon, I.*, Data-driven Robust Optimization for Minimum Nitrogen Oxide Emission Under Process Uncertainty. *Chemical Engineering Journal*. **2022**, 428, 130971.

13. Shin, S., Choi, S., **Na, J.**, Jung, I., Kim, M.-K, Park, M.-Y.*, Lee, W.B.*, CFD modeling for the prediction of molecular weight distribution in the LDPE autoclave reactor: Effects of non-ideal mixing. *Chemical Engineering Journal*. **2022**, 427, 131829.

14. Kim, H., **Na, J.***, & Lee, W. B.* (2021). Generative Chemical Transformer: Neural Machine Learning of Molecular Geometric Structures from Chemical Language via Attention. *Journal of Chemical Information and Modeling*, 61(12), 5804-5814.

[Highlights on Back Cover Article]

15. Jung, B.†, Park, S.†, Lim, C., Lee, W.H., Lim, Y., **Na, J.**, Lee, C.-J., Oh, H.-S.*, Lee, U.*, Design methodology for mass transfer-enhanced large-scale electrochemical reactor for CO_2 reduction. *Chemical Engineering Journal*, **2021**, *424*, 130265.

16. Kim, D., Choi, W., Lee, H.W., Lee, S.Y., Choi, Y., Lee, D.K., Kim, W., **Na, J.**, Lee, U.*, Hwang, Y.J.*, Won, D.H.*, Electrocatalytic Reduction of Low Concentrations of CO_2 Gas in a Membrane Electrode Assembly Electrolyzer. *ACS Energy Letters*. **2021**, 6(10), 3488-3495.

17. Shams, M.H., Niaz, H., **Na, J.**, Anvari-Moghaddam, A.*, Liu J., Machine learning-based utilization of renewable power curtailments under uncertainty by planning of hydrogen systems and battery storages. *Journal of Energy Storage.* **2021**, 41, 103010.

18. **Na, J.**, Bak, J.H., Sahinidis, N.*, Efficient Bayesian inference using adversarial machine learning and low-complexity surrogate models. *Computers & Chemical Engineering,* **2021**, 151, 107322.
[Computers & Chemical Engineering: 2021 Best Paper Award]

19. Lee, D., **Na, J.**, Park, D., Lee, J.M.*, Bayesian Optimization of Semicontinuous Carbonation Process Operation Recipe. *Industrial & Engineering Chemistry Research*. **2021**, *60(27),* 9871-9884.

20. Park, S., Atwair, M., Kim, K., Lee, U., **Na, J.**, Zahid, U.*, Lee, C.-J.*, Bayesian optimization of industrial-scale toluene diisocyanate liquid-phase jet reactor with 3-D computational fluid dynamics model. *Journal of Industrial and Engineering Chemistry*, **2021,** *98*, 327-339.

21. Park, D., **Na, J.**, Lee, J.M.*, Clustered Manifold Approximation and Projection for Semisupervised Fault Diagnosis and Process Monitoring. *Industrial & Engineering Chemistry Research*. **2021**, *60(26),* 9521-9531.

22. Jang, K., Hong, S., Kim, M., **Na, J.***, & Moon, I.* (2021). Adversarial Autoencoder Based Feature Learning for Fault Detection in Industrial Processes. *IEEE Transactions on Industrial Informatics*, *18*(2), 827-834.

23. Back, S.†, **Na, J.†**, & Ulissi, Z.*, Efficient Discovery of Active, Selective, and Stable Catalysts for Electrochemical H_2O_2 Synthesis through Active Motif Screening. *ACS Catalysis,* **2021**, *11(5)*, 2483-2491.

24. Park, S.†, Wijaya, D. T.†, **Na, J.***, & Lee, C. W.* Towards the Large-Scale Electrochemical Reduction of Carbon Dioxide. *Catalysts*, **2021**, *11(2)*.

25. Kim, J.†, **Na, J.†**, Kim, K., Bak, J.H., Lee, H., & Lee, U.* Learning the properties of a water-lean amine solvent from carbon capture pilot experiments. *Applied Energy,* **2021,** *283*, 116213.

26. Back, S.†, **Na, J.†**, Tran, K. & Ulissi, Z. W. In silico discovery of active, stable, CO-tolerant and cost-effective electrocatalysts for hydrogen evolution and oxidation. *Physical Chemistry Chemical Physics*. **2020**, *22*, 19454-19458.

27. Sa, Y. J.†, Lee, C. W.†, Lee, S. Y.†, **Na, J.**, Lee, U.*, & Hwang, Y. J.* Catalyst–electrolyte interface chemistry for electrochemical CO_2 reduction. *Chemical Society Reviews*. **2020**, 49, 6632-6665.

28. Kim, K., Lee, W. H., **Na, J.**, Hwang, Y. J., Oh, H.-S., & Lee, U.*, Data driven pilot optimization for electrochemical CO mass production. *Journal of Materials Chemistry A*. **2020**, *44,* 8781–8798.

29. Lee, H. W., Kim, K., An, J., **Na, J.**, Kim, H., Lee, U.* Toward the practical application of direct CO2 hydrogenation technology for methanol production. *International Journal of Energy Research*. **2020**, *44(11)*, 1– 18.

30. Nguyen, D. L. T.†, Lee, C. W.†, **Na, J.†**, Kim, M.-C. Tu, N. D. K., Lee, S. Y., Sa, Y. J., Won, D.

H., Oh, H.-S., Kim, H., Han, S. S., Min, B. K., Lee, U.[*], Hwang Y. J.[*], Mass transport control by surface graphene oxide for selective CO production from electrochemical CO_2 reduction. *ACS Catalysis,* **2020**, *10(5),* 3222-3231.

31. **Na, J.**, Seo, B., Kim, J., Lee, C. W., Lee, H., Hwang, Y. J., Min, B. K., Lee, D. K., Oh, H.-S.[*], Lee, U[*], General technoeconomic analysis for electrochemical coproduction coupling carbon dioxide reduction with organic oxidation. *Nature Communications.* **2019**, *10*, 5193.
[Also appeared in *Nature Research Device and Materials Engineering Community*, 2019]
[Editor's Highlights in Nature Communications]

32. Lee, Y., Jeon, K., Cho, J., **Na, J**, Park J., Jung, I., Park, J., Park, M.J., Lee, W.B.[*], Multicompartment Model of an Ethylene–Vinyl Acetate Autoclave Reactor: A Combined Computational Fluid Dynamics and Polymerization Kinetics Model. *Industrial & Engineering Chemistry Research.* **2019**, *58*, 16459-1641.

33. Hwang, J., Kim, J., Lee, H. W., **Na, J.**, Ahn, B. S., Lee, S. D., Kim, H.S., Lee, H., Lee, U.[*], An experimental based optimization of a novel water lean amine solvent for post combustion CO2 capture process. *Applied Energy.* **2019**, *248*, 174-184.

34. **Na, J**.†, Park, S.†, Bak, J. H., Lee, D., Yoo, Y., Kim, I., Park, J., Lee, U., Lee, J.M.[*], Bayesian Parameter Estimation of Aqueous Mineral Carbonation Kinetics. *Industrial & Engineering Chemistry Research*. **2019**, *58(19)*, 8246-8259.

35. Jeon, K., Yang, S., Kang, D., **Na, J.**, Lee, W.B.[*], Development of surrogate model using CFD and deep neural networks to optimize gas detector layout. *Korean Journal of Chemical Engineering*. **2019**, *36(3)*, 325-332.

36. Lee, Y.†, **Na, J.**†, Lee, W.B.[*], Robust design of ambient-air vaporaizer based on time-series clustering. *Computers & Chemical Engineering.* **2018,** *118*, 236-247

37. Park, S., **Na, J.**, Kim, M., Lee, J.M.[*], Multi-objective Bayesian optimization of chemical reactor design using computational fluid dynamics. *Computers & Chemical Engineering.* **2018,** *119*, 25-37.

38. Lee, W.-J.†, **Na, J.**†, Kim, K., Lee, C., Lee, Y., Lee, J.M.[*], NARX Modeling for Real-Time Optimization of Air and Gas Compression Systems in Chemical Processes. *Computers & Chemical Engineering.* **2018**, *115,* 262-274.

39. **Na, J.**†, Kshetrimayum, K. S.†, Jung, I., Park, S., Lee, Y., Kwon, O., Mo, Y., Chung, J., Yi, J., Lee, U., Han, C.[*], Pilot Scale Compact Gas-to-Liquid Process: Design and Operation of Microchannel Reactor for Fischer-Tropsch Synthesis. *Chemical Engineering and Processing: Process Intensification*. **2018**, *128,* 63-76.

40. **Na, J.**†, Jeon, K.†, Lee, W.-B.[*], Toxic gas release modeling for real-time analysis using variational autoencoder with convolutional neural networks. *Chemical Engineering Science*, **2018**. *181,* 68-78.

41. Kim, M., **Na, J.**, Park, S., Park, J.-H., Han, C.[*], Modeling and validation of a pilot-scale aqueous mineral carbonation reactor for carbon capture using computational fluid dynamics. *Chemical Engineering Science*, **2018**, *177,* 301-312.

42. An, J.†, **Na, J.**†, Lee, U.[*], Han, C.[*], Design of carbon dioxide dehydration process using derivative-free superstructure optimization. *Chemical Engineering Research and Design* **2018,** *129*, 344-355.

43. Shin, S., Lee, G., Ahmed, U., Lee, Y., **Na, J.**, Han, C.[*], Risk-based underground pipeline safety management considering corrosion effect. *Journal of Hazardous Materials* **2018,** *342* (Supplement C), 279-289.

44. Kshetrimayum, K., **Na, J.**, Park, S., Jung, I., Lee, Y., Han, C., Intensified Low-Temperature

Fischer-Tropsch Synthesis Using Microchannel Reactor Block: A Computational Fluid Dynamics Simulation Study. *Journal of the Korean Institute of Gas* **2017,** *21* (4), 92-102.

45. **Na, J.**, Lim, Y., Han, C.*, A modified DIRECT algorithm for hidden constraints in an LNG process optimization. *Energy* **2017,** *126*, 488-500.

46. **Na, J.**, Kshetrimayum, K. S., Lee, U.*, Han, C.*, Multi-objective optimization of microchannel reactor for Fischer-Tropsch synthesis using computational fluid dynamics and genetic algorithm. *Chemical Engineering Journal* **2017,** *313*, 1521-1534.

47. Jung, I., **Na, J.**, Park, S., Jeon, J., Mo, Y.-G., Yi, J.-Y., Chung, J.-T., Han, C.*, Optimal design of a large scale Fischer-Tropsch microchannel reactor module using a cell-coupling method. *Fuel Processing Technology* **2017,** *159*, 448-459.

48. Park, S., **Na, J.**, Kim, M., An, J., Lee, C., Han, C., CO2 Mineral Carbonation Reactor Analysis using Computational Fluid Dynamics: Internal Reactor Design Study for the Efficient Mixing of Solid Reactants in the Solution. *Korean Chemical Engineering Research* **2016,** *54* (5), 612-620.

49. Shin, S., Lee, Y., Song, K., **Na, J.**, Park, S., Lee, Y., Lee, C.-J., Han, C.*, Design and economic analysis of natural gas hydrate regasification process combined with LNG receiving terminal. *Chemical Engineering Research and Design* **2016,** *112*, 64-77.

50. Park, S., Jung, I., Lee, Y., Kshetrimayum, K. S., **Na, J.**, Park, S., Shin, S., Ha, D., Lee, Y., Chung, J., Lee, C.-J.*, Han, C.*, Design of microchannel Fischer–Tropsch reactor using cell-coupling method: Effect of flow configurations and distribution. *Chemical Engineering Science* **2016,** *143*, 63-75.

51. Kshetrimayum, K. S., Jung, I., **Na, J.**, Park, S., Lee, Y., Park, S., Lee, C.-J.*, Han, C.*, CFD Simulation of Microchannel Reactor Block for Fischer–Tropsch Synthesis: Effect of Coolant Type and Wall Boiling Condition on Reactor Temperature. *Industrial & Engineering Chemistry Research* **2016,** *55* (3), 543-554.

52. Jung, I., Kshetrimayum, K. S., Park, S., **Na, J.**, Lee, Y., An, J., Park, S., Lee, C.-J.*, Han, C.*, Computational Fluid Dynamics Based Optimal Design of Guiding Channel Geometry in U-Type Coolant Layer Manifold of Large-Scale Microchannel Fischer–Tropsch Reactor. *Industrial & Engineering Chemistry Research* **2016,** *55* (2), 505-515.

53. Lee, Y., Jung, I., **Na, J.**, Park, S., Kshetrimayum, K. S., Han, C., Analysis on Thermal Effects of Process Channel Geometry for Microchannel Fischer-Tropsch Reactor Using Computational Fluid Dynamics. *Korean Chemical Engineering Research* **2015,** *53* (6), 818-823.

54. Park, S., Jung, I., Lee, U., **Na, J.**, Kshetrimayum, K. S., Lee, Y., Lee, C.-J.*, Han, C.*, Design and modeling of large-scale cross-current multichannel Fischer–Tropsch reactor using channel decomposition and cell-coupling method. *Chemical Engineering Science* **2015,** *134*, 448-456.

55. **Na, J.**, Jung, J., Park, C., Han, C.*, Simultaneous synthesis of a heat exchanger network with multiple utilities using utility substages. *Computers & Chemical Engineering* **2015,** *79*, 70-79.

56. **Na, J.**, Jung, I., Kshetrimayum, K. S., Park, S., Park, C., Han, C., Computational Fluid Dynamics Study of Channel Geometric Effect for Fischer-Tropsch Microchannel Reactor. *Korean Chemical Engineering Research* **2014,** *52* (6), 826-833.

57. Park, C., Jung, I., Park, S., **Na, J.**, Kshetrimayum, K., Han, C., Lee, J. Y., Jung, J., Modeling of Liquid Hold-up in Fixed-bed Reactor for Fischer-Tropsch Synthesis. *Journal of the Korean Institute of Gas* **2014,** *18* (4), 63-67.

58. Park, S., Park, C., Lee, U., Jung, I., **Na, J.**, Kshetrimayum, K. S., Han, C.*, Comparative Study of Process Integration and Retrofit Design of a Liquefied Natural Gas (LNG) Regasification Process Based on Exergy Analyses: A Case Study of an LNG Regasification Process in Republic of Korea. *Industrial & Engineering Chemistry Research* **2014,** *53* (37), 14366-14376.

59. Jung, I., Park, C., Park, S., **Na, J.**, Han, C.[*], A Comparative Study of Various Fuel for Newly Optimized Onboard Fuel Processor System under the Simple Heat Exchanger Network. *Korean Chemical Engineering Research* **2014,** *52* (6), 720-726.

60. Jung, J., Song, K., Park, S., **Na, J.**, Han, C.[*], Optimal operation strategy of batch vacuum distillation for sulfuric acid recycling process. *Computers & Chemical Engineering* **2014,** *71,* 104-115.

[First and corresponding authored papers featured as journal covers/highlights]

Proceedings, Reports, and Expositions

1. **Na, J.** Autonomous discovery in the process systems design. *NICE (News & Information for Chemical Engineers)* **2021**, *39.2,* 207-216.

2. **Na, J.**, Lee, U. Research trends of process optimization using machine learning and its applications. *NICE (News & Information for Chemical Engineers)* **2018**, *36.1,* 4-8.

3. Lee, Y., **Na, J.**, Lee, W.-B. Optimal Design of an Ambient Air Vaporizer using Numerical Model and DIRECT Algorithm. *Computer Aided Chemical Engineering* **2018**, *44* (eds Mario R. Eden, Marianthi G. Ierapetritou, & Gavin P. Towler), 1795-1800.

4. **Na, J.**, Jung, J., Park, C., Han, C., Simultaneous Optimization Models for Heat Exchanger Network Synthesis with Multiple Utilities: A New Strategy by Using Utility Sub-stage. *Computer Aided Chemical Engineering* **2015,** *33 (eds Jiří Jaromír Klemeš, Petar Sabev Varbanov, & Peng Yen Liew),* 1675-1680.

5. Kshetrimayum, K. S., Park, S., Jung, I., **Na, J.**, Han, C. Simulation Study of Heat Transfer Enhancement due to Wall Boiling Condition in a Microchannel Reactor Block for Fischer-Tropsch Synthesis. *Computer Aided Chemical Engineering* **2015,** *37 (eds Krist V. Gernaey, Jakob K. Huusom, & Rafiqul Gani),* 1355-1360.

PATENT	1. **KR 1020210149307** "DEVICE FOR DESIGNING MATERALS" (2021.11.03 Application)
	2. **KR 1021552360000** "Ether-functional Diamine-based Carbon Dioxide Absorbents having a Low Regeneration Energy" (2020.09.07 Registered)
	3. **KR 1021968200000** "APPARATUS AND METHOD FOR RELEASE MODELING OF TOXIC GASES" (2020.12.23 Registered)
	4. **KR 1017114660000** "CARBON DIOXIDE COLLECTING APPARATUS USING ROTATING REACTOR" (2017.02.23 Registered)

INVITED CONFERENCE TALKS	• *Taiwan-Japan-Korea-Czech International Symposium on Chemical Engineering (2022 TJKC-ISCE),* "Autonomous Product and Process Design Using Reinforcement Learning", Dec. 2-3, 2022. Tamkang University, Taiwan.
	• *Korean Society of Industrial and Engineering Chemistry Fall Meeting, JPI-KSIEC Joint Symposium*, "Can electrochemical processes compete with conventional petrochemical industry?", Nov. 3, 2022, Daejon, Republic of Korea.
	• *Conference of The Korean Society of Clean Technology*, "Electrochemical chemical production processes in terms of circular economy", Sep. 22, 2022. Jeju Island, Republic of Korea.
	• *Practical View of Artificial Photosynthesis,* "Electrochemistry-based chemical production processes as circular economy", Aug. 26, 2022. Busan, Republic of Korea.
	• *Mathematics in (bio)Chemical Kinetics and Engineering (MaCKiE),* "Generative Chemical Transformer: Neural Machine Learning of Molecular Geometric Structures from Chemical Language via Attention", Oct. 25, 2021. Shanghai, China.
	• *Invited Flash Presentation.* "General technoeconomic analysis for electrochemical coproduction coupling carbon dioxide reduction with organic oxidation". Nov. 13, Emerging Junior Investigator Open Innovation Forum', Hanwha Travel Award at 2019 AIChE Annual Meeting, Orlando, USA.
	• *KSASF in Korea Science Academy, Invited sectional lecturer. "What are Differences between Science and "Engineering": How Your Course Works Can Be Applied in The Real Engineering Industry?".* Aug. 16th, 2015. Korea Science Academy of KAIST, Busan, Republic of Korea.

INVITED SEMINARS AND COLLOQUIA	• *Invited Seminar. "Digital transformation through CFD compartment modeling & physics-informed ML". Aug*. 10, 2022. SK Innovation, Daejeon, Republic of Korea.
	• *Invited Seminar. "Optimization-based process design in process systems engineering". Jul*. 08, 2022. SK Innovation, Daejon, Republic of Korea
	• *Invited Seminar*. "Autonomous discovery for process and product design". Jul. 12, 2022. Korea Research Institute of Chemical Technology (KRICT), Daejeon, Republic of Korea.
	• *Invited Seminar*. "Physics-informed deep learning for data-driven solutions of computational fluid dynamics". Jun. 21, 2022. Hyundai Motors, Pangyo, Republic of Korea.
	• *Invited Seminar. "Autonomous Discovery for Process and Product Design". May*. 24, 2022. UNIST, Ulsan, Republic of Korea
	• *Colloquium. "Electrochemcial Carbon Dioxide Reduction: Device and Process". Feb*. 07, 2022. Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea
	• *Invited Seminar. "Autonomous Design of Products and Processes". Dec*. 30, 2021. EDRC, Seoul National University, Seoul, Republic of Korea
	• *Invited Seminar*. "Pilot Scale compact GTL Process: Design and Operation of Microchannel Fischer-Tropsch Reactor". Dec. 09, 2021. Korea Institute of Machinery & Materials (KIMM), Daejeon, Republic of Korea
	• *Invited Seminar*. "Artificial Intelligence for Process and Product Design". Dec. 01, 2021. Seoul National University College of Medicine, Seoul National University, Seoul, Republic of Korea
	• *Invited Seminar*. "Explainable Artificial Intelligence for Process and Product Design". May. 13,

2021. Korea Research Institute of Chemical Technology (KRICT), Daejeon, Republic of Korea

- *Invited Seminar. "Machine Learning Technologies Towards Enhancing Interpretability in Process Systems Engineering". Jan*. 13, 2021. EDRC, Seoul National University, Seoul, Republic of Korea
- *Invited Seminar. "Machine Learning and Multiscale Simulations Towards Enhancing Interpretability in Chemical Engineering". Apr*. 01, 2020. Ewha Womans University, Seoul, Republic of Korea
- *Invited Seminar. "Digital Twin: Manufacturing of Thin Films for Pharmaceutical Applications". Nov*. 05, 2020. Process Systems & Safety Engineering Laboratory, Chung-Ang University, Seoul, Republic of Korea
- *Invited Seminar. "Stochastic multiscale model-based optimal design and control via Bayesian inference and polynomial chaos expansion".* Nov. 19, 2019. Process Systems & Safety Engineering Laboratory, Chung-Ang University, Seoul, Republic of Korea
- *Invited Seminar. "Stochastic multiscale model-based optimal design and control via Bayesian inference and polynomial chaos expansion".* Nov. 19, 2019. Process Systems & Safety Engineering Laboratory, Chung-Ang University, Seoul, Republic of Korea
- *Invited Seminar.* "Computational science approach for applying artificial intelligence to process systems engineering field". Feb. 29, 2019. Yonsei University, Seoul Republic of Korea
- *SNU-KIST joint Seminar*, Invited speaker. "General techno-economic analysis for paired electrolysis of CO_2 reduction and anodic oxidation". Feb. 15, 2019. Seoul National University, Seoul Republic of Korea
- *NTNU-SNU-KIST joint Seminar, Invited speaker*. "Stochastic model development using Bayesian inference and its applications". Oct. 19, 2018. Seoul National University, Seoul Republic of Korea
- *Invited Seminar. "Current issues on autoclave reactor multi-scale modeling and simulation for polyethylene and its copolymers (EVA, EAA)".* Oct. 1st, 2018. SK Innovation, Daejeon, Republic of Korea
- *Invited Seminar. "Toxic gas release modeling for real-time analysis using variational autoencoder with convolutional neural networks".* Aug. 8th, 2018. Process Systems & Safety Engineering Laboratory, Chung-Ang University, Seoul, Republic of Korea
- *Invited Seminar. "Derivative-free optimization using modified DIRECT algorithm for black-box models with hidden constraints".* Mar. 28th, 2016. Offshore Process Systems Engineering Laboratory, Seoul National University, Seoul, Republic of Korea

INVITED LECTURE SERIES

- *Invited Short Courses. "Introduction to Reinforcement Learning". Dec*. 28, 2021. EDRC, Seoul National University, Seoul, Republic of Korea
- *Invited Short Courses.* "인공지능과 빅데이터 활용 에너지 시스템 최적화 연구". Nov. 25, 2021. Dongkuk University, Gyeongju, Republic of Korea
- *Invited Lecturer. "Introduction to process systems engineering and related software (Aspen Plus, Hysys, Fluent)",* Apr. 20th, 2016. Engineering Development Research Center, Seoul National University, Seoul, Republic of Korea

OTHER CONFERENCES ATTENDED AS A PARTICIPANT

[International]
- AIChE Phoenix, United States. Nov. 2022.
  "Decision-Making Optimization of Hybrid Energy Management System for Curtailed Renewable Energy through Deep Reinforcement Learning"
- AIChE Virtual meeting, United States. Nov. 2020.
  "Efficient Bayesian Inference for First-Principle Simulation Via Adversarial Networks and Low-Complexity Surrogate Models"

- *AIChE* Orlando, FL, United States. Nov. 2019.
  "General Techno-Economic Analysis for Electrochemical Coproduction of CO_2 Reduction and Anodic Oxidation"
- *AIChE* Pittsburgh, PA, United States. Oct. 2018.
  "Stochastic Multiscale Model-Based Predictive Control Via Polynomial Chaos Theory: Manufacturing of Thin Films for Pharmaceutical Applications"
- *PSE ASIA* Tokyo, Japan. Jul. 2016.
  "Derivative-Free Optimization Using Modified DIRECT Algorithm for Black-Box Models with Unknown Infeasible Region"
- *AIChE* Salt Lake City, Utah, United States. Nov. 2015.
  "Multi-Objective Optimization for High Heat Removal and Productivity in Fischer-Tropsch Synthesis Microchannel Reactor Using Discrete Catalyst Dilution Zone"
- *ESCAPE* Budapest, Hungary. Jun. 2014
  "Simultaneous Optimization Models for Heat Exchanger Network Synthesis with Multiple Utilities: A New Strategy by Using Utility Sub-stage"

[Domestic]
- *KSIEC* Daegu, Repulic of Korea. Nov. 2021
  "Conceptual design of non-equilibrium ultrasonic separation for clean chemical processes"
- *KSIEC* Busan, Repulic of Korea. May. 2021
  "Conditional variational de novo molecular generation based on a deep understanding of chemical language"
- *KSBB* Jeju Island, Repulic of Korea. Apr. 2021
  "Process design and assessment of electrochemical carbon and nitrogen reduction processes"
- *KIChE* Busan, Republic of Korea. Apr. 2021
  "Supervised machine learning techniques for process and reactor modeling"
- *KIChE Online*, Republic of Korea. Oct. 2020
  "Efficient Bayesian Inference for First-Principle Simulation Via Adversarial Networks and Low-Complexity Surrogate Models"
- *KSIEC* Gwangju, Repulic of Korea. Oct. 2020
  "Physics-informed deep learning for data-driven solutions of computational fluid dynamics"
- *KIChE* Daegu, Republic of Korea. Oct. 2018
  "The electrochemical CO_2 reduction process using solar energy: multi-scale simulation, techno-economic analysis, and pilot plant"
- *KIChE* Changwon, Republic of Korea. Apr. 2018.
  "Toxic gas release modeling for real-time analysis using variational autoencoder with convolutional neural networks"
- *KIChE* Daejun, Republic of Korea. Oct. 2016.
  "A Model of Mineral Carbonation Kinetics for Carbon Capture, Utilization and Storage (CCUS) Technology"
- *KIChE* Busan, Republic of Korea. Apr. 2016.
  "Developing simultaneous design procedure for carbonation reactor and CCU process using integrated platform of process simulator and CFD"
- *KIChE* Jeju, Republic of Korea. Apr. 2015.
  "Multi-Objective Optimization in Discrete Catalyst Dilution Zone of Fischer-Tropsch Microchannel Reactor"
- *KIChE* Daejeon, Republic of Korea. Oct. 2014.
  "Text Analytics in Chemical Accident Databases for Extracting Knowledge"
- *KIChE* Changwon, Republic of Korea. Apr. 2014.
  "Computational Fluid Dynamics Study of Channel Geometric Effect for Fischer-Tropsch

Microchannel Reactor"
- *KIGAS* Jeju, Republic of Korea. Nov. 2013.
"Quantitative Analysis of Heat Exchanger Network Synthesis for Applying Theoretical Networks to the Gas Industry"
- *KIChE* Daegu, Republic of Korea. Oct. 2013.
"Simultaneous Optimization Models for Multiple Utility Heat Exchanger Networks"

RESEARCH GRANT

- [산업체, Feb. 2023 – May. 2023] SK E&S:
CCUS를 위한 광물탄산화 다상반응기 전산유체역학 시뮬레이션
- [산업체, Aug. 2022] SK Innovation:
암모니아 제조 공정의 기술 타당성 검토.
- [산업체, Mar. 2022 – Feb. 2023] 삼성전자:
Diffusion 공정의 ALD 표면 화학반응 시뮬레이션 모델 개발.
- [NRF, Apr. 2022 – Dec. 2026] 원천연구개발사업 – 바이오·의료기술개발사업:
목질계 바이오매스의 통합 e-Biorefinery 기술개발.
- [NRF, Jun. 2021 – Feb. 2024] 이공분야기초연구사업 – 기초연구실:
지속가능 AI 기반 실시간 동적 한국형 수소공급망 설계 플랫폼 개발.
- [KIAT, Apr. 2021 – Dec. 2025] 제조분야 온실가스 미세먼지 동시저감 기술개발사업:
석유화학공정 휘발성유기화합물의 촉매연소와 동적 시뮬레이션 기반 공정효율 최적화 기술개발.
- [NRF, Mar. 2021 – Feb. 2025] 이공분야기초연구사업 – 우수신진연구:
화학 제품 및 공정 자율설계를 위한 폐루프 인공지능 시스템 개발.
- [NRF, Jan. 2021 – Feb. 2024] 원천연구개발사업 – C1 가스 리파이너리 사업:
셰일가스로부터 BTX 제조를 위한 촉매기술 및 연속공정 개발.
Methane-to-PHA and CO-to-formate 공정 TEA/LCA 분석
- [KIAT, Jan. 2021 – Dec. 2021] 산업기술혁신사업:
산업단지 폐부산물 폐쇄순환 그리드 시스템 개발.
- [NRF, Sep. 2020 – Aug. 2027] 4단계BK21사업 – 혁신인재양성:
4IR (4th industrial Revolution)-기반 헬스케어 전문인력 양성사업단.
- [NRF, Jul. 2020 – Jan. 2025] 원천기술개발사업 – Carbon to X 기술개발사업:
이산화탄소 전환 포름산제조 반응기 설계를 위한 멀티스케일 모델링 및 시뮬레이션.
- [NRF, Jun. 2020 – May. 2021] 이공분야기초연구사업 – 기본연구:
전기화학적 공생산과 비평형 초음파 분리를 이용한 차세대 청정화학공정 개념설계 및 기술경제성평가.

PROFESSIONAL ACTIVITIES & SERVICE

Professional affiliations
- American Institute of Chemical Engineers, 2015 – present
- Korea Institute of Chemical Engineers, 2013 – present
  - 공정시스템 부문위원회 학술간사, Jan. 2021 – Dec. 2021
  - 공정시스템 부문위원회 교육간사, Jan. 2022 – Dec. 2022
- Korean Society of Industrial and Engineering Chemistry, 2020 – present
  - 화학공정분과 재무간사, Jan. 2022 – Dec. 2022

Public service

- Referee for journals
  - *Computers & Chemical Engineering*
  - *Energy and Environmental Science*
  - *Industrial & Engineering Chemistry Research*
  - *Chemical Engineering Science*
  - *Chemical Engineering Research and Design*
  - *Korean Journal of Chemical Engineering*
  - *Korean Chemical Engineering Research*

TEACHING
EXPERIENCE

Courses
- Ewha Womans University, Seoul, Republic of Korea
  - Chemical process design (2020 spring, 2021 spring, 2022 spring)
  - Process control systems (2020 fall, 2021 fall, 2022 fall)
  - Applied mathematics (2020 spring, 2021 spring, 2022 spring)
  - Chemical engineering experiment I (2022 fall)
  - Computer-aided design in chemical engineering (2020 fall)
  - Reinforcement learning for systems engineering (2021 fall, 2022 fall)
  - Introduction to system health for BK21 (2021 spring, 2022 spring)

Adviser and Mentorship
- **Ewha Womans University**, Seoul, Republic of Korea
  - Ph.D. Students
    Juyeon Kim, 2021 – present
    Areum Han, 2022 – present
  - M.S. Students
    Yesong Lee, 2021 – present
    Doeun Kang, 2021 – present
    Chaeeun Lee, 2021 – present
    Haeyeon Choi, 2022 – present
    Daeun Shin, 2022 – present
    Yubin Ryu, 2022 – present
    Sunyoung Lee, 2022 – present
    Suhyun Lee, 2022 – present
    Jiwoo Ha, 2022 – present
    Sumin Hwangbo, 2022 – present
    Yuna Ko, 2022 – present
    Youngwon Lee, 2022 – present
  - Adviser, process design Olympiad by KIChE
    최우수상 with team 여름이었다 (Daeun Lee, Soojeong Ahn, Hwajin Yu), 2022

    입선 with team WEGO (Hyerim kim, Yurim Jeong, Nakyung Chae), 2022

    장려상 with team Lumos (Jiin Na, Yejin Yu, Hayeon Kim, Somin Chae), 2021

    입선 with team 비기너스럭 (Seoyeon Kim, Heejin Koo, Yoonseo Kim, Hakyung Lee), 2021

    대상 with Team O.A.O (Daeun Shin, Jiwoo Ha, Shihyun Woo, Sohyun Park), 2020

    우수상 with Team N.D.G (Myungsun Kim, Hayoung Jeong, Jungmin An, Jiyoon Jang), 2020
  - Adviser, LG Chem. Petrochemical Olympiad
    Gold medal at productivity optimization section with Team Ptime (Heesu Woo, Yuhyeon Kim, Chaewon Yoon), 2022

Silver medal at process safety section with Team DARK DIMENSION (Yoona Ko, Sukyung Kim, Yungwon Lee), 2022

- **Carnegie Mellon University**, Pittsburgh, PA, United States
    - *Adviser*, MS. students (Swapnil Agrawal, Lihan Liu, Kanishk Mair, Muyi Song, Yao Zhao) graduation projects related to "black-box optimization", Jul. 2019 – Present.
- **Korea Institute of Science and Technology**, Seoul, Republic of Korea
    - *Adviser*, Ph.D. candidates (Donggu Han, Hee Won Lee, Michael Shincheon Jee) projects related to "electrochemical CO_2 reduction and C1 chemicstry", Mar. 2018 – Jun. 2019.
- **Yeonsei University**, Seoul, Republic of Korea
    - *Co-Adviser with Prof. Il Moon*,
    Minsu Kim (2020 – present)
    Kyojin Jang (2020 – present)
- **Seoul National University**, Seoul, Republic of Korea
    - *Co-Adviser with Prof. Won Bo Lee*,
    Seungwoo Kim (2021 – present)
    Hyunseung Kim (2020 – present)
    Woojin Kang (2020 – present)
    Sunkyu Shin (2020 – present)
    Seung Jae Kwak (2019 – 2021)
    Changjoon Ko (2019 – 2020)
    - *Adviser*, MS. Exchange program by EDRC, Mar. 2016 – Jul. 2016.
    - *Adviser*, process design Olympiad by KIChE, Jun. 2015 – Aug. 2015.
    - *Adviser*, process design Olympiad by KIChE, Jun. 2014 – Aug. 2014.

Short Courses
- KIChE Tutorial Series
    - *Speaker*, Introduction to Techno-economic Analysis and Life-cycle Assessment for Chemical Process I and II, 2022
    - *Organizer/Chair/Specker*, Artificial Intelligence Based Chemical Process Technologies, 2021

Teaching assistant
- Seoul National University, Seoul, Republic of Korea
    - Chemical & biological engineering process experiment, Spring 2015.
    - Chemical & biological engineering basic experiment, Fall 2014.
- EDRC (Engineering Development Research Center), Seoul National University, Seoul, Republic of Korea
    - Thermodynamics for chemical engineering, Apr. 2016.
    - Advanced oil&gas process design, Mar. 2016.
    - Advance reactor design, Aug. 2015.
    - Conceptual design and techno-economic analysis, Jan. 2015.

TECHNICAL SKILLS
- Programming Language: Matlab, GAMS, Python, Fortran, C++
- Simulations: Aspen (Plus/HYSYS), gPROMS, CFD (Fluent/CFX/COMSOL/OpenFOAM), Tensorflow, Keras, PyTorch, KMC (Zacros), DFT (VASF)

REFERENCES

Nikolaos V. Sahinidis (Postdoc advisor)
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H. Milton Stewart School of Industrial & Systems Engineering
and School of Chemical & Biomolecular Engineering
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Ung Lee (Postdoc advisor)
Principal Research Scientist
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Seoul, 02792, Republic of Korea
ulee@kist.re.kr
http://kist-cepl.com