

# Shannon Q. Fernandes

✉ shanferns12@gmail.com    🌐 shanferns.github.io    GitHub    Google Scholar

## STATEMENT

Shannon develops computationally efficient, physics-based compartmental models—incorporating electrophysiology, soft tissue mechanics, and fluid dynamics—to simulate stomach motility and gastric emptying at a systems level. His work enables real-time, closed-loop control of gastrointestinal function and extends to modeling diseased states and gut-brain interactions, including vagal regulation. He is currently focused on integrating vagal nerve stimulation (VNS) into personalized therapies, in collaboration with institutions such as Emory University and Harvard Medical School.

Digital Twins • Physics-Informed Modeling • Reduced-Order Multi-Physics Simulation • Closed-Loop Physiological Control (NMPC) • Neuromodulation (VNS/taVNS) • Hybrid AI–Mechanistic Models • MRI Analysis and 4D Segmentation • CFD and Molecular dynamics

## EDUCATION

<b>Lehigh University</b> — Ph.D. in Chemical and Biomolecular Engineering	Pennsylvania, USA
CGPA: 3.91/4.0 — 2024–2025: John C. Chen Fellow (Prof. Kothare's Lab)	Aug. 2020 – 2025 (Expected)
<b>Thesis Title:</b> Gastric emptying initiated by neural stimuli- A Compartmental Modeling Approach	
<b>Abu Dhabi University</b> — B.Sc. in Chemical Engineering	Abu Dhabi, UAE
CGPA: 3.99/4.0 — 2016–2020: Dean's List in All Academic Semesters	Sept. 2016 – June 2020
<b>Design Project:</b> Natural Gas (NG) Purification	

## RESEARCH EXPERIENCE

- **Fernandes, S. Q.**, & Kothare, M. V. (2025). Nonlinear Model Predictive Control Framework to Improve Gastric Function using Vagal Nerve Stimulation. *Submitted to: American Control Conference, IFAC & IEEE, 2025*
- **Fernandes, S. Q.**, Kothare, M. V., Sclocco R. & Mahmoudi B. (2025). Impact of Slow Wave Abnormalities and Impaired Coordination of Pyloric Closure and Antral Contraction on Gastric Emptying: A Compartmental Modeling Study. *bioRxiv, 2025-11*.
- **Fernandes, S. Q.**, & Kothare, M. V. (2025). A Compartmental Model for Simulating the Gut-Brain Axis in Gastric Function Regulation. *bioRxiv, 2025-06*.
- **Fernandes, S. Q.**, Kothare, M. V., & Mahmoudi, B. (2024). A novel compartmental approach for modeling stomach motility and gastric emptying. *Computers in Biology and Medicine, Elsevier, 181, 109035*.
- Madhuranthakam, C. M. R., **Fernandes, S. Q.**, Piozzi, A., & Francolini, I. (2022). Mechanical Properties and Diffusion Studies in Wax–Cellulose Nanocomposite Packaging Material. *International Journal of Molecular Sciences, 23(16), 9501*.
- **Fernandes, S. Q.**, & Madhuranthakam, C. M. R. (2021). Molecular Dynamics Simulation of a Superhydrophobic Cellulose Derivative Targeted for Eco-Friendly Packaging Material. *Macromolecular Theory and Simulations, 30(1), 2000056*.
- Madhuranthakam, C. M. R., Thomas, A., Akhter, Z., **Fernandes, S. Q.**, & Elkamel, A. (2021). Removal of chromium (VI) from contaminated water using untreated moringa leaves as biosorbent. *Pollutants, 1(1), 51-64*.
- Khalifeh, H. A., Alkhedher, M., & **Fernandes, S. Q.** (2021). Two dimensional computational fluid dynamics simulations of three-phase hydrodynamics in turbulent bed contactor. *Intl. Review on Modelling and Simulations, 14(4), 281-290*.
- Khalifeh, H. A., Alkhedher, M., & **Fernandes, S. Q.** (2019). A CFD Simulation for a Two-Phase Turbulent Bed Contactor. *(2019) 8th International Conference on Modeling Simulation and Applied Optimization (ICMSAO) (pp. 1-4). IEEE*.

## PROJECTS

- **Hybrid Mechanistic–Neural Network Model for Predicting Gastric ICC Activity:** Developed a hybrid model linking cholinergic neural stimulation to ICC slow-wave frequency and amplitude by combining mechanistic equations with a residual-learning MLP. Validated trends using literature and generated synthetic data to capture biological variability. The hybrid approach improved RMSE over purely mechanistic baselines by modeling core physiology mechanistically while learning subject-specific deviations with the neural network.

- **Physics-based pipeline + modified 3D U-Net for stomach MRI segmentation:** Built an image-processing workflow (denoising, registration, Otsu thresholding, morphology) to generate high-quality 4D MRI stomach masks. Trained a customized 3D U-Net with class-imbalance weighting, BatchNorm, a lightweight two-level encoder, and full skip connections. Applied sigmoid + thresholding for inference and used on unseen MRI volumes to check the model's credibility.
- **Image processing + data science to study VNS effects on gastric motility:** Applied motion correction, segmentation, thresholding, and spatiotemporal imaging to extract gastric metrics, then evaluated logistic regression, LDA, QDA, and KNN to determine which best captures VNS-induced changes.
- **Modeling afferent vagal nerve + action potential propagation:** Extended a Hodgkin–Huxley model for rat vagal afferents and used cable theory to simulate action potential propagation along the nerve.
- **Shear deformation of armchair CNTs via molecular dynamics:** Compared effects of chirality, temperature, strain rate, and double-walled structures. Found CNTs fracture only under very high stress, with double-walled CNTs showing greater strength. All simulations used the AIREBO potential.
- **Methanol synthesis reactor modeling over  $Cu/ZnO/Al_2O_3$ :** Modeled  $CO_2$  hydrogenation using a 1D pseudo-homogeneous reactor and Vanden Bussche–Froment kinetics. Identified dissociative  $CO_2$  adsorption and formate hydrogenation as rate-limiting steps; model matches industrial data with < 1% error.

## EXPERIENCE

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<b>Rossin Research Scholars: Compartmental Model to Explain Duodenum Function</b>	Jan 2025 – Present
<i>Lehigh University</i>	<i>Bethlehem, PA</i>
• Authored a grant proposal to support two undergraduate researchers.	
• Developed teaching modules on computational neuroscience and tissue mechanics for organ-level modeling.	
<b>Teaching Assistant- Process control / Physical chemistry</b>	Aug 2023 – Dec 2023 / Aug 2022 – Dec 2022
<i>Lehigh University</i>	<i>Bethlehem, PA</i>
• Graded assignments, assisted in exam proctoring, and provided feedback to students.	
• Conducted office hours and tutorials focused on using MATLAB and SIMULINK.	
<b>Internship in Abu Dhabi Polymers: Worked on polyethylene (PE) plant</b>	Jun 2019 – Aug 2019
<i>Borouge</i>	<i>Abu Dhabi, UAE</i>
• Modeled fluid dynamics through a heated 200-meter flash pipe in a polyolefin plant, focusing on decompression from 65 to 26 barg.	
• Involves a loop reactor (65 barg) and gas-phase reactor (19 barg), with polymer separation in a flash tank (20 barg).	
• Computational analysis used ASPEN HYSYS (SRK fluid package) and ANSYS Fluent (Euler granular model).	
<b>Vice President, AIChE – ADU Student Chapter</b>	Dec 2017 – Oct 2019
<i>Abu Dhabi University</i>	<i>Abu Dhabi, UAE</i>
• Co-founded the AIChE Student Chapter at Abu Dhabi University, establishing its foundational structure and objectives.	
• Developed by-laws, promotional materials, and operational guidelines to support chapter activities.	
• Organized industrial field visits to local chemical companies, including Neopharma, to enhance student exposure to real-world applications.	

## ACCOMPLISHMENTS

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- Invited speaker at Abu Dhabi University on “Modeling of Gastric Function.”
- 1st place, 7th Undergraduate Research Competition (middle east region), for “2-D Simulation of Turbulent Bed Contactor with Non-Newtonian Liquids.”
- Reviewed papers for journals including Computers in Biology and Medicine, Neurogastroenterology and Motility, and the International Journal of Medical Sciences

## TECHNICAL SKILLS

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**Software experience:** COMSOL, ANSYS Fluent, C++, Java, Python (PyTorch, NumPy, Pandas, SciPy, scikit-learn), Javascript, HTML5, MATLAB, SIMULINK, Aspen HYSYS, LAMMPS, Ovito, NEURON, VMD, Microsoft Visio

**Communication skills:** Writing technical documents, tutoring, fluent public speaker and leadership qualities

**Courses:** Advanced Engineering Mathematics, Advanced Thermodynamics, Applied Data Science (In Python), Linear Control, Neural Modeling, Non-linear Control, Non-linear Optimization, Reaction Engineering (advanced), Soft Material Mechanics, Transport Phenomena, Natural Gas Processing, Object Oriented Programming, Industrial Wastewater Treatment

**Languages:** Fluent in English, Hindi and Konkani