Shannon Q. Fernandes

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Statement

During my undergraduate studies in Chemical Engineering, I conducted research on computational fluid dynamics (CFD) in packed bed systems under the supervision of Prof. Khalifeh and Prof. Alkhedher. I later explored sustainable materials by studying lotus-based cellulose-derived (ADULOSE) packaging using all-atom molecular dynamics (MD) simulations with Prof. Madhuranthakam.

In my PhD, my research focuses on systems-level modeling of gastric regulation. I develop computationally efficient, physics-based compartmental models—constructed entirely using ordinary differential equations (ODEs) and algebraic equations—to simulate electrophysiology, soft tissue mechanics, and fluid dynamics of the stomach. These mechanistic models capture key aspects of gastric motility, gastric emptying, and gut–brain (vago–vagal) reflex pathways. Several of my reduced-order ODE formulations have been validated using finite element and finite volume analyses in COMSOL Multiphysics, and the generalized equations can be adapted to other organ systems.

My work also emphasizes real-time, closed-loop control of gastrointestinal function. I have implemented a real-time invasive vagal nerve stimulator within a nonlinear model predictive control (NMPC) framework to investigate vagus nerve stimulation (VNS) as a therapeutic modality for gastrointestinal disorders and to study autonomic regulation of gastric function.

Currently, I am validating these models using experimental datasets, including MRI and fMRI scans. I have developed an end-to-end pipeline that incorporates physics-based methods for image registration and segmentation, along with a modified U-Net architecture for stomach organ segmentation from MRI images. I am also developing hybrid mechanistic–neural network models—such as a framework that combines cholinergic-driven mechanistic equations with a residual-learning MLP—to capture both physiological dynamics and subject-specific variability. These hybrid approaches integrate physics-based equations with data-driven learning, supporting personalized and precision medicine.

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

Education

Lehigh University — Ph.D. in Chemical and Biomolecular Engineering — Pennsylvania, USA
CGPA: 3.89/4.0 — 2024–2025: John C. Chen Fellow (Prof. Kothare's Lab) — Aug. 2020 – 2025 (Expected)
Thesis Title: Gastric emptying initiated by neural stimuli- A Compartmental Modeling Approach

Abu Dhabi University — 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
Design Project: 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.*

  Developed the first closed-loop framework for regulating gastric function using vagus nerve stimulation (VNS) integrated with a physiologically informed compartmental stomach model.
  Designed a nonlinear model predictive control (NMPC) strategy to adaptively tune invasive VNS parameters within physiological limits, enhancing gastric motility and emptying efficiency.
  Incorporated the vago-vagal reflex loop to simulate brain–stomach communication and vagal feedback control, advancing model-based closed-loop neuromodulation for gastrointestinal (GI) disorders such as functional dyspepsia.

- **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.*

  Developed a computationally efficient gastric compartmental model to simulate diseased stomach function by altering antral–pyloric coordination and slow wave dynamics.
  Incorporated enhanced flow coupling and regional slow wave variability (bradygastria, tachygastria, and quiescent activity) to evaluate motility, gastric emptying, and mixing efficiency under healthy and impaired conditions.

Demonstrated that abnormal slow wave patterns delay gastric emptying, induce retrograde transpyloric flow, and reduce mixing efficiency—providing a mechanistic and fast-executing platform for model-based closed-loop neurostimulation therapy design.

- **Fernandes, S. Q.**, & Kothare, M. V. (2025). A Compartmental Model for Simulating the Gut-Brain Axis in Gastric Function Regulation. *bioRxiv, 2025-06.*

  Developed the first complete computational model of the vago-vagal reflex loop that simulates parasympathetic vagal pathways regulating gastric motility and pyloric sphincter relaxation during the gastric emptying phase.
  Introduced a gut–brain axis model integrating vagal and enteric nervous system (ENS) pathways within a computationally efficient compartmental framework, capturing afferent and efferent feedback dynamics across the fundus, antrum, and pylorus.
  Derived equations to simulate neurotransmitter release and neuromuscular coupling, reproducing physiological responses such as excitatory gastric emptying during parasympathetic activation and inhibitory activity under sympathetic modulation—providing a foundation for closed-loop vagal stimulation therapies for gastrointestinal (GI) disorders.

- **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.*

  Developed a cost-efficient multi-compartmental model of the human stomach that integrates electrophysiology, muscle mechanics, and fluid dynamics to simulate gastric motility and emptying at the organ level.
  Represented the proximal, middle, and terminal antrum and pyloric sphincter using coupled ODE-based compartments with electro-mechanical coupling to capture slow-wave–driven peristalsis and retrograde flow dynamics.
  Validated model predictions against experimental and computational studies, demonstrating accurate electro-mechanical correlations, realistic emptying and mixing behavior, and rapid simulation performance (180 s simulated in 2.7 s), enabling applications in neuromodulation therapy design for gastric disorders.

- 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.*

  Performed molecular dynamics simulations to estimate the mechanical properties of cellulose–wax nanocomposites, demonstrating improved strength and modulus of elasticity compared to conventional polymer packaging materials.
  Evaluated thermal stability via glass transition temperature, providing insights into the glassy and rubbery states for eco-friendly packaging applications.
  Analyzed transport properties of oxygen, nitrogen, and water by estimating diffusion volumes and coefficients, linking diffusion behavior to interaction energies with cellulose and wax constituents.

- **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.*

  Designed a lotus leaf–inspired cellulose derivative (Adulose) by layering cellulose with nonacosan-10-ol and nonacosane-5,10-diol to achieve superior hydrophobicity while maintaining physical strength and reusability.
  Constructed an atomistic model with 24 cellulose chains and 48 molecules of each wax component, performing molecular dynamics simulations using LAMMPS under isothermal–isobaric conditions to study material behavior.
  Evaluated mechanical and surface properties, showing ultimate stress comparable to polyethylene and contact angles over 150°, confirming excellent nonwettability for eco-friendly packaging applications.

- Madhuranthakam, C. M. R., & **Fernandes, S. Q.** (2021). Docking and Molecular Dynamic Simulations of Cholecalciferol (Vitamin D3) as a Promising Inhibitor of Main Protease of Coronavirus to Prevent COVID-19 Infection. *In Proceedings of the 13th International Conference on Computer Modeling and Simulation, pp. 50–57.*

  Conducted molecular docking studies to investigate the binding of Cholecalciferol (Vitamin D3), Resveratrol, and Curcumin to the COVID-19 main protease, identifying VD3 as a promising, low-cost inhibitor.
  Performed molecular dynamics (MD) simulations using LAMMPS with the CHARMM force field to evaluate binding stability and interactions, including RMSD, RMSF, and hydrogen bonding.
  Demonstrated that Vitamin D3 exhibits comparable docking affinity to hydroxychloroquine and plays a key role in inhibiting the main protease, highlighting its potential as a naturally derived therapeutic candidate.

- 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.*

  Investigated biosorption of Cr(VI) from industrial wastewater using raw Moringa Oleifera leaf powder as a sustainable, low-cost biosorbent.
  Evaluated adsorption efficiency across varying Cr(VI) concentrations (1–20 ppm) and biosorbent dosages (0.5–2.5 g), achieving 30–90% metal removal within 30–90 minutes.
  Modeled experimental results with Langmuir, Freundlich, and Redlich–Peterson isotherms and confirmed metal binding to carboxylate and hydroxyl groups using FTIR analysis and molecular docking simulations.

- 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.*

  Developed a two-dimensional multiphase Eulerian computational model to simulate the hydrodynamic behavior of three-phase (air–water–beads) turbulent bed contactors under various operating conditions.
  Analyzed the impact of superficial gas velocity, static bed height, and liquid flow rate on bed pressure drop, providing insights into critical design and operational parameters.
  Validated simulation results against experimental data, demonstrating high accuracy and enhancing understanding of efficiency optimization in turbulent bed contactors for process industry applications.

- 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.*

  Developed a two-phase CFD model to simulate hydrodynamics in turbulent bed contactors, focusing on gas–solid interactions and pressure drop behavior.
  Investigated the effect of varying operational parameters including gas velocity, bed height, and particle size on the bed hydrodynamics.
  Validated simulation results against experimental data, providing insights into design and operational optimization for process industry applications.

Projects

- **Hybrid Mechanistic–Neural Network Model for Predicting Gastric ICC Activity from Cholinergic Pathway Stimulation**: Developed a physiologically grounded hybrid model combining mechanistic equations that relate cholinergic vagal stimulation to Interstitial Cells of Cajal (ICC) slow-wave frequency and amplitude. Because experimental datasets showed substantial subject-to-subject variability, I validated baseline trends using published literature and generated synthetic data to better represent realistic biological variation. Built a residual-learning Multi-Layer Perceptron (MLP) in PyTorch to model deviations from the mechanistic prediction. This hybrid mechanistic–ML framework improved RMSE over purely mechanistic baselines by capturing both the nonlinear dynamics mechanistically and inter-individual variability through the data-driven component.
- **Developed both a physics-based pipeline and a modified 3D U-Net for stomach organ segmentation from MRI**: Built a traditional image-processing workflow—denoising, rigid registration, binary Otsu thresholding, and morphological refinement—to generate high-quality stomach masks from 4D MRI datasets. Using these curated masks, designed and trained a modified 3D U-Net with organ-specific enhancements: class-imbalance handling using `BCEWithLogitsLoss`, BatchNorm in all convolutional blocks for MRI intensity stabilization, a lightweight architecture with only two downsampling stages to reduce GPU memory while preserving organ structure, and full skip connections to maintain spatial detail. Applied sigmoid and thresholding at inference to produce binary masks and validated the model on unseen MRI volumes to assess segmentation generalization and robustness.
- **Using image processing and applied data science to study the effect of vagal nerve stimulation (VNS) on gastric motility**: Using image-processing techniques—including motion correction, segmentation, Otsu thresholding, and spatiotemporal imaging—to extract quantitative data, followed by applying data-science methods such as logistic regression, LDA, QDA, and KNN to evaluate which approach best captures the effects of VNS on gastric motility.
- **Modeling the afferent vagal nerve of a rat and the action potential propagation**: Extending the existing Hodgkin–Huxley model to represent the afferent vagal nerve in rats, and using cable theory to model action potential propagation along the nerve.
- **A Comparative Study of Armchair Carbon Nanotubes under Shear Deformation using Molecular Dynamics Simulation**: A comparative study of carbon nanotube (CNT) shear deformation—across chirality, temperature, strain rates, and double-walled structures—showed that CNTs fracture only under very high stress, with double-walled CNTs displaying greater mechanical strength. All simulations used the AIREBO potential, which models covalent bonding and long-range van der Waals interactions.
- **Modeling of a reactor for Methanol Synthesis using $Cu/ZnO/Al_2O_3$ catalyst**: Methanol synthesis—an exothermic hydrogenation of CO_2 over a $Cu/ZnO/Al_2O_3$ catalyst—proceeds primarily through two rate-determining steps: CO_2 dissociative adsorption and formate hydrogenation, with formate as the dominant intermediate. A 1D pseudo-homogeneous reactor model using the Vanden Bussche–Froment kinetics best matches industrial data (error <1%) and remains the most accurate for commercial multi-tubular reactor conditions.

Experience

Rossin Research Scholars: Compartmental Model to Explain Duodenum Function Jan 2025 – Present
Lehigh University *Bethlehem, PA*

- Authored a grant proposal to support two undergraduate researchers.
- Developed teaching modules on computational neuroscience and tissue mechanics for organ-level modeling.

Teaching Assistant- Process control / Physical chemistry Aug 2023 – Dec 2023/ Aug 2022 – Dec 2022
Lehigh University *Bethlehem, PA*

- Graded assignments, assisted in exam proctoring, and provided feedback to students.
- Conducted office hours and tutorials focused on using MATLAB and SIMULINK.

Internship in Abu Dhabi Polymers: Worked on polyethylene (PE) plant Jun 2019 – Aug 2019
Borouge *Abu Dhabi, UAE*

- 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).

Vice President, AIChE – ADU Student Chapter Dec 2017 – Oct 2019
Abu Dhabi University *Abu Dhabi, UAE*

- 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.

Talks and Poster Presentations

- **Fernandes, S. Q.**, Kothare, M. V. Vagal Nerve Stimulation for Gastric Function via Model Based Closed Loop Control. American Institute of Chemical Engineers (AIChE), Boston, MA, 2025.
- **Fernandes, S. Q.**, Kothare, M. V., Sclocco R. & Mahmoudi B. Evaluating the Effects of Slow Wave Abnormalities and Impaired Antral-Pyloric Sphincter Coordination on Gastric Emptying and Stomach Motility Using Compartmental Modeling Framework. Society for Neuroscience (SfN), Chicago, IL, 2024.
- **Fernandes, S. Q.**, Kothare, M. V., Sclocco R. & Mahmoudi B. Compartmental Modeling of the Vagus Nerve Pathway that Connects the Nucleus Tractus Solitarii to the Stomach with the Potential Application to Treat GI Disorders. SfN, Washington, DC, 2023.
- **Fernandes, S. Q.**, Kothare, M. V., Horn C. C. & Mahmoudi B. Compartmental Modeling of the GI System to Simulate Retrograde Contractions with Potential Application to Modeling of Emesis, SfN, San Diego, CA, 2022.
- **Fernandes, S. Q.** & Kothare, M. V., Mahmoudi B. Gastric Emptying Initiated by Neural Stimuli – A Compartmental Model Approach. Abu Dhabi University, Abu Dhabi, UAE, *Invited talk*, 2022.
- **Fernandes, S. Q.**, Kothare, M. V., Mahmoudi B. & Horn C. C. Compartmental Modeling of the Gastrointestinal (GI) Tract: Model Development and Validation in Predicting Gastric Emptying of Liquids. AIChE, Phoenix, AZ, 2022.
- **Fernandes, S. Q.**, Kothare, M. V. & Mahmoudi B. Sparc: gastric emptying of liquids initiated by neural stimuli – a compartmental modeling approach. SfN, Virtual, 2021.

Accomplishments

- 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

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 Programing, Industrial Wastewater Treatment
Languages: Fluent in English, Hindi and Konkani

Activities and societies

- Coordinator of Impromptu Category in Speaker's Society.
- Member of Developing Student Learning Communities.
- Member of ADU Hands volunteering group.
- Members of SfN and AIChE societies.