Timoteo Dinelli

Contact Informations

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Current Position

Ph.D. Candidate Politecnico di Milano, Milano, Italy.

Research Interests

I am in my third year of Ph.D. at Politecnico di Milano, affiliated with the Department of Chemistry, Materials, and Chemical Engineering Giulio Natta. My research takes place within the CRECK modeling laboratory, under the supervision of Professor Alessandro Stagni. My Ph.D. work centers on enhancing chemical kinetics models for predicting combustion and pyrolysis behaviors of complex fuels using data-driven methods.

Education

Ph.D., Chemical Engineering, Politecnico di Milano, Milano, Italy **2021-present**

Dissertation Advisor: Prof. Alessandro Stagni

M.Sc., Chemical Engineering, Politecnico di Milano, Milano, Italy **2019-2021**

Thesis Title: "*Development of an automatic framework for kinetic model validation.*" (link).

Thesis Advisors: Prof. Alessandro Stagni and Prof. Matteo Pelucchi.

B.Sc., Chemical Engineering, Politecnico di Milano, Milano, Italy **2016-2019**

Thesis Title: "*Applicazioni della stampa 3D per l'ingegnieria chimica.*".

Thesis Advisor: Prof. Giulia Luisa Bozzano.

Visting Positions

Visiting Ph.D. student, Stanford University, Stanford CA, USA **Oct 2023-Jun 2024**

Visiting Ph.D. student at Stanford University's FxLab, under the guidance of Professor Matthias Ihme. My research focuses on implementing Data Assimilation methods for the joint estimation of state and parameters within chemical kinetic dynamical systems.

Teaching

Teacher assistant, Politecnico di Milano

Calcoli di Processo dell'Ingegneria Chimica. Course given to undergraduate students in Chemical Engineering. Covering introductory numerical methods applied to chemical engineering problems. Samples of the practical sessions can be found on the GitHub repository (link). **A.Y. 22-23, 24-25.**

Laboratorio Progettuale di Ingegneria Chimica. Course given to undergraduate students in Chemical Engineering. Covering fundamental aspects of modeling chemical process from first principles to industrial size plants. **A.Y. 21-22, 22-23.**

Tutor, Politecnico di Milano

Laboratorio Progettuale di Ingegneria Chimica. Support activity during the final project of the course. **A.Y. 22-23.**

Publications

Refereed Publications

5. **Timoteo Dinelli**, Alessandro Pegurri, Andrea Bertolino, Alessandro Parente, Tiziano Faravelli, Marco Mehl, and Alessandro Stagni. "A data-driven, lumped kinetic modeling of OME2-5 pyrolysis and oxidation". In: *Proceedings of the Combustion Institute* 40.1 (2024), p. 105547. ISSN: 1540-7489. DOI: https://doi.org/10.1016/j.proci.2024.105547.

4. Andrea Nobili, Niccolò Fanari, **Timoteo Dinelli**, Edoardo Cipriano, Alberto Cuoci, Matteo Pelucchi, Alessio Frassoldati, and Tiziano Faravelli. "Kinetic modeling of carbonaceous particle morphology, polydispersity and nanostructure through the discrete sectional approach". In: *Combustion and Flame* 269 (2024), p. 113697. ISSN: 0010-2180. DOI: https://doi.org/10.1016/j.combustflame.2024.113697.

3. Alessandro Pegurri, **Timoteo Dinelli**, Luna Pratali Maffei, Tiziano Faravelli, and Alessandro Stagni. "Coupling chemical lumping to data-driven optimization for the kinetic modeling of dimethoxymethane (DMM) combustion". In: *Combustion and Flame* 260 (Feb. 2024), p. 113202. ISSN: 0010-2180. DOI: 10.1016/j.combustflame.2023.113202.

2. **Timoteo Dinelli**, Luna Pratali Maffei, Alessandro Pegurri, Amedeo Puri, Alessandro Stagni, and Tiziano Faravelli. "Automated Kinetic Mechanism Evaluation for e-Fuels Using SciExpeM: The Case of Oxymethylene Ethers". en. In: Capri, Italy, Aug. 2023, pp. 2023–24–0092. DOI: 10.4271/2023-24-0092.

1. Edoardo Ramalli, **Timoteo Dinelli**, Andrea Nobili, Alessandro Stagni, Barbara Pernici, and Tiziano Faravelli. "Automatic validation and analysis of predictive models by means of big data and data science". en. In: *Chemical Engineering Journal* 454 (Feb. 2023), p. 140149. ISSN: 13858947. DOI: 10.1016/j.cej.2022.140149.

Conferences and Presentations

8. 40th International Symposium on Combustion, Milano Italy. Oral contribution based on the paper, "*A data-driven, lumped kinetic modeling of $OME_{2\text{-}5}$ pyrolysis and oxidation*". **Dinelli, T.**, Pegurri, A, Bertolino, A, Parente, A, Faravelli, T., Mehl, M, Stagni, A., 22-26 July 2024.

7. 19th International Conference on Numerical Combustion, Kyoto Japan. Oral contribution, "*Leveraging data assimilation techniques to integrate experimental and synthetic measurements in the kinetic mechanisms of e-fuels.*". **Dinelli, T.**, Faravelli, T., Stagni, A., Ihme, M., 07-10 May 2024.

6. Math2Product, Taormina, Italy. Oral contribution, "*Comparative assessment of optimization algorithms for kinetic model optimization*". **Dinelli, T.**, Stagni, A., 30 May-1 June 2023.

5. 45th Meeting of the Italian Section of the Combustion Institute, Firenze, Italy. Oral contribution, "*Automatic validation and optimization of a kinetic model for alcohols combustion*". **Dinelli, T.**, Pegurri, A., Stagni, A., Pelucchi, M., 28-31 May 2023.

4. 11th European Combustion Meeting, Rouen, France. Conference paper and poster prsentation, "*Developing a compact kinetic model for dimethoxymethane (DMM) combustion through a novel chemical lumping method*". Pegurri, A., **Dinelli, T.**, Stagni, A., 26-28 April 2023.

3. 11th European Combustion Meeting, Rouen, France. Conference paper and poster presentation, "*Data-driven, class-based optimization methodology for the kinetic modeling of oxymethylene ethers (OME_{1-4}) combustion*". Puri, A., **Dinelli, T.**, Pegurri, A., Stagni, A., 6-8 March 2023.

2. AI4Energy (KAUST), Jeddah, Saudi Arabia. Poster presentation, "*Data ecosystems for kinetic model reduction*". **Dinelli, T.**, Ramalli, E., Pegurri, A., Pernici, B., Faravelli, T., Stagni, A., 26-28 April 2023.

1. 18th International Conference on Numerical Combustion, San Diego CA, USA. Oral contribution, "*From detailed kinetics to large-scale simulations: integrating data ecosystems in the skeletal reduction framework*". **Dinelli, T.**, Ramalli, E., Pegurri, A., Pernici, B., Faravelli, T., Stagni, A., 08-11 May 2022.

Professional Activities, Outreach, and Service

Journal referee

Proceedings of the Combustion Institute, International Journal of Hydrogen Energy.

Mentoring/ Supervision

Master Students (Politecnico di Milano)

Lorenzo Paggetta, co-supervised with Prof. Alessandro Stagni and Prof. Marco Mehl, Present.

Matteo Lea Casagrande, co-supervised with Prof. Matteo Pelucchi and Prof. Carlo Cavallotti, Present.

Sara Meraviglia, co-supervised with Prof. Matteo Pelucchi and Eng. Matteo Primi. Thesis title: "Implementation of recent theoretical findings in hydrogen combustion model" (link).

Federico Marino, co-supervised with Prof. Matteo Pelucchi. Thesis title: "Automatic data management and model validation of ammonia-hydrogen and methane-hydrogen mixture combustion through the framework SciExpeM" (link).

Amedeo Puri, co-supervised with Prof. Alessandro Stagni and Eng. Alessandro Pegurri. Thesis title: "Data-driven, class-based kinetic modeling of oxymethylene ethers combustion" (link).

Haithem Tej, co-supervised with Prof. Matteo Pelucchi. Thesis title: "Validation and optimization of a kinetic model for alcohols combustion using an automatic framework" (link).

Computer Skills

Languages— Proficient in C/C++, Python, Matlab. Experience in Fortran, Julia. Markup languages: LaTeX, HTML, CSS, Markdown.

Software—Most of the contributions can be found at https://github.com/tdinelli. During my PhD, together with Edoardo Ramalli, I was the main developer and actual maintainer of the SciExpeM ecosystem, which integrates and orchestrates various programs and software. I have actively contributed to the development of OpenSMOKE++. My contributions include significant enhancements to the core library, as well as the development of functionality for the ideal reactor and one-dimensional flame solvers, DoctorSMOKE++ and OptiSMOKE++. I have developed a Python interface, OpenSMOKEpp_Intrefaces, which exposes the core functionality of the `OpenSMOKE++` library. In addition, I have created a comprehensive post-processing suite, pySMOKEPostProcessor. Currently I am working on the development of the `CurveMatching` framework, which is tailored for functional data analysis, with a special focus on chemical kinetic data.

Honors and Awards

Travel student fellowship. KAUST. Jeddah, Saudi Arabia 2023

PhD scholarship. Italian Ministry of Education (MIUR). Milano, Italy 2021

Additional Contact Links

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LinkedIn	www.linkedin.com/in/timoteo-dinelli
Github	www.github.com/tdinelli

References

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