Timoteo Dinelli

Contact Information

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Short Bio

I am a fifth year Ph.D. student 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.

Experiences

Graduate Researcher, *Politecnico di Milano, Milano, Italy* **Oct. 2021-present**

Advised by Prof. Alessandro Stagni, working on the development of data-driven modeling strategies of complex chemical kinetics models for combustion and pyrolysis of renewable fuels.

Visiting Graduate Student, *Stanford University, Stanford CA, USA* **Oct. 2023-Jun. 2024**

Visiting Graduate 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.

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: "*Applications of 3D printing for chemical engineering*".

Thesis Advisor: Prof. Giulia Luisa Bozzano.

Publications

Journal Publications (refereed)

8. P. Crepaldi, A. Nobili, **T. Dinelli**, L. Pratali Maffei, A. Cuoci, and T. Faravelli. "Effect of ammonia on soot volume fraction and morphology in laminar flames: modeling the impact of NH_2 radicals". *Fuel* 409 (2026), p. 137695. DOI: 10.1016/j.fuel.2025.137695.

7. **Timoteo Dinelli**, Alessandro Stagni, and Matthias Ihme. "Learning chemical kinetics through data assimilation: Theory and application to ammonia oxidation". *Chemical Engineering Journal* 524 (2025), p. 168863. DOI: 10.1016/j.cej.2025.168863.

6. Alessandro Stagni and **Timoteo Dinelli**. "Impact of third-body colliders on ammonia pyrolysis and oxidation: Detailed kinetic modeling and mechanistic insights". *Chemical Engineering Journal* 526 (2025), p. 170737. DOI: 10.1016/j.cej.2025.170737.

5. **Timoteo Dinelli**, Alessandro Pegurri, Andrea Bertolino, Alessandro Parente, Tiziano Faravelli, Marco Mehl, and Alessandro Stagni. "A data-driven, lumped kinetic modeling of $OME_{2\text{-}5}$ pyrolysis and oxidation". *Proceedings of the Combustion Institute* 40.1 (2024), p. 105547. DOI: 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". *Combustion and Flame* 269 (2024), p. 113697. DOI: 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". *Combustion and Flame* 260 (Feb. 2024), p. 113202. 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". *16th International Conference on Engines & Vehicles*. SAE International, Aug. 2023. 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". *Chemical Engineering Journal* 454 (Feb. 2023), p. 140149. DOI: 10.1016/j.cej.2022.140149.

Conference Publications (not—refereed)

1. Guillaume Vignat, Yichi Ma, Jen Zen Ho, Younghwa Cho, Nozomu Hashimoto, **Timoteo Dinelli**, Taekeun Yoon, Colette Fisher, and Matthias Ihme. "Effect of Synthetic Aviation Fuels on the Stochastic Ignition of Fuel Droplets on Hot Surfaces". *AIAA SCITECH 2025 Forum*. DOI: 10.2514/6.2025-0741.

Talks, Lectures, Conferences and Presentations

Invited Lectures

1. COST CYPHER Training School on the Analysis, uncertainty quantification, validation, optimization and reduction of combustion kinetic mechanisms. Budapest, Hungary. 02-05 September 2025.

Conferences

12. 20th International Conference on Numerical Combustion, Rome, Italy. Oral contribution, "*Advancing sustainable fuel models: Data Assimilation Techniques for combustion chemical kinetics.*". **Dinelli, T.**, Stagni, A., Ihme, M., 14-17 October 2025.

11. 20th International Conference on Numerical Combustion, Rome, Italy. Oral contribution, "*Automated Validation of Combustion Kinetic Mechanisms through Curve Matching: A Functional Data Analysis Approach for Large and Incomplete Datasets*". **Dinelli, T.**, Sangalli, L.M., Faravelli, T., Stagni, A., 14-17 October 2025.

10. 47th Meeting of the Italian Section of the Combustion Institute, Pisa, Italy. Oral contribution, "*Beyond Conventional Models: Implementation of LMR-R Framework for Multi-Collider Systems in Hydrogen Combustion*". **Dinelli, T.**, Primi, M., Pratali Maffei, L., Cuoci, A., Cavallotti, C., Pelucchi, M., 12-15 May 2025.

9. 12th European Combustion Meeting, Edinburgh, Scotland UK. Conference paper and poster presentation, "*Reconciling theory, experiments and gas-phase kinetic models. A case study on rigorous implementation of pressure dependent reactions in hydrogen combustion.*". **Dinelli, T.**, Primi, M., Casagrande, M.L., Pratali Maffei, L., Cuoci, A., Cavallotti, C., Pelucchi, M., 07-10 April 2025.

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.

Workshops

1. 7th International Workshop on Flame Chemistry, Milano, Italy. Poster presentation, "*Assessment and Validation of recent theoretical findings in Hydrogen combustion kinetics: Master Equation and Mixture Rules*". **Dinelli, T.**, Primi, M., Pratali Maffei, L., Cuoci, A., Cavallotti, C., Pelucchi, M., 20-21 July 2024.

Professional Activities, Outreach and Service

Journal referee

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

Honors and Awards

Travel student fellowship. KAUST. Jeddah, Saudi Arabia **Apr. 2023**

PhD scholarship. Italian Ministry of Education (MIUR). Milano, Italy **2021-2025**

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 of the course (link). **A.Y. 22-23, 24-25, 25-26.**

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.**

Mentoring/Supervision

Master Students (Politecnico di Milano)

10. *Maryam Pasandidehnia.*, co-supervised with Prof. Matteo Pelucchi and Doct. Luna Pratali Maffei.
9. *Sahar Niroumand.*, co-supervised with Prof. Matteo Pelucchi and Doct. Luna Pratali Maffei.
8. *Filippo Bonfanti.*, co-supervised with Prof. Matteo Pelucchi and Prof. Marco Mehl. Present.
7. *Nicola Bernardi*, co-supervised with Prof. Alessandro Stagni. Present.
6. *Lorenzo Paggetta*, co-supervised with Prof. Alessandro Stagni. Thesis title: "Simplified kinetic models for methane/air combustion" (link).
5. *Matteo Lea Casagrande*, co-supervised with Prof. Carlo Cavallotti, Prof. Matteo Pelucchi, Doct. Luna Pratali Maffei, Eng. Matteo Primi. Thesis title: "Reconciling theory, experiments and gas-phase kinetic models. A case study on rigorous implementation of pressure dependent reactions in hydrogen combustion." (link).
4. *Sara Meraviglia*, co-supervised with Prof. Matteo Pelucchi and Eng. Matteo Primi. Thesis title: "Implementation of recent theoretical findings in hydrogen combustion model" (link).

3. *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).
2. *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).
1. *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— I have contributed to several scientific software tools during my research work. My contributions are available via my GitHub. During my PhD, I collaborated with Edoardo Ramalli as developers of the SciExpeM ecosystem, which integrates various scientific programs for experimental research. As part of this work, I helped enhance the OpenSMOKE++ library and developed functionalities for reactor and flame solvers, including also DoctorSMOKE++ and OptiSMOKE++. To make these tools more accessible, I created OpenSMOKEpp_Interfaces, providing Python bindings to the core library. Additionally, I developed pySMOKEPostProcessor for analyzing and visualizing simulation data. Currently, I am working on the CurveMatching framework, which uses functional data analysis techniques for chemical kinetic applications.

Additional Contact Links

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

References

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