

# TIMOTEO DINELLI

## Contact Informations

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## Research Interests

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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. My academic pursuits revolve around the following areas of interest:

- Developing and overseeing an automatic framework (SciExpeM) to systematically gather and analyze scientific data and kinetic models. [Project link](#).
- Creating robust pipelines to develop and validate detailed kinetic models. Models undergoing rigorous testing against extensive experimental datasets using data science methodologies.
- Designing automated routines to simplify the optimization of complex kinetic schemes, thus boosting the effectiveness of physics-based approaches.
- Implementing algorithms for the inverse modeling of high-dimensional problems, with the goal of improving predictive capabilities in complex systems.

## Education

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**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*.”.

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'ingegneria chimica*.”.

Thesis Advisor: Prof. Giulia Luisa Bozzano.

## Visting Positions

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**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.

## Honors and Awards

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Travel student fellowship. KAUST. Jeddah, Saudi Arabia	2023
PhD scholarship. Italian Ministry of Education (MIUR). Milano, Italy	2021

## Teaching Experience

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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 associated GitHub repository (link). **2022-2023**

*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. **2021-2023**

Tutor, Politecnico di Milano

*Laboratorio Progettuale di Ingegneria Chimica.* Support activity during the final project of the course. **2022-2023**

## Publications

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### Submitted Publications

- [1] **T. Dinelli**, A. Pegurri, A. Bertolino, A. Parente, T. Faravelli, M. Mehl, and A. Stagni. “A data-driven, lumped kinetic modeling of OME2-5 pyrolysis and oxidation”. In: *Proceedings of the Combustion Institute* 40 (2024).
- [2] A. Nobili, N. Fanari, **T. Dinelli**, E. Cipriano, A. Cuoci, M. Pelucchi, A. Frassoldati, and T. Faravelli. “Kinetic modeling of carbonaceous particle morphology, polydispersity and nanostructure through the discrete sectional approach”. In: *Combustion and Flame* (2024).

### Refereed Publications

- [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.
- [4] **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.
- [5] 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

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7. 19<sup>th</sup> International Conference on Numerical Combustion, Kyoto JP. 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. 45<sup>th</sup> 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. 11<sup>th</sup> European Combustion Meeting, Rouen, France. Conference paper and poster presentation, “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. 11<sup>th</sup> European Combustion Meeting, Rouen, France. Conference paper and poster presentation, “Data-driven, class-based optimization methodology for the kinetic modeling of oxymethylene ethers (OME<sub>1-4</sub>) 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. 18<sup>th</sup> 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.

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## Professional Activities, Outreach, and Service

### Journal referee

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

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### 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).

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## Computer Skills

**Languages**— Proficient in C/C++, Python, Matlab. Experience in Fortran, Julia. Markup languages: L<sup>A</sup>T<sub>E</sub>X, 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.

## Addition Contact Links

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Google scholar	<a href="https://www.scholar.google.com">www.scholar.google.com</a>
ORCID	0000-0003-1660-2965
Research Gate	<a href="https://www.researchgate.net/profile/Timoteo_Dinelli">www.researchgate.net/profile/Timoteo_Dinelli</a>
LinkedIn	<a href="https://www.linkedin.com/in/timoteo-dinelli">www.linkedin.com/in/timoteo-dinelli</a>
Github	<a href="https://www.github.com/tdinelli">www.github.com/tdinelli</a>

## References

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