Timoteo Dinelli

Contact Information

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Research Interests

I am a third-year Ph.D. candidate enrolled at Politecnico di Milano, affiliated with the Department of Chemistry, Materials, and Chemical Engineering Giulio Natta. I am actively engaged in research within the CRECK modeling laboratory, under the guidance of Professor Alessandro Stagni. My doctoral research is primarily centered on leveraging data-driven methodologies to advance the development of chemical kinetics mechanisms aimed at predicting combustion and pyrolysis behaviors of complex fuels. My academic pursuits revolve around several key areas of interest:

- Establishing and managing an automated framework for the systematic collection and analysis of scientific data and kinetic models (SciExpeM).
- Constructing robust pipelines for the creation and validation of detailed kinetic mechanisms, which are rigorously benchmarked against extensive experimental datasets employing data science methodologies.
- Designing automated routines to streamline the optimization of complex kinetic schemes, thereby enhancing the efficacy of physics-based approaches.
- Implementing various algorithms for conducting inverse modeling of high-dimensional problems, with a focus on enhancing predictive capabilities in complex systems.

Education

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

Dissertation Advisor: Prof. Alessandro Stagni

M.S., 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.S., 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.

Visiting position

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

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

Teaching Experience

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**

Submitted Publications

4. **Dinelli, T.**, Pegurri, A., Bertolino, A., Parente, A., Faravelli, T., Mehl, M., Stagni, A., (2024) *A data-driven, lumped kinetic modeling of $OME_{2\text{-}5}$ pyrolysis and oxidation*, Proceedings of the Combustion Institute 40.

Refereed Publications

3. Pegurri, A., **Dinelli, T.**, Pratali Maffei, L., Faravelli, T., Stagni, A., (2024) *Coupling chemical lumping to data-driven optimization for the kinetic modeling of dimethoxymethane (DMM) combustion*, Combustion and Flame **260**, 113202.
2. **Dinelli, T.**, Pratali Maffei, L., Pegurri, A., Puri, A., Stagni, A., Faravelli, T., (2023) *Automated Kinetic Mechanism Evaluation for e-Fuels Using SciExpeM: The Case of Oxymethylene Ethers*, SAE Techincal Paper.
1. Ramalli, E., **Dinelli, T.**, Nobili, A., Stagni, A., Pernici, B., Faravelli, T., (2023) *Automatic validation and analysis of predictive models by means of big data and data science*, Chemical Engineering Journal **454**, 140149.

Conferences and Presentations

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 ($OME_{1\text{-}4}$) 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

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 contributions can be found at `https://github.com/tdinelli`. During my PhD I have been, together with Edoardo Ramalli, the main developer and actual mantainer of the SciExpeM ecosystem, which involves and orchestrates different programs and software. I actively contributed to the development of OpenSMOKE++ ecosystem. My contributions include significant enhancements to the core library, as well as the development of functionalities for the ideal reactor and one-dimensional flame solvers, `DoctorSMOKEpp`, and the creation of OptiSMOKEpp. I have developed a python interface, OpenSMOKEpp_Intrefaces, which exposes the key functionalities of the core `OpenSMOKEpp` library. Additionally I have created comprehensive post-processing suite, pySMOKEPostProcessor. Presently, I am engaged in the development of the `CurveMatching` framework, which is tailored towards functional data analysis, with a specific emphasis on chemical kinetic data. Furthermore, I am working on `daSMOKE`, a collection of Data Assimilation routines designed to address the joint state parameters estimation problem within chemical kinetic dynamical systems.

Additional contact links

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Research Gate	www.researchgate.net/profile/Timoteo_Dinelli
Linkedin	www.linkedin.com/in/timoteo-dinelli
Github	github.com/tdinelli

References

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Tiziano Faravelli, Full Professor of Chemical Engineering, Politecnico di Milano
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