

Curriculum Vitae

MATTEO PELUCCHI

1. PERSONAL DATA

Name: Matteo Pelucchi
Date of birth: 19th May 1988
Place of birth: Vaprio D'Adda (Milano, Italy)
Work Address: CRECK Modeling Lab, Department of Chemistry, Materials, and Chemical Engineering "G. Natta", Politecnico di Milano, Piazza Leonardo Da Vinci 32, 20133 Milano (MI)
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2. CURRENT AND PREVIOUS POSITIONS

2017-Present

Assistant Professor at Politecnico di Milano,

Department of Chemistry, Materials and Chemical Engineering

Scientific Disciplinary Sector: ING-IND/26 *"Teoria dello sviluppo dei processi chimici"- "Theory of development of chemical processes"*

2016-2017

Post-doctoral researcher at Politecnico di Milano

Department of Chemistry, Materials and Chemical Engineering

3. EDUCATION

2013-2016

Ph.D. (cum laude) in Industrial Chemistry and Chemical Engineering at Politecnico di Milano

Graduation Date: 15th February 2017.

Title of the Thesis: *"Development of kinetic mechanisms for the combustion of renewable fuels."*

Advisor: Prof. Tiziano Faravelli.

2010-2012

Master Degree (cum Laude) in Chemical Engineering at Politecnico di Milano

Graduation Date: 22nd April 2013.

Final Mark: 110/110 cum laude.

Title of the Thesis: “*Experimental and kinetic modelling study of n-butanal and n-pentanal auto-ignition in a shock tube*”.

Advisors: Prof. Tiziano Faravelli, Prof. Eliseo Ranzi, Prof. Henry J. Curran.

2007-2010

Bachelor Degree in Chemical Engineering at Politecnico di Milano

Graduation Date: 21st September 2010

Final mark: 101/110.

Title of the Thesis: “*Modelli di surrogati per combustibili aeronautici*”-“*Surrogate fuels for avio applications*”

Advisors: Prof. Tiziano Faravelli, Prof. Alberto Cuoci.

4. AWARDS and GRANTS

2020

National Scientific Habilitation to Associate Professor in Chemical Engineering

Scientific Sectors: i) 09/D2 “Sistemi metodi e tecnologie dell’ingegneria chimica e di processo” (Systems, methods and technologies of chemical and process engineering); ii) 09/D3 “Impianti e processi industriali chimici” (Plants and processes of industrial chemistry)

2020

Front cover of *Reaction Chemistry and Engineering* with the paper titled “Theoretical study of sensitive reactions in phenol decomposition”

2020

The paper titled “Electronic Structure-based rate rules for H ipso addition-elimination reactions on mono-aromatic hydrocarbons with single and double OH/CH₃/OCH₃/CHO/C₂H₅ substituents: a systematic theoretical investigation” selected as **2020 HOT PCCP article** by the *Physical Chemistry Chemical Physics* Editors.

2019

Front cover of *Reaction Chemistry and Engineering* with the paper titled “Detailed kinetics of substituted phenolic species in pyrolysis bio-oils”

2018

Front cover of *Physical Chemistry Chemical Physics* issue “Kinetics in the Real World” with the paper titled “H-Abstraction reactions by OH, HO₂, O, O₂ and benzyl radical addition to O₂ and their implications for kinetic modelling of toluene oxidation”

2017

2nd position, PhD Award

Issued by the Doctoral School in Industrial Chemistry and Chemical Engineering, Politecnico di Milano.

2013-2016

PhD scholarship

Issued by Italian Ministry of Education (MIUR), Italy

2012-2013

Master Degree scholarship for thesis projects abroad – National University of Ireland Galway (Prof. H. Curran)

Issued by Politecnico di Milano

5. VISITING POSITIONS

2016 (January-August)

Visiting PhD at Argonne National Laboratory, IL, USA. Chemical Science and Engineering Division

Supervisor: Dr. S.J. Klippenstein

2015 (February)

Visiting PhD Student at National University of Ireland Galway, School of Chemistry

Supervisor: Prof. H.J. Curran

2013 (October)

Visiting PhD Student at National University of Ireland Galway, School of Chemistry

Supervisor: Prof. H.J. Curran

2012 (March-September)

Visiting Master Student at National University of Ireland Galway, School of Chemistry

Supervisor: Prof. H.J. Curran

6. TEACHING ACTIVITIES

2018-Present: Lecturer of “*Dynamics and Control of Chemical Processes*”

Master Degree in Chemical Engineering and Automation Engineering.

2013-Present: Teaching assistant of “*Principi di Combustione*” (*Combustion fundamentals*)

Bachelor Degree in Chemical Engineering

2018-2019: Teaching assistant of “*Sperimentazione Industriale*” (*Error propagation and analysis for industry*)

Bachelor Degree in Chemical Engineering

2014-2016: Teaching assistant of “*Combustion and Pollutant Formation*”

Master Degree in Chemical Engineering

2013-Present: Supervision of M.Sc. and B.Sc. students.

Supervisor of 2 PhD students (Luna Pratali Maffei, 2018-present; Francesco Serse, 2020-present)

Supervisor of 8 M.Sc. students in Chemical Engineering

Supervisor of >15 B.Sc. students in Chemical Engineering

Co-advisor of 7 M.Sc. students in Chemical Engineering

Co-advisor of 10 B.Sc. students in Chemical Engineering.

7. OTHER INSTITUTIONAL ACTIVITIES

2016-Present:

- Chemical Engineering POLIMI-OpenDay Organizer. *Yearly orientation activity for high school students.*

2019-Present:

- Author of the Quarterly Newsletter reaching out to professors in the BS and MS in Chemical Engineering to periodically communicate news and ongoing efforts from the School of Industrial and Information Engineering, Politecnico di Milano.

2020-Present:

- Member of the Working Group on the analysis and reinforcement of laboratory activities. MS in Chemical Engineering, Politecnico di Milano.
- Member of the Committee on Student Exchange Programs (incoming, outgoing, double degree agreements). MS in Chemical Engineering, Politecnico di Milano.

8. INVITED TALKS/LECTURES and Conference presentations.

8th July 2015: Young Researchers Colloquium, Clean Air Conference 2015, Lisbon, Portugal

“Detailed kinetic mechanisms for practical applications: new reaction classes and model reduction”

20th January 2021: International Sooting Flames Workshop. Invited presentation: *“Reflections on PAH/Soot chemistry as raised from the 2020 Flame Chemistry Workshop: challenges and perspectives in theoretical and modeling efforts”* Adelaide, Australia, remote presentation.

Over 20 oral presentations at international conferences and meetings.

Over 10 poster presentations at international conferences and meetings.

9. CONFERENCES/WORKSHOPS ORGANIZATION

21st August – 26^h July 2024, Politecnico di Milano, Mi-CO, Milan, Italy *“40th International Symposium on Combustion”*. Bid Proposal leader and organizing committee member. Awarded.

30th August – 4th September 2020, Politecnico di Milano, Milan, Italy *“XXIV International Conference on Chemical Reactors-CHEMREACTOR24”*. Organizing committee member. Postponed to August 2021.

23rd-24th April 2018, Politecnico di Milano, Milan, Italy *“Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules”*. Organizing committee member.

27th July 2018, Trinity College Dublin, Dublin, Ireland *“Fourth International Rapid Compression Machine workshop”*. Technical committee member.

7th May 2019, Aachen, Germany. Chair of Mini-Symposium on *“High Performance Computing: Towards High Throughput Kinetics and Combustion Model Development”* Numerical Combustion Meeting.

10. SCIENTIFIC INTERESTS

My research activity is focused on the development of chemical kinetic models for the pyrolysis and combustion of gas, liquid and solid fuels (e.g. plastics, biomass, coal). In particular:

1. Detailed kinetic mechanisms of homogeneous gas phase reactions and theoretical calculations

The activity is focused on the development, iterative validation and improvement of detailed kinetic mechanisms describing the **pyrolysis, oxidation and combustion of hydrocarbon and oxygenated fuels**. A particular focus is dedicated to the formation of **PAHs** and of **pollutants** such as **NO_x** and carbonaceous particles (**soot**). To achieve the goal of modeling fuels combustion and pollutant formation, **theoretical ab initio and DFT methods** are used to estimate rate constant and kinetic parameters, in a reaction class-based approach. My research also deals with the development of **tools for the automatic theoretical calculation of rate constants** for various reaction classes.

2. Theoretical kinetics for heterogeneous gas/solid reactive systems

The focus of this activity is the estimation of accurate reaction parameters for **gas solid interactions using DFT**. This activity involves different processes such as thermal conversion of coal and biomass, graphene and carbonaceous materials synthesis, CVD and CVI, soot formation/oxidation.

3. Kinetic Modelling of plastic polymer pyrolysis.

Solid plastic wastes recovery through chemical recycling is of industrial interest in the perspective of circular economy. My research activity in the area has been focused on the analysis of the degradation process of mixtures of SPW through semi-detailed kinetic models, and on the development of new subsets for polyesters (i.e. PET) and polyamide (i.e. Nylon-6).

4. Automatic tools for mechanism development and comparison

Recently my research efforts have also been devoted to the implementation of **automatic validation tools** based on **curve comparisons** algorithm to support the iterative development of kinetic models. Such tools have been implemented in automatic routines for kinetic mechanism development and analysis also developed during the last 2 years of activity.

5. Data management, standardization and database development

I am involved in activities related to the **standardization of combustion experimental data** as well as in the development of **data repositories**. In particular, I am part of the Data Exchange task force within the Smartcats COST Action of the EU and involved in the Rapid Compression Machine and Shock Tube Initiatives.

11. PARTICIPATION IN PUBLIC AND INDUSTRIAL RESEARCH PROJECTS

2020-2021.

“A modular and hierarchical kinetic framework for the thermo-catalytic pyrolysis of methane for VACS production: an application to carbon-nanotubes (CNT)” Politecnico di Milano/Rice University “Carbon-Hub” Project Leader. ~50 k€. Duration: 1 year.

2019-2020.

Individuazione processo per eliminazione Cloro da Plasmix fino a livello di 5-10 ppm. ODL 4310328956, Politecnico di Milano/ENI Spa. (EN: "Reduction of Chlorine content from Municipal Solid Plastic Waste up to 5-10 ppm"). Project Leader. ~250 k€. Duration: 6 months.

2018-2019.

DOE-Exascale Computing Project: automatic rate constant calculations and automatic model development and validation tools.

2018-2020.

2nd initiative of the RCM/ST Network. Chair of WP#3 on Data Exchange.

2018-Present.

Computational Chemistry Consortium, Converge Science Inc. Madison-Wisconsin, USA.

2017-2020.

JETSCREEN (JET Fuel SCREENing and Optimization), H2020 European Project [GA No. 723525]

2016-2019.

Residue2Heat (Renewable residential heating with fast pyrolysis bio-oil), H2020 European Project [GA No. 654650]

2017-2020.

IMPROOF (Integrated model guided process optimization of steam cracking furnaces, H2020 European Project [GA No. 723706]

2015-2019.

SMARTCATs COST ACTION CM1404. Detailed kinetic mechanisms development and "task force" on combustion data standardization.

12. BIBLIOMETRY (7th January 2021)

Scopus Papers: 41, Citations: 664, h-index: 15

Google Scholar Papers: 58, Citations: 946, h-index: 16

13. PUBLICATIONS (*corresponding author)

2021

1. O. Dogu, **M. Pelucchi**, R. Van de Vijver, P.H.M. Van Steenberge, D. R. D'hooge, A. Cuoci, M. Mehl, A. Frassoldati, T. Faravelli, K. M. Van Geem "The chemistry of chemical recycling of solid plastic waste: state-of-the-art, challenges, and future directions of pyrolysis and gasification" *Progress in Energy and Combustion Science*, 2021, in press.

2020

2. **M. Pelucchi**, P. Osswald, W. Pejpichestakul, A. Frassoldati, M. Mehl "On the combustion and sooting behavior of standard and hydro-treated jet fuels: An experimental and modeling study on the compositional effects" *Proceedings of The Combustion Institute*, in press.
3. **M. Pelucchi***, C. Cavallotti, E. Ranzi, A. Frassoldati, P. Glarborg, T. Faravelli "Theoretical and kinetic modelling study of chloromethane (CH₃Cl) pyrolysis and oxidation." *International Journal of Chemical Kinetics*, 2020, published online, doi.org/10.1002/kin.21452.
4. **M. Pelucchi***, S. Namysl, E. Ranzi, A. Rodriguez, C. Rizzo, K. P. Somers, Y. Zhang, O. Herbinet, H.J. Curran, F. Battin-Leclerc, T. Faravelli "Combustion of n-C₃-C₆ linear alcohols: an experimental and kinetic

- modeling study. Part II: speciation measurement in a jet stirred reactor, ignition delay time measurement in a rapid compression machine, model validation and kinetic analysis" *Energy and Fuels*, 2020, published online, doi.org/10.1021/acs.energyfuels.0c02252.
5. **M. Pelucchi***, S. Namysl, E. Ranzi, A. Rodriguez, C. Rizzo, K. P. Somers, Y. Zhang, O. Herbinet, H.J. Curran, F. Battin-Leclerc, T. Faravelli "Combustion of n-C3–C6 linear alcohols: an experimental and kinetic modeling study. Part I: reaction classes, rate rules, model lumping and validation." *Energy and Fuels*, 2020, published online, doi.org/10.1021/acs.energyfuels.0c02251.
 6. L. Pratali Maffei, C. Cavallotti, T. Faravelli, **M. Pelucchi*** "Electronic Structure-based rate rules for H ipso addition-elimination reactions on mono-aromatic hydrocarbons with single and double OH/CH3/OCH3/CHO/C2H5 substituents: a systematic theoretical investigation" *Physical Chemistry Chemical Physics*, 2020. DOI: [10.1039/D0CP03099F](https://doi.org/10.1039/D0CP03099F)
 7. L. Pratali Maffei, **M. Pelucchi**, T. Faravelli, C. Cavallotti "Theoretical Study of Sensitive Reactions in Phenol Decomposition" *Reaction Chemistry and Engineering*, 2020, DOI: [10.1039/C9RE00418A](https://doi.org/10.1039/C9RE00418A).
 8. G. Bagheri, E. Ranzi, **M. Pelucchi**, A. Parente, A. Frassoldati, T. Faravelli "Comprehensive kinetic study of combustion technologies for low environmental impact: MILD and OXY-fuel combustion of methane" *Combustion and flame*, 2020. DOI: [10.1016/j.combustflame.2019.10.014](https://doi.org/10.1016/j.combustflame.2019.10.014)
 9. S. Namysl, **M. Pelucchi**, L. Pratali Maffei, O. Herbinet, A. Stagni, T. Faravelli, F. Battin-Leclerc "Experimental and modeling study of benzaldehyde oxidation" *Combustion and Flame*, 2020, DOI: [10.1016/j.combustflame.2019.09.024](https://doi.org/10.1016/j.combustflame.2019.09.024)

2019

10. **M. Pelucchi**, L. Cai, W. Pejpichestakul, R. Tripathi, S.W. Wagon, K. Zhang, M. Raju, M. Mehl, T. Faravelli, W. J. Pitz, H. Pitsch, H. Curran, P. K. Senecal "Computational Chemistry Consortium: Surrogate Fuel Mechanism Development, Pollutants Submechanisms and Components Library", *SAE Technical Paper*, 2020, DOI:[10.4271/2019-24-0020](https://doi.org/10.4271/2019-24-0020)
11. **M. Pelucchi**, C. Cavallotti, A. Cuoci, T. Faravelli, A. Frassoldati, E. Ranzi "Detailed kinetics of substituted phenolic species in pyrolysis bio-oils", *Reaction Chemistry and Engineering*, 2019, Royal Society of Chemistry. DOI: [10.1039/C8RE00198G](https://doi.org/10.1039/C8RE00198G)
12. S. Namysl, **M. Pelucchi***, O. Herbinet, A. Frassoldati, T. Faravelli, F. Battin-Leclerc "A first evaluation of butanoic and pentanoic acid oxidation kinetics", *Chemical Engineering Journal*, 2019, Elsevier. DOI: [10.1016/j.cej.2019.05.090](https://doi.org/10.1016/j.cej.2019.05.090).
13. **M. Pelucchi**, A. Stagni, T. Faravelli "Addressing the complexity of combustion kinetics: Data management and automatic model validation" in "Mathematical Modelling of Gas-Phase Complex Reaction Systems: Pyrolysis and Combustion" *Computer Aided Chemical Engineering*, 2019, Elsevier. DOI: [10.1016/B978-0-444-64087-1.00015-2](https://doi.org/10.1016/B978-0-444-64087-1.00015-2)
14. C. Cavallotti, **M. Pelucchi**, Y. Georgievskii, S.J. Klippenstein, "EStokTP: Electronic Structure to Temperature and Pressure Dependent Rate Constants; A Code for Automatically Predicting the Thermal Kinetics of Reactions", *Journal of Chemical Theory and Computation*, 2019, American Chemical Society. DOI: [10.1021/acs.jctc.8b00701](https://doi.org/10.1021/acs.jctc.8b00701)
15. W. Pejpichestakul, A. Cuoci, A. Frassoldati, **M. Pelucchi**, A. Parente, T. Faravelli. "Buoyancy effect in sooting laminar premixed ethylene flame", *Combustion and Flame*, 2019, Elsevier. DOI: [10.1016/j.combustflame.2019.04.001](https://doi.org/10.1016/j.combustflame.2019.04.001).
16. M. Keçeli, S. Elliott, Y-P Li, M. Johnson, C. Cavallotti, Y. Georgievskii, W.H. Green, **M. Pelucchi**, J.M. Wozniak, A.W. Jasper, S.J. Klippenstein "Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics" *Proceedings of the Combustion Institute*, 2019, Elsevier
DOI: [10.1016/j.proci.2018.07.113](https://doi.org/10.1016/j.proci.2018.07.113)

17. W. Pejpichestakul, E. Ranzi, **M. Pelucchi**, A. Frassoldati, A. Cuoci, A. Parente, T. Faravelli, "Examination of a soot model in premixed laminar flames at fuel-rich conditions" *Proceedings of the Combustion Institute*, 2019, Elsevier
DOI: [10.1016/j.proci.2018.06.104](https://doi.org/10.1016/j.proci.2018.06.104)
18. **M. Pelucchi***, S. Namysl, E. Ranzi, A. Frassoldati, O. Herbinet, F. Battin-Leclerc, T. Faravelli, "An experimental and kinetic modelling study of n-C4-C6 aldehydes oxidation in a jet-stirred reactor" *Proceedings of the Combustion Institute*, 2019, Elsevier
DOI: [10.1016/j.proci.2018.07.087](https://doi.org/10.1016/j.proci.2018.07.087)
19. C. Cavallotti, **M. Pelucchi**, A. Frassoldati, "Analysis of acetic acid gas phase reactivity: Rate constant estimation and kinetic simulations" *Proceedings of the Combustion Institute*, 2019, Elsevier
DOI: [10.1016/j.proci.2018.06.137](https://doi.org/10.1016/j.proci.2018.06.137)
20. G. Mairinger, A. Frassoldati, A. Cuoci, **M. Pelucchi**, E. Pucher, K. Seshadri "Experimental and computational investigation of autoignition of jet fuels and surrogates in nonpremixed flows at elevated pressures" *Proceedings of the Combustion Institute*, 2019, Elsevier. DOI: [10.1016/j.proci.2018.06.224](https://doi.org/10.1016/j.proci.2018.06.224)
21. G. Bagheri, M. Lubrano Lavadera, E. Ranzi, **M. Pelucchi**, P. Sabia, M. de Joannon, T. Faravelli. "Thermochemical oscillation of methane MILD combustion diluted with N₂/CO₂/H₂O" *Combustion Science and Technology*, 2019. DOI: [10.1080/00102202.2018.1452411](https://doi.org/10.1080/00102202.2018.1452411)

2018

22. Z-B. Ding, E. Di Marco, **M. Pelucchi**, T. Faravelli, M. Maestri, "First-principles assessment of the analogy between gas-phase and gas-solid H-abstraction reactions at graphene edges" *Chemical Engineering Journal*, 2018, Elsevier. DOI: [10.1016/j.cej.2018.08.077](https://doi.org/10.1016/j.cej.2018.08.077)
23. M. Lubrano Lavadera, Y. Song, P. Sabia, O. Herbinet, **M. Pelucchi**, A. Stagni, T. Faravelli, F. Battin-Leclerc, M. de Joannon, "Oscillatory behavior in methane combustion: on the influence of the operating parameters" *Energy & Fuels*, 2018, American Chemical Society. DOI: [10.1021/acs.energyfuels.8b00967](https://doi.org/10.1021/acs.energyfuels.8b00967)
24. **M. Pelucchi***, C. Cavallotti, T. Faravelli, S.J. Klippenstein. "H-Abstraction reactions by OH, HO₂, O, O₂ and benzyl radical addition to O₂ and their implications for kinetic modelling of toluene oxidation" *Physical Chemistry Chemical Physics*, 20, 10607-10627, 2018. DOI: [10.1039/C7CP07779C](https://doi.org/10.1039/C7CP07779C)
25. M. Singla, M.L. Rasmussen, H. Hashemi, H. Wu, P. Glarborg, **M. Pelucchi**, T. Faravelli, P. Marshall. "Ab Initio Calculations and Kinetic Modeling of Thermal Conversion of Methyl Chloride: Implications for Gasification of Biomass" *Physical Chemistry Chemical Physics*, 20, 10741-10752, 2018. DOI: [10.1039/C7CP07552A](https://doi.org/10.1039/C7CP07552A)
26. G. Scalia, **M. Pelucchi**, A. Stagni, T. Faravelli, B. Pernici. "Storing Combustion Data Experiments: New Requirements Emerging from a First Prototype: Position Paper". *Lecture Notes in Computer Science*, 2018, Springer. DOI: [10.1007/978-3-030-01379-0_10](https://doi.org/10.1007/978-3-030-01379-0_10).

2017

27. A. Carrera, **M. Pelucchi**, A. Stagni, A. Beretta, G. Groppi. "Catalytic partial oxidation of n-octane and iso-octane: Experimental and modeling results" *International Journal of Hydrogen Energy* 42 (39), 24675-24688, 2017. DOI: [10.1016/j.ijhydene.2017.08.020](https://doi.org/10.1016/j.ijhydene.2017.08.020)
28. **M. Pelucchi***, M. Bissoli, C. Rizzo, Y. Zhang, K. Somers, A. Frassoldati, H.J. Curran, T. Faravelli, "A Kinetic Modelling Study of Alcohols Operating Regimes in a HCCI Engine" *SAE International Journal of Engines* 10, 2354-2370, 2017. DOI: [10.4271/2017-24-0077](https://doi.org/10.4271/2017-24-0077)

29. G. Mairinger, A. Frassoldati, A. Cuoci, **M. Pelucchi**, E. Pucher, K. Seshadri. "Experimental and computational investigation of autoignition of jet fuels and surrogates in nonpremixed flows at elevated pressures" *Fall Technical Meeting of the Western States Section of the Combustion Institute*, 2017. <http://hdl.handle.net/11311/1043115>

30. **M. Pelucchi**, E. Ranzi, A. Frassoldati, T. Faravelli. "Alkyl radicals rule the low temperature oxidation of long chain aldehydes" *Proceedings of the Combustion Institute*, 36(1), 393-401, 2017. DOI: [10.1016/j.proci.2016.05.051](https://doi.org/10.1016/j.proci.2016.05.051)

2016

31. "Detailed kinetic mechanism of gas-phase reactions of volatiles released from biomass pyrolysis" P. E. A. Debiagi, G. Gentile, **M. Pelucchi**, A. Frassoldati, A. Cuoci, T. Faravelli, E. Ranzi. *Biomass and bioenergy*, 93, 60-71, 2016. DOI: [10.1016/j.biombioe.2016.06.015](https://doi.org/10.1016/j.biombioe.2016.06.015)

32. **M. Pelucchi**, C. Cavallotti, E. Ranzi, A. Frassoldati, T. Faravelli. "Relative Reactivity of Oxygenated Fuels: Alcohols, Aldehydes, Ketones, and Methyl Esters" *Energy & Fuels*, 30(10), 8665-8679, 2016. DOI: [10.1021/acs.energyfuels.6b01171](https://doi.org/10.1021/acs.energyfuels.6b01171)

33. M.S. Bernardi, **M. Pelucchi**, A. Stagni, L.M. Sangalli, A. Cuoci, A. Frassoldati, P. Secchi, T. Faravelli. *Combustion and Flame* 168, 186-203, 2016. "Curve matching, a generalized framework for models/experiments comparison: An application to n-heptane combustion kinetic mechanisms" DOI: [10.1016/j.combustflame.2016.03.019](https://doi.org/10.1016/j.combustflame.2016.03.019)

34. D. Nativel, **M. Pelucchi**, A. Frassoldati, A. Comandini, A. Cuoci, E. Ranzi, N. Chaumeix, T. Faravelli. *Combustion and Flame* 166, 1-18, 2016. "Laminar flame speeds of pentanol isomers: An experimental and modeling study" DOI: [10.1016/j.combustflame.2015.11.012](https://doi.org/10.1016/j.combustflame.2015.11.012)

2015

35. **M. Pelucchi**, A. Frassoldati, T. Faravelli, B. Ruscic, P. Glarborg. "High-temperature chemistry of HCl and Cl₂" *Combustion and Flame* 162 (6), 2693-2704, 2015. DOI: [10.1016/j.combustflame.2015.04.002](https://doi.org/10.1016/j.combustflame.2015.04.002)

36. E. Ranzi, C. Cavallotti, A. Cuoci, A. Frassoldati, **M. Pelucchi**, T. Faravelli. "New reaction classes in the kinetic modeling of low temperature oxidation of n-alkanes" *Combustion and Flame* 162 (5), 1679-1691, 2015. DOI: [10.1016/j.combustflame.2014.11.030](https://doi.org/10.1016/j.combustflame.2014.11.030)

37. "An experimental and kinetic modeling study of the pyrolysis and oxidation of n-C₃-C₅ aldehydes in shock tubes" **M. Pelucchi***, K.P. Somers, K. Yasunaga, U. Burke, A. Frassoldati, E. Ranzi, H.J. Curran, T. Faravelli. *Combustion and Flame* 162 (2), 265-286, 2015. DOI: [10.1016/j.combustflame.2014.07.027](https://doi.org/10.1016/j.combustflame.2014.07.027)

2014

38. "Improved kinetic model of the low-temperature oxidation of n-heptane" **M. Pelucchi**, M. Bissoli, C. Cavallotti, A. Cuoci, T. Faravelli, A. Frassoldati, A. Stagni, E. Ranzi *Energy & Fuels* 28 (11), 7178-7193, 2014. DOI: [10.1021/ef501483f](https://doi.org/10.1021/ef501483f)
 39. "Reduced kinetic schemes of complex reaction systems: fossil and biomass-derived transportation fuels" E. Ranzi, A. Frassoldati, A. Stagni, **M. Pelucchi**, A. Cuoci, T. Faravelli *International Journal of Chemical Kinetics* 46 (9), 512-542, 2014. DOI: [10.1002/kin.20867](https://doi.org/10.1002/kin.20867)
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14. Contributions to conferences and symposia (*presenter)

2020

1. "On the combustion and sooting behavior of standard and hydro-treated jet fuels: An experimental and modeling study on the compositional effects" **M. Pelucchi***, P. Oswald, W. Pejpichestakul, A. Frassoldati, M. Mehl. 38th International Symposium on Combustion, Adelaide, Australia. 24th-29th January 2021. Oral presentation.
2. "An experimental and kinetic modelling study of alpha-methylnaphthalene combustion" **M. Pelucchi***, A. Nobili, M. Mehl, A. Frassoldati, A. Comandini, N. Chaumeix. 38th International Symposium on Combustion, Adelaide, Australia. 24th-29th January 2021. Poster presentation.
3. "An experimental and kinetic modelling study of alpha-methylnaphthalene combustion" A. Nobili, L. Pratali Maffei, **M. Pelucchi**, M. Mehl, A. Frassoldati, A. Comandini, N. Chaumeix. 43rd Meeting of The Italian Section of the Combustion Institute, joint Italian-Polish meeting. Postponed to April 2021, Ischia, NA, Italy. Oral.
4. "Thermal degradation of Nylon-6 and real mixtures of solid plastic waste. An experimental and kinetic modelling study." **M. Pelucchi***, R. Batista da Silva, M. Mehl, A. Cuoci, A. Frassoldati, A. Beretta, L. Lietti, T. Faravelli. XXIV International Conference on Chemical Reactors-CHEMREACTOR24, Politecnico di Milano, Milan, Italy. Postponed to August 2021.
5. "Thermal degradation of nylon-6 and real mixtures of solid plastic waste: an experimental and kinetic modelling study." **M. Pelucchi***, R. Batista da Silva, M. Mehl, A. Cuoci, A. Frassoldati, A. Beretta, L. Lietti, T. Faravelli. 43rd Meeting of The Italian Section of the Combustion Institute, joint Italian-Polish meeting. Postponed to April 2021, Ischia, NA, Italy. Oral.
6. "Kinetics of the formation of first and second aromatic ring in premixed and counterflow flames: a comparative analysis" L. Pratali Maffei, A. Nobili, Q. Mao, **M. Pelucchi**, H. Pitsch, T. Faravelli. 5th International Flame Chemistry Workshop. 30th November-4th December 2020, remote.

2019

7. "Computational chemistry consortium: surrogate fuel mechanism development, pollutants submechanism and components library" **M. Pelucchi***, L. Cai, W. Pejpichestakul, R. Tripathi, S. Wagnon, R. Mandhapaty, K. Zhang, W.J. Pitz, H. Pitsch, T. Faravelli, K. Senecal, H.J. Curran. 14th International Conference on Engines & Vehicles. Capri, Napoli (Italy) September 15-19, 2019. Oral presentation.
8. "Theoretical and kinetic modelling study of the oxidation of oxygenated aromatic hydrocarbons: reaction classes and rate rules" S. Caruso, G. Cislighi, L. Pratali Maffei, W. Pejpichestakul, C. Cavallotti, A. Frassoldati, T. Faravelli, **M. Pelucchi***. 42nd meeting of the Italian Section of the Combustion Institute. Ravenna, 8-11 Settembre 2019. Oral presentation.
9. "Kinetic modelling of a standard jet fuel oxidation in a flow reactor" M.Mehl, P. Oswald, **M. Pelucchi**. 42nd meeting of the Italian Section of the Combustion Institute. Ravenna, 8-11 Settembre 2019. Oral presentation.

10. "Modellazione cinetica del degrado termico di materie plastiche e miscele: stato dell'arte e sviluppi volti a migliorare l'efficienza di processi di pirolisi e gassificazione." Convegno GRICU 2019 (Chemical Engineering Italian Meeting), Palermo, Italy, 2019. ***M. Pelucchi**, A. Cuoci, A. Frassoldati, M. Mehl, T. Faravelli. Oral presentation.
11. "A systematic kinetic modelling study of mono-aromatic hydrocarbons: towards the definition of reaction classes and rate rules" ***M. Pelucchi**, L. Pratali Maffei, R. Buttgen, A. Frassoldati, K.A. Heufer, T. Faravelli. 11th International Conference on Chemical Kinetics 2019, Orleans, France. Oral presentation.
12. "A Theoretical and Kinetic Analysis of Phenol Pyrolysis" L. Pratali Maffei, **M. Pelucchi**, T. Faravelli, C. Cavallotti. 11th International Conference on Chemical Kinetics 2019, Orleans, France. Oral presentation. Oral presentation.
13. "Fast Pyrolysis Bio-Oil Combustion Characteristics and Challenges for Kinetic Modeling" A. Frassoldati, **M. Pelucchi**, A.E. Saufi, C. Cavallotti, A. Cuoci, T. Faravelli, E. Ranzi. 11th International Conference on Chemical Kinetics 2019, Orleans, France. Oral presentation.
14. ***Chair and organizer of** "High Performance Computing: Towards High Throughput Kinetics and Combustion Model Development" Mini-Symposium, Numerical Combustion Meeting, May 2019, Aachen, Germany.
15. "Predictive Automated Combustion Chemistry: A DOE-Exascale Project" S. J. Klippenstein, ..., **M. Pelucchi**. Mini-Symposium on "High Performance Computing: Towards High Throughput Kinetics and Combustion Model Development" Numerical Combustion Meeting, May 2019, Aachen, Germany.
16. "Towards an automated and generalized approach to the validation of kinetic models" A. Stagni, **M. Pelucchi**, G. Scalia, T. Faravelli, B. Pernici. 17th Numerical Combustion Meeting, 2019, Aachen, Germany. Oral presentation.
17. "From Electronic Structure to Temperature and Pressure Dependent Rate Constants: ESTokTP. A Code for Automatically Predicting the Thermal Kinetics of Reactions" C. Cavallotti, **M. Pelucchi**, Y. Georgievskii, S. J. Klippenstein. Mini-symposium on "New Techniques in Computational Kinetics", 17th Numerical Combustion Meeting, 2019, Aachen, Germany. Oral presentation.
18. "HO₂ + HO₂: High Level Theory and the Role of Singlet Channels" S. J. Klippenstein, R. Sivaramakrishnan, U. Burke, K. Somers, H. J. Curran, L. Cai, H. Pitsch, **M. Pelucchi**, T. Faravelli, P. Glarborg. 11th U. S. National Combustion Meeting, Pasadena, USA. Oral presentation.
19. "Towards a common C0-C2 mechanism: a critical evaluation of rate constants for syngas combustion kinetics" ***M. Pelucchi**, U. Burke, K. P. Somers, L. Cai, P. Glarborg, T. Turanyi, H. Pitsch, T. Faravelli, S. J. Klippenstein. 1st International Conference on Smart Energy Carriers, Università Federico II, Napoli, Italy. Oral presentation.
20. "Theoretical and kinetic modelling study of phenol and phenoxy radical decomposition to CO and C₅H₆/C₅H₅ in pyrolysis conditions" L. P. Maffei, **M. Pelucchi**, C. Cavallotti, T. Faravelli. 1st International Conference on Smart Energy Carriers, Università Federico II, Napoli, Italy. Poster presentation.
21. "Experimental and kinetic modelling study of benzaldehyde oxidation in JSR", S. Namysl, **M. Pelucchi**, A. Stagni, O. Herbinet, T. Faravelli, F. Battin-Leclers. 1st International Conference on Smart Energy Carriers, Università Federico II, Napoli, Italy. Poster presentation.
22. "Assessment of the Analogy between Gas-Phase and Gas-Solid Reactions for the Microkinetic Modeling of Reactions at the Graphene Edges" Z.-B. Ding, **M. Pelucchi**, T. Faravelli, M. Maestri. 2019 North American Catalysis Society Meeting, Chicago, IL, USA, 23rd-28th June 2019. Poster presentation.
23. "Towards a better understanding of the combustion of oxygenated aromatic hydrocarbons in rapid compression machine" R. D. Buttgen, L. Pratali Maffei, **M. Pelucchi**, T. Faravelli, A. Frassoldati, K.A. Heufer. 9th European Combustion Meeting, Lisbon, Portugal, 14th-17th April 2019. Poster presentation.

24. "Mechanism Comparison for PAH Formation in Pyrolysis and Laminar Premixed Flames" W. Pejpichestakul, R. Tripathi, **M. Pelucchi**, L. Cai, H. Pitsch, E. Ranzi, T. Faravelli. 9th European Combustion Meeting, Lisbon, Portugal, 14th-17th April 2019. Poster presentation.
25. "Evaluation of Polycyclic Aromatic Hydrocarbon Formation in Counterflow Diffusion Flames" R. Tripathi, W. Pejpichestakul, L. Cai, **M. Pelucchi**, T. Faravelli, H. Pitsch. 9th European Combustion Meeting, Lisbon, Portugal, 14th-17th April 2019. Poster presentation.
26. "Experimental and modelling study of the oxidation of methane doped with ammonia" Y. Song, O. Herbinet, **M. Pelucchi**, A. Stagni, T. Faravelli, F. Battin-Leclerc. 9th European Combustion Meeting, Lisbon, Portugal, 14th-17th April 2019. Poster presentation.

2018

27. "An experimental and kinetic modelling study of c4-c5 carboxylic acids pyrolysis and oxidation in a jet stirred reactor" ***M. Pelucchi**, S. Namysl, O. Herbinet, T. Faravelli, F. Battin-Leclerc. ChemReactor-23, Ghent, Belgium. Oral presentation.
28. "Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics" M. Keçeli, S. Elliott, Y-P Li, M. Johnson, C. Cavallotti, Y. Georgievskii, W.H. Green, **M. Pelucchi**, J.M. Wozniak, A.W. Jasper, S.J. Klippenstein. 37th International Symposium on Combustion, Dublin, Ireland. Oral presentation.
29. "Examination of a soot model in premixed laminar flames at fuel-rich conditions" W. Pejpichestakul, E. Ranzi, **M. Pelucchi**, A. Frassoldati, A. Cuoci, A. Parente, T. Faravelli. 37th International Symposium on Combustion, Dublin, Ireland. Oral presentation.
30. "Analysis of acetic acid gas phase reactivity: Rate constant estimation and kinetic simulations" C. Cavallotti, **M. Pelucchi**, A. Frassoldati. 37th International Symposium on Combustion, Dublin, Ireland. Oral presentation
31. "An experimental and kinetic modelling study of n-C4C6 aldehydes oxidation in a jet-stirred reactor" ***M. Pelucchi**, S. Namysl, E. Ranzi, A. Frassoldati, O. Herbinet, F. Battin-Leclerc, T. Faravelli. 37th International Symposium on Combustion, Dublin, Ireland. Oral presentation.
32. "A critical evaluation of rate constants for syngas combustion kinetics" U. Burke, ***M. Pelucchi**, L. Cai, P. Glarborg, T. Turanyi, H. Pitsch, T. Faravelli, S. J. Klippenstein. International Flame Chemistry Workshop, Trinity College, Dublin, Ireland. Oral presentation.
33. "Best Practices – Measurements, Repositories, Standards for Rapid Compression Machines" ***M. Pelucchi**, S. Dooley, S. Goldsborough. 4th International RCM Workshop, Trinity College, Dublin, Ireland. Oral presentation.
34. "From electronic structure calculations to temperature and pressure dependent rate constants: a new computational environment" C. Cavallotti, **M. Pelucchi**, Y. Georgievskii, S. J. Klippenstein. Oral presentation. International Symposium on Chemical Reaction Engineering (ISCRE18), Firenze, Italy.
35. "H-Abstraction reactions by OH, HO₂, O, O₂ and benzyl radical addition to O₂ and their implications for kinetic modelling of toluene oxidation" ***M. Pelucchi**, C. Cavallotti, T. Faravelli, S.J. Klippenstein. BUNSENTAGUNG 2018 - KINETICS IN THE REAL WORLD, Leibniz University, Hannover.
36. "Reaction Classes Characterizing Oxygenated Fuels Combustion: alcohols, aldehydes and carboxylic acids" M. Pelucchi, S. Namysl, O. Herbinet, F. Battin-Leclerc, T. Faravelli. Workshop on "Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules", 23-24 April 2018, Milan, Italy

2017

37. "Ab Initio and Kinetic Modelling Study of Toluene Oxidation" ***M. Pelucchi**, C. Cavallotti, T. Faravelli, S.J. Klippenstein. 10th International Conference on Chemical Kinetics, University of Illinois, Chicago, USA. Oral presentation. Oral presentation.

38. "A kinetic modelling study of alcohols operating regimes in a HCCI engine" ***M. Pelucchi**, M. Bissoli, C. Rizzo, A. Frassoldati, T. Faravelli, K.P. Somers, Y. Zhang, H.J. Curran. International Conference on Internal Combustion Engines-SAE Napoli, Capri, Italy. Oral presentation.
39. "Experimental and computational investigation of autoignition of jet fuels and surrogates in nonpremixed flows at elevated pressures". G. Mairinger, A. Frassoldati, A. Cuoci, **M. Pelucchi**, E. Pucher, K. Seshadri. 2017 Fall Technical Meeting of the Western States Section of the Combustion Institute. Wyoming, USA. Oral presentation.
40. "Exploring the reactivity of C4-C6 linear alcohols: from jet stirred reactor and rapid compression machine experiments to operating regimes in a hcci engine" ***M. Pelucchi**, M. Bissoli, C. Rizzo, A. Frassoldati, T. Faravelli, K.P. Somers, Y. Zhang, H.J. Curran, F. Battin-Leclerc, S. Namysl, O. Herbinet. Third Annual Meeting of the SMARTCATs COST Action, J. Heyrovský Institute of Physical Chemistry, Czech Academy of Science, Prague, Czech Republic. Oral presentation.
41. "Towards a community standard data exchange: an application to RCM measurements and simulations" ***M. Pelucchi**, A. Matriciano, S. Dooley. Third Annual Meeting of the SMARTCATs COST Action, J. Heyrovský Institute of Physical Chemistry, Czech Academy of Science, Prague, Czech Republic. Oral presentation.

2016

42. "Towards a fully automated system to develop, validate and evaluate combustion kinetic mechanisms" ***M. Pelucchi**, A. Rigamonti, A. Frassoldati, B. Pernici, T. Faravelli. Second Annual Meeting of the SMARTCATs COST Action, Instituto Tecnico Superior, Lisbon, Portugal. Oral presentation.
43. "Data exchange: towards a community standard" ***M. Pelucchi**, A. Stagni, A. Frassoldati, A. Cuoci, E. Ranzi, T. Faravelli. Second Annual Meeting of the SMARTCATs COST Action, Instituto Tecnico Superior, Lisbon, Portugal. Workshop on data exchange. Oral presentation.
44. "Alkyl radicals rule the low temperature oxidation of aldehydes" ***M. Pelucchi**, E. Ranzi, A. Frassoldati T. Faravelli. 36th International Symposium on Combustion, Seoul, South Korea. Oral presentation.

2015

45. "Curve Matching, a generalized framework for combustion models validation" ***M. Pelucchi**, M. Bernardi, A. Stagni, L. M. Sangalli, P. Secchi, T. Faravelli. European Combustion Meeting 2015, Budapest, Hungary. Workshop "Taming uncertainty in combustion chemistry: experiments and models". Oral presentation.
46. "Detailed kinetic mechanisms for practical applications: new reaction classes and model reduction" ***M. Pelucchi**, A. Stagni, A. Frassoldati, A. Cuoci, M. Bissoli, E. Ranzi, T. Faravelli. **Invited talk** at Young Researchers Colloquium, Clean Air Conference 2015, Lisbon, Portugal. Oral Presentation.
47. "Kinetic modeling of the low temperature cool flames of acetaldehyde in a well stirred reactor" ***M. Pelucchi**, A. El Ziani, M. Mensi, E. Ranzi, A. Frassoldati T. Faravelli. 28th Italian Combustion Meeting, Università di Lecce, Italy. Oral and poster presentation.
48. "Oxidation of C3 and n-C4 aldehydes at low temperatures" ***M. Pelucchi**, E. Ranzi, A. Frassoldati T. Faravelli. 28th Italian Combustion Meeting, Università di Lecce, Italy. Oral and poster presentation.

2014

49. "Kinetic modeling of biofuels: aldehydes oxidation" ***M. Pelucchi**, A. Frassoldati, E. Ranzi, T. Faravelli. 1st International conference on Biomass. Firenze, Italy. Oral presentation.

2013

50. "Experimental and kinetic modeling study of C3-C5 n-aldehydes auto-ignition and pyrolysis in shock tubes" ***M. Pelucchi**, K. P. Somers, U. Burke, C. Saggese, K. Yasunaga, A. Frassoldati, E. Ranzi, H. J.

Curran, T. Faravelli. 4th Annual meeting of COST Action CM0901, Università di Perugia, Perugia, Italy. Oral Presentation.

15. Reviewer and Editor activities

2020-2021

Guest Editor for:

1. Energies MDPI Special Issue: *“Kinetic Modeling of E-fuels combustion”*, Deadline for paper submission July 2021. Co-editor: Prof. Liming Cai (RWTH Aachen, DE and Tongji University, CHN)
2. Frontiers in Mechanical Engineering Special Issue: *“Chemical kinetics for fuel combustion: from theoretical kinetics to real world applications”*, Deadline for paper submission November 2021. Co-editor: Prof. Nicole Labbe (University of Colorado, Boulder, USA) and Dr. Ruben Van de Vijver (Ghent University, Belgium)

2016-Present.

Reviewer for different journals in the field of energy, combustion, chemical reaction engineering, chemical kinetics, renewable energy, physical chemistry: *Combustion and Flame, Fuel, Energy and Fuels, Physical Chemistry Chemical Physics, Reaction Chemistry and Engineering, RSC Advances, Proceedings of the Combustion Institute, Chemical Engineering Journal, Chemical Engineering Communications, Combustion Theory and Modelling, International Journal of Chemical Kinetics, International Journal of Hydrogen Energy, Journal of Physical Chemistry A, Biomass and Bioenergy.*