

## LIST OF PUBLICATIONS 2013

### LABORATORY OF COMBUSTION RESEARCH (5300)

#### TEACHING ACTIVITIES (lectures)

Dr. S.M.A. Biollaz

*Biomass: Options for technical use*

Renewable Energy Technologies I, ETH Zürich, Zürich, November 26, 2013.

Dr. S.M.A. Biollaz

*Biomass: Fuel production*

Renewable Energy Technologies I, ETH Zürich, Zürich, December 03, 2013.

Dr.-Ing. P. Jansohn

*Gasturbinen: Prozesse und Verbrennungssysteme*

(Vorlesung für höhere Semester/Master in den Studiengängen Maschineningenieurwissenschaften und Energy Science & Technology)

ETH Zürich, FS 2013.

Dr.-Ing. P. Jansohn

*Verbrennung in Gasturbinen - neue Herausforderungen durch Wasserstoff*

(Ringvorlesung „Ausgewählte Kapitel der Turbomaschinen“)

RWTH Aachen, (13.11.2013) WS 2013.

PD Dr. J. Mantzaras, Dr. C. Frouzakis<sup>1</sup>

*Theoretical and Numerical Combustion*

ETH Zürich, HS 2013.

<sup>1</sup> ETH Zürich

#### PUBLICATIONS

##### Books and Reviewed Book Chapters

P. Jansohn (Ed.)

*Modern Gas Turbine Systems*

Woodhead Publishing Series in Energy: Number 20

ISBN: 978-1-84569-728-0

Woodhead Publishing Ltd. (2013).

M. Rüdüsüli, T.J. Schildhauer, S.M.A. Biollaz, J.R. van Ommen<sup>1</sup>

*Measurement, monitoring and control of fluidized bed combustion and gasification*

Fluidized bed technologies for near-zero emission combustion and gasification, F. Scala (Ed.), Woodhead (2013).

<sup>1</sup> TU Delft, The Netherlands

##### Peer Reviewed Papers

A.M. Bernhard, D. Peitz, M. Elsener, T.J. Schildhauer, O. Kröcher

*Catalytic urea hydrolysis in the selective catalytic reduction of NOx: catalyst screening and kinetics on anatase TiO<sub>2</sub> and ZrO<sub>2</sub>*

Catalysis Science and Technology **3**, 942-951 (2013).

S. Biollaz

*Stand der Technik und Trends bei der Erzeugung von Strom und Treibstoffen aus Holz*

Schweiz Z Forstwes **164**, 12, 398–407 (2013).

A. Bodi, P. Hemberger, T. Gerber

*A robust link between the thermochemistry of urea and isocyanic acid by dissociative photoionization*

doi:10.1016/j.jct.2012.11.013, J. Chem. Thermody. **58**, 292-299 (2013).

- A. Bodi, P. Hemberger, D. L. Osborn, B. Sztaray  
*Mass-Resolved isomer-Selective chemical analysis with imaging photoelectron photoion coincidence spectroscopy*  
 doi:10.1021/jz401500c, J. Phys. Chem. Lett. **4**, 2948-2952 (2013).
- P. Bornhauser, Y. Sych, G. Knopp, T. Gerber, and P.P. Radi  
*Re-visiting the observation of the vibronic sequence of the C2 swan system*  
 doi:10.1016/j.cplett.2013.04.011, J. Phys. Chem. Lett. **572**, 16-20 (2013).
- I. Czekaj, K. Kacprzak, J. Mantzaras  
*CH<sub>4</sub> combustion cycles at Pd/Al<sub>2</sub>O<sub>3</sub> - important role of support and oxygen access*  
 doi:10.1039/c3cp51085a, Phys. Chem. Chem. Phys. **15**, 11368-11374 (2013).
- I. Czekaj, K. Kacprzak, J. Mantzaras  
*Methane catalytic combustion on Pd<sub>9</sub>/γ-Al<sub>2</sub>O<sub>3</sub> with different degrees of Pd oxidation*  
 doi:10.2533/chimia.2013.271, Chimia **67**, 271-274 (2013).
- S. Daniele, J. Mantzaras, P. Jansohn, A. Denisov, K. Boulouchos<sup>1</sup>  
*Flame front/turbulence interaction for syngas fuels in the thin reaction zones regime: turbulent and stretched laminar flame speeds at elevated pressures and temperatures*  
 doi:10.1017/jfm.2013.141, J. Fluid Mech. **724**, 36-68 (2013).
- <sup>1</sup> ETHZ/LAV
- A. Denisov, G. Colmegna, P. Jansohn,  
*Temperature measurements in sooting counterflow diffusion flames using laser-induced fluorescence of flame-produced nitric oxide*  
 Applied Physics B, Online First, 2013.  
 doi:10.1007/s00340-013-5697-6
- K. H. Fischer, P. Hemberger, A. Bodi, I. Fischer  
*Photoionisation of the tropyli radical*  
 doi:10.3762/bjoc.9.77, Beilstein J. Org. Chem. **9**, 681-688 (2013).
- T. Gerber, Y. Liu, G. Knopp, P. Hemberger, A. Bodi, P.P. Radi, Y. Sych  
*Charged particle velocity map Image reconstruction with one-dimensional projections of spherical functions*  
 doi:10.1063/1.4793404, Rev. Sci. Instrum. **84**, 033101-10 (2013).
- J. Harvey, P. Hemberger, A. Bodi, R.P. Tuckett  
*Vibrational and electronic excitations in fluorinated ethene cations from the ground up*  
 doi:10.1063/1.4795428, J. Chem. Phys. **138**, (2013).
- P. Hemberger, A. Bodi, T. Gerber, M. Wurtemberger, U. Radius  
*Unimolecular reaction mechanism of an imidazolin-2-ylidene: An iPEPICO study on the complex dissociation of an arduengo-type carbene*  
 doi:10.1002/chem.201204465, Chem. Eu. J. **19**, 7090-7099 (2013).
- P. Hemberger, A. J. Trevitt, E. Ross, G. da Silva  
*Direct observation of para-Xylylene as the decomposition product of the meta-Xylyl radical using VUV Synchrotron radiation*  
 doi:10.1021/jz401207z, J. Phys. Chem. Lett. **4**, 2546-2550 (2013).
- F. Holzmeier, M. Lang, K. Hader, P. Hemberger, I. Fischer  
*H<sub>2</sub>CN<sup>+</sup> and H<sub>2</sub>CNH<sup>+</sup>: New insight into the structure and dynamics from mass-selected threshold photoelectron spectra*  
 doi:10.1063/1.4808050, J. Chem. Phys. **138**, (2013).
- J. Kang, N. Prasianakis, J. Mantzaras  
*Lattice Boltzmann model for thermal binary-mixture gas flows*  
 doi:10.1103/PhysRevE.87.053304, Phys. Rev. E **87**, 053304 (2013).
- C.F.J. König, P. Schuh<sup>1</sup>, T.J. Schildhauer, M. Nachtegaal  
*High-temperature sulfur removal from biomass-derived synthesis gas over bifunctional molybdenum catalysts*  
 Chem. Cat. Chem **5**, 3700-3711(2013).
- <sup>1</sup> TU München, Germany

- C.F.J. König, T.J. Schildhauer, M. Nachtegaal  
*Methane synthesis and sulfur removal over a Ru catalyst probed in situ with high sensitivity X-ray absorption spectroscopy*  
*J. Catal.* **305**, 92-100 (2013).
- C.F.J. König, M. Nachtegaal, M. Seemann, F. Clemens<sup>1</sup>, N. van Garderen<sup>1</sup>, S.M.A. Biollaz, T.J. Schildhauer  
*Mechanistic studies of chemical looping desulfurization of Mn-based oxides using in situ X-ray absorption spectroscopy*  
*Appl. Energy* **113**, 1895-1901 (2014).  
<sup>1</sup> Empa, Dübendorf
- J. Kopyscinski, M.C. Seemann, R. Moergeli<sup>1</sup>, S.M.A. Biollaz, T.J. Schildhauer  
*Synthetic natural gas from wood: Reactions of ethylene in fluidised bed methanation*  
*Appl.Catal. A: General* **462–463**, 150-156 (2013).  
<sup>1</sup> CTU AG Winterthur
- J. Kiefer, P.P. Radi  
*Development and applications of nonlinear optical spectroscopy: The joint 11th ECONOS and 31st ECW meeting in Aberdeen, Scotland*  
 doi:10.1002/jrs.4397, *J. Raman Spectrosc.* **44**, 1317–1318 (2013).
- D.N. Kozlov, D.A. Sadovskii, P.P. Radi  
*Laser-induced grating spectroscopy of highly excited overtone and combination vibrational states of methane*  
 doi:10.1016/j.jms.2013.04.005, *J. Mol. Spectrosc.* **291**, 23–32 (2013).
- P. Kyrtatos<sup>1</sup>, K. Hoyer, P. Obrecht<sup>1</sup>, K. Boulouchos<sup>1</sup>  
*Apparent effects of in-cylinder pressure oscillations and cycle-to-cycle variability on heat release rate and soot concentration under long ignition delay conditions in diesel engines.*  
*International Journal of Engine Research* published online 28 June 2013,  
 doi: 10.1177/1468087413483288,  
<sup>1</sup> ETH Zürich
- M. Lang, F. Holzmeier, I. Fischer, P. Hemberger  
*Threshold photoionization of fluorenyl, benzhydryl, diphenylmethylene, and their dimers*  
 doi:10.1021/jp403158z, *J. Phys. Chem. A* **117**, 5260-5268 (2013).
- Y.-C Lin, S. Daniele, P. Jansohn, K. Boulouchos<sup>1</sup>  
*Turbulent Flame Speed as an Indicator for Flashback Propensity of Hydrogen-Rich Fuel Gases,*  
*Journal of Engineering for Gas Turbines and Power* **135**(11), 111503, (2013).  
 [doi: 10.1115/1.4025068]  
<sup>1</sup> ETH Zürich
- F. Lucci, C. Frouzakis<sup>1</sup>, J. Mantzaras  
*Three-dimensional direct numerical simulation of turbulent channel flow catalytic combustion of hydrogen over platinum*  
 doi:10.1016/j.proci.2012.06.110, *Proc. Combust. Inst.* **34**, 2295-2302 (2013).  
<sup>1</sup> ETH/LAV Zürich
- Y. Liu, T. Gerber, Y. Sych, P.P. Radi, G. Knopp  
*Real-time observation of ultrafast internal conversion in ethylbenzene by femtosecond time-resolved photoelectron imaging*  
 doi:10.1364/OE.21.016639, *Opt. Express* **21**,16639 (2013).
- Y. Liu, G. Knopp, P. Hemberger, Y. Sych, P.P. Radi, A. Bodi, T. Gerber  
*Ultrafast imaging of electronic relaxation in O-xylene: a new competing intersystem crossing channel*  
 doi:10.1039/C3CP53004C, *Phys. Chem. Chem. Phys.* **15**, 18101–18107 (2013).
- P. Maksyutenko, P. P. Radi, D. N. Kozlov, and A. P. Kouzov  
*Polarization- and time-resolved DFWM spectroscopy of the A 2Σ<sup>+</sup>- X 2Π (0,0) band transitions of nascent OH radicals generated by 266 Nm laser photolysis of H<sub>2</sub>O<sub>2</sub>*  
 doi:10.1002/jrs.4299, *J. Raman Spectrosc.* **44**, 1349–1355 (2013).

J. Mantzaras

*New directions in advanced modelling and in situ measurements near reacting surfaces*

doi:10.1007/s10494-012-9394-z, Flow Turbul. Combust. **90**, 681-707 (2013).

P. M. Mayer, D. Staedter, V. Blanchet, P. Hemberger, A. Bodi

*Comparing femtosecond multiphoton dissociative ionization of tetrathiafulvene with imaging photoelectron photoion coincidence spectroscopy*

doi:10.1021/jp311066y, J. Phys. Chem. A **117**, 2753-2759 (2013).

N. Prasianakis, T. Rosen, J. Kang, J. Eller, J. Mantzaras, F.N. Buechi

*Simulation of 3D porous media flows with application to polymer electrolyte fuel cells*

doi:10.4208/cicp.341011.310112s, Commun. Comput. Phys. **13**, 851-866 (2013).

U. Rhyner, P. Edinger, T.J. Schildhauer, S.M.A. Biollaz

*Applied kinetics for modeling of reactive hot gas filters*

Appl. Energy **113**, 766-780 (2014).

U. Rhyner, R. Mai<sup>1</sup>, H. Leibold<sup>1</sup>, S.M.A. Biollaz

*Dynamic pressure measurements of a hot gas filter as a diagnostic tool to assess the time dependent performance*

Biomass and Bioenergy **53**, 72-80 (2013).

<sup>1</sup> KIT, Karlsruhe, Germany

Y. Sych, P. Bornhauser, G. Knopp, Y. Liu, T. Gerber, R. Marquardt, and P. P. Radi

*Perturbation facilitated two-color four-wave-mixing spectroscopy of C3*

doi:10.1063/1.4825198, J. Chem. Phys. **139**, 154203 (2013).

M. Schultze, J. Mantzaras, R. Bombach, K. Boulouchos<sup>1</sup>

*An experimental and numerical investigation of the hetero-/homogeneous combustion of fuel-rich hydrogen/air mixtures over platinum*

doi:10.1016/j.proci.2012.05.029, Proc. Combust. Inst. **34**, 2269-2277, (2013).

<sup>1</sup> ETHZ/LAV

M. Schultze, J. Mantzaras

*Hetero-/homogeneous combustion of hydrogen/air mixtures over platinum: fuel-lean versus fuel-rich combustion modes*

doi:10.1016/j.ijhydene.2013.06.069, Int. J. Hydrogen Energy **38**, 10654-10670 (2013).

X. Zheng, J. Mantzaras, R. Bombach

*Homogeneous combustion of fuel-lean syngas mixtures over platinum at elevated pressures and preheats*

doi:10.1016/j.combustflame.2012.09.001, Combust. Flame **160**, 155-169 (2013).

X. Zheng, J. Mantzaras, R. Bombach

*Hetero-/homogeneous combustion of ethane/air mixtures over platinum at pressures up to 14 bar*

doi:10.1016/j.proci.2012.05.028, Proc. Combust. Inst. **34**, 2279-2287 (2013).

X. Zheng, M. Schultze, J. Mantzaras, R. Bombach

*Effects of hydrogen addition on the catalytic oxidation of carbon monoxide over platinum at power generation relevant temperatures*

doi:10.1016/j.proci.2012.06.118, Proc. Combust. Inst. **34**, 3343-3350, (2013).

## TALKS

### Invited Talks

S. Biollaz

*Progress in R&D for next generation methanation technologies*

SGC International Seminar on Gasification 2013, Goteborg, Sweden, October 16-17, 2013.

P. Hemberger

*Threshold ionization of reactive Intermediates: from combustion to catalysis*

Laboratoire de Chimie Physique Group Seminar, Universite Paris Sud Orsay, France, July 5, 2013.

P. Jansohn  
*(trockene) Biomasse: Umwandlung zu Wärme, Strom und (synthet.) Erdgas*  
 SVUT-Forum, Cleantech City, Bern, 20. März 2013.

P. Jansohn  
*Combustion Research: Contributions to efficient & low emission energy conversion*  
 Advisory Board Meeting, CCEM, Novotel Zürich Airport Messe, Zürich, 25. April 2013.

J. Mantzaras  
*Catalytic combustion modeling and simulation*  
 Haldor Topsoe Catalysis Forum (HTC), Lyngby, Denmark, August 28-19, 2013.

## THESES

### Dissertations

F. Grygier  
*Influence of Rotational Energy Transfer on Quantitative O<sub>2</sub> Laser-Induced Fluorescence Measurements in Flames*  
 Ph.D. Thesis, No. xxxx, ETH Zürich, December 2013.

J. Kang  
*Lattice Boltzmann method for reactive thermal multicomponent flows*  
 Ph.D. Thesis No. 21435, ETH Zürich, September 2013.

U. Rhyner  
*Reactive hot gas filter for B-IGFC systems*  
 Ph.D. Thesis, No. 21102, ETH Zürich, May 2013.

M. Schultze  
 An experimental and numerical investigation of the hetero-/homogeneous combustion of H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> and H<sub>2</sub>/CO/O<sub>2</sub>/N<sub>2</sub> mixtures over platinum at fuel-rich stoichiometries  
 Ph.D. Thesis No. 21555, ETH Zürich, November 2013

Y Sych  
*Four-wave mixing spectroscopy of small carbon clusters*  
 Ph.D. Thesis, No. xxxx, ETH Zürich, December 2013.

### Diploma / Master Theses

M. End  
*Perspektive 2020 für Holz-BHKW in der Schweiz*  
 Hochschule Luzern (HSLU), AEW and PSI, June, 2013.

S. Wiedner  
*Umsetzung von SNG-Anlagen in der Schweiz: Modellierung des Business Case und Erarbeitung von Handlungsempfehlungen*  
 FA Konstanz and PSI, October, 2013.

### Bachelor / Semester Theses

T. Fink  
*Validierung eines Simulationsprogramms für die Druckentwicklung während eines Abreinigungsverfahrens mittels Coupled Pressure Pulse Reinigungsverfahren*  
 FA Konstanz and PSI, February, 2013.

## Conference Proceedings / Other Papers

F. Bolanos<sup>1</sup>, D. Winkler<sup>1</sup>, F. Piringer<sup>1</sup>, T. Griffin<sup>1</sup>, R. Bombach, J. Mantzaras  
*Study of a rich/lean staged combustion concept for hydrogen at gas turbine relevant conditions*  
 ASME 2013-94420, San Antonio, USA, June 3-7 (2013).

<sup>1</sup> FHNW

P. Kyrtatos<sup>1</sup>, K. Hoyer, P. Obrecht<sup>1</sup>, K. Boulouchos<sup>1</sup>  
*Recent developments in the Understanding of the Potential of In-Cylinder NOx Reduction through Extreme Miller Valve Timing*, Paper No. 225, CIMAC Congress 2013, Shanghai

<sup>1</sup> ETH Zurich

Y.-C Lin, P. Jansohn, K. Boulouchos<sup>1</sup>

*Turbulent Flame Speed as an Indicator for Flashback Propensity: An Example for Wet Gas Turbine Applications*, Proceedings of the European Combustion Meeting, Lund, Sweden (2013).

<sup>1</sup> ETH Zürich

Y.-C Lin, S. Daniele, P. Jansohn, K. Boulouchos<sup>1</sup>

*Turbulent Flame Speed as an Indicator for Flashback Propensity of Hydrogen-Rich Fuel Gases*, paper # GT2013-95518, Proceedings of ASME Turbo Expo, San Antonio, Texas, USA (2013).

<sup>1</sup> Labor für Aerothermochemie und Verbrennungssysteme, Institut für Energietechnik, ETH Zürich

Y.-C Lin, P. Jansohn, K. Boulouchos<sup>1</sup>

*Turbulent Flame Speed as an Indicator for Flashback Propensity: Effects of Preheat Temperature*, 26th German Flame Day - Combustion and Furnaces, Duisburg, Germany (2013).

<sup>1</sup> ETH Zürich

S. Maurer, M. Rüdüsüli, T.J. Schildhauer, S.M.A. Biollaz, J.R. van Ommen<sup>1</sup>

*Scale-up of bubbling fluidized bed reactors with vertical internals: a new approach accounting for chemistry and hydrodynamics*

Proceedings of the 14th International Conference on Fluidization, Noordwijkerhout (2013).

<sup>1</sup> TU Delft, The Netherlands

S.L. Teske, I. Couckuyt<sup>1</sup>, T.J. Schildhauer, S.M.A. Biollaz, F. Maréchal<sup>2</sup>

*Integrating rate based models into multi-objective optimisation of process designs using surrogate models*  
 proceedings of the international conference on efficiency, cost, optimization, simulation and environmental impact of Energy Systems (2013).

<sup>1</sup> University of Ghent, Belgium

<sup>2</sup> EPF Lausanne

## CONFERENCES, WORKSHOPS & EXHIBITIONS

N.I. Prasianakis, J. Kang, J. Roth, V. Vargek, J. Mantzaras, F. N. Büchi

*Numerical simulation of the flow in the cathode channel and porous diffusion layer (GDL) of a micro fuel cell*, 5th International Conference on Porous Media and Annual Meeting (InterPore), Prague, Czech Republic (21-24 May 2013).

J. Kang, N.I. Prasianakis, J. Mantzaras

*Lattice Boltzmann simulations of catalytic reactive flows with large temperature variations*, 10th International Conference for Mesoscopic Methods in Engineering and Science (ICMMES 2013), Oxford, UK, (22-26 July 2013).

M. Schultze; R. Bombach; J. Mantzaras; F. Bolanos<sup>1</sup>, D. Winkler<sup>1</sup>, T. Griffin<sup>1</sup>

*Experimental and Numerical Investigation of the Catalytic Fuel-rich / Gaseous Fuel-lean Combustion of Hydrogen/air Mixtures*, Fachhochschule Nordwestschweiz, Institut fuer Thermo- und Fluid-Engineering, Windisch, European Combustion Meeting (ECM) 2013, Lund, Sweden (25-28 June 2013).