

# Publications

## Thesis

- [1] M. Klein. *Towards LES as an Engineering Tool*, Habilitation, Technische Universität Darmstadt. 2009.
- [2] M. Klein. *Direkte Numerische Simulation des primären Strahlzerfalls in Einstoffzerstäuberdüsen*. PhD thesis, Technische Universität Darmstadt, 2002.

## Journal Articles

- [3] Linus Engelman, Riccardo Concetti, Daeyoung Jun, Bok Jik Lee, Markus Klein, and Josef Hasslberger. Interaction of ammonia droplets with spherically expanding laminar lean hydrogen-air flames. *International Journal of Hydrogen Energy*, 2026, accepted.
- [4] Andreas Iberl, Elias Trautner, Markus Klein, and Josef Hasslberger. Simulation of particle deposition in bubbly flows using an Eulerian-Lagrangian framework. *International Journal of Multiphase Flow*, 2026, accepted.
- [5] Markus Klein, Artur Tyliczszak, Josef Hasslberger, and Massimo Germano. Isotropy and homogeneity of the Taylor-Green vortex at late stages using different initial conditions. *Journal of Fluid Mechanics*, 2026, accepted.
- [6] Vishnu Mohan, Ruslan Khamedov, Hong. G. Im, Markus Klein, and Nilanjan Chakraborty. Interrelation between dilatation rate and displacement speed in premixed turbulent flames. *Flow Turbulence and Combustion*, 2025, accepted.
- [7] Vinzenz Silvester Wehrmann, Nilanjan Chakraborty, Markus Klein, and Josef Hasslberger. On local equivalence ratio dependence of the burning rate in premixed turbulent lean hydrogen/air flames: A direct numerical simulation analysis. *Flow Turbulence and Combustion*, 2025, accepted.
- [8] Dario Kotzlowski, Eike Tangermann, Markus Klein, Tony Di Fabbio, Yuan Fang, and Richard D. Sandberg. Enhancing one-equation turbulence model for delta wing flows by gene expression programming. *AIAA Journal*, 2025, accepted.
- [9] Marianne Abdelsayed and Markus Klein. Effect of thixotropy on primary jet breakup - A DNS study. *International Journal of Multiphase Flow*, 2025, accepted.
- [10] Marco Herbert, Oussama Chaib, Isaac Boxx, Simone Hochgreb, Nilanjan Chakraborty, and Markus Klein. Lewis number effects on weakly turbulent premixed Bunsen flames: A comparison between DNS and experimental investigations. *Proc. Comb. Inst.*, 2025, accepted.
- [11] E. Trautner and M. Klein. LES of liquid jet breakup using an eulerian-lagrangian approach extended by a primary atomization model. *Flow Turbulence and Combustion*, 2025, accepted.
- [12] Magnus Schweiger, Markus Klein, Francisco Alcantara-Avila, Sergio Hoyas, and Josef Hasslberger. A-priori evaluation of sub-grid scale heat flux models in large eddy simulation for low to high Prandtl numbers. *International Journal of Heat and Mass Transfer*, 2025, accepted.

- [13] Lorenzo Folcarelli, Riccardo Concetti, Fabio Cozzi, Andrea Ferrero, Filippo Masseni, Dario Pastrone, Josef Hasslberger, and Markus Klein. A chemical reactor network methodology for estimating NO<sub>x</sub> emissions under non-premixed lean hydrogen combustion with water injection. *International Journal of Hydrogen Energy*, 2025, accepted.
- [14] N. Chakraborty and M. Klein. On the interrelation of the fractal description and the ratio of the 3D and 2D flame wrinkling for turbulent premixed flames. *Flow Turbulence and Combustion*, 2025, accepted.
- [15] Andreas Iberl, Elias Trautner, Markus Klein, and Josef Hasslberger. A-posteriori assessment of mixed models for large eddy simulation of polydisperse multiphase flows. *International Journal of Multiphase Flow*, 2025, accepted.
- [16] Josef Hasslberger, Maximilian Reissmann, Richard D. Sandberg, and Markus Klein. Exploiting semantic back-propagation to impose near-wall scaling constraints in machine-learned symbolic subgrid-scale closures. *Physics of Fluids*, 2025, accepted.
- [17] Riccardo Concetti, Josef Hasslberger, and Markus Klein. Direct numerical simulations with multi-step chemistry of liquid water interaction with laminar spherically expanding premixed hydrogen/air flames. *International Journal of Hydrogen Energy*, 2025, accepted.
- [18] T. Hehn, F. Zimmer, M. Klein, and J. Holtmannspötter. An optimized additive manufacturing strategy for low-impedance electronics. *Electronics*, 2025, accepted.
- [19] Min Son, Alexander Doehring, Markus Klein, Lars Zigan, Michael Pfitzner, and Tobias Sander. Experimental and numerical investigation of cyclopentane sprays in transcritical environment. *Atomization and Sprays*, 2025, accepted.
- [20] Rixin Yu, Marco Herbert, Markus Klein, and Erdzan Hodzic. Koopman theory-inspired method for learning time advancement operators in unstable flame front evolution. *Physics of Fluids*, 2025, accepted.
- [21] T. Hehn, F. Zimmer, M. Klein, and J. Holtmannspötter. Enhancing electrical high-frequency performance by an optimized additive manufacturing strategy. *International Journal of Advanced Manufacturing Technology*, 2025, accepted.
- [22] L. Schier, B. Blau, C. Heinrich, and M. Klein. Experimental analysis of microscopic spray properties of non-stabilized water-in-gasoline emulsions using shadowgraph imaging. *Atomization and Sprays*, 2024, accepted.
- [23] M. Klein and N. Chakraborty. Relation between 3D and 2D wrinkling factors in turbulent premixed flames. *Flow Turbulence and Combustion*, 2024, accepted.
- [24] Elias Trautner, Josef Hasslberger, and Markus Klein. Towards LES of liquid jet atomization using an Eulerian-Lagrangian multiscale approach. *Flow Turbulence and Combustion*, 2024, accepted.
- [25] M. Klein. Synthetic turbulence with prescribed probability density function and application to scalar quantities occurring in reactive flows. *Flow Turbulence and Combustion*, 2024, accepted.
- [26] Elfego Ruiz-Gutierrez, Josef Hasslberger, Markus Klein, Kenny Dalgarno, and Nilanjan Chakraborty. Binary droplet collisions in bioprinting: Influence of material properties on mixing and repeatability. *Flow Turbulence and Combustion*, 2024, accepted.
- [27] Umair Ahmed, Nilanjan Chakraborty, and Markus Klein. Effects of laminar burning velocity to friction velocity ratio on turbulent premixed flame-wall interaction within turbulent boundary layers. *Physical Review Fluids*, 2024, accepted.

- [28] Sanjeev Kumar Ghai, Umair Ahmed, Nilanjan Chakraborty, and Markus Klein. Multiscale analysis of Reynolds stresses and its dissipation rates for premixed flame wall interaction. *Physics of Fluids*, 2024, accepted.
- [29] Marianne Abdelsayed, Elias Trautner, Jakob Berchtenbreiter, and Markus Klein. Primary atomization of shear-thinning liquid jets: A direct numerical simulation study. *Scientific Reports*, 2024, accepted.
- [30] Vinzenz Silvester Wehrmann, Markus Klein, and Josef Hasslberger. Direct numerical simulation and modeling of the flame propagation characteristics in lean premixed turbulent h<sub>2</sub>/co/air combustion. *International Journal of Hydrogen Energy*, 2024, accepted.
- [31] Riccardo Concetti, Josef Hasslberger, Nilanjan Chakraborty, and Markus Klein. Effects of water mist on the initial evolution of turbulent premixed hydrogen/air flame kernels. *Energies*, 2024, accepted.
- [32] Ruiyun Ji, Stephan Kelm, and Markus Klein. An efficient method for input uncertainty propagation in CFD and the application to buoyancy-driven flows. *Nuclear Engineering and Design*, 2024, accepted.
- [33] Tony Di Fabbio, Yuan Fang, Eike Tangermann, Richard D. Sandberg, and Markus Klein. Strategies for enhancing one-equation turbulence model predictions using gene-expression programming. *Fluids*, 9:191, 2024.
- [34] Marianne Abdelsayed, Josef Hasslberger, Moritz Ertl, Bernhard Weigand, and Markus Klein. Towards large eddy simulation of shear-thinning liquid jets: A-priori analysis of subgrid scale closures for multiphase flows. *Physics of Fluids*, 36:085130, 2024.
- [35] Antony Premkumar, Francesca Loffredo, Heinz Pitsch, and Markus Klein. Towards direct numerical simulations of a reactivity-controlled compression ignition engine using n-octanol/ethanol fuel blends. *Flow Turbulence and Combustion*, 2024.
- [36] Riccardo Concetti, Josef Hasslberger, Nilanjan Chakraborty, and Markus Klein. Effects of liquid water addition on turbulent premixed hydrogen/air combustion. *Fuel*, 373:132314, 2024.
- [37] Maximilian Bambauer, Michael Pfitzner, and Markus Klein. LES of premixed turbulent combustion using filtered tabulated chemistry. *Flow Turbulence and Combustion*, 2024.
- [38] Vinzenz Silvester Wehrmann, Nilanjan Chakraborty, Markus Klein, and Josef Hasslberger. Choice of reaction progress variable under preferential diffusion effects in turbulent syngas combustion based on detailed chemistry direct numerical simulations. *Scientific Reports*, 14:14861, 2024.
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- [40] Alexander Doehring, Theresa Trummler, Michael Pfitzner, and Markus Klein. Two-dimensional DNS study of multicomponent mixing with phase transition in a transcritical shear layer. *Physics of Fluids*, 36:065141, 2024.
- [41] E. Ruiz-Gutierrez, J. Hasslberger, M. Klein, K. Dalgarno, and N. Chakraborty. Physically consistent modelling of surface tension forces in the volume-of-fluid method for three or more phases. *Journal of Computational Physics*, 513:113149, 2024.

- [42] Karthick Rajkumar, Tony Di Fabbio, Eike Tangermann, and Markus Klein. Physical aspects of vortex-shock dynamics in delta-wing configurations. *Physics of Fluids*, 36:066112, 2024.
- [43] Benjamin Blau, Oscar Krzeczek, Christoph Heinrich, and Markus Klein. Analysis of water-in-gasoline emulsions using experiments and direct numerical simulations. *Experimental and Computational Multiphase Flow*, 7:178–196, 2025.
- [44] Riccardo Concetti, Josef Hasslberger, Thomas Sattelmayer, and Markus Klein. On the chemical effect of steam addition to premixed hydrogen flames with respect to NO<sub>x</sub> emissions and flame speed. *Flow Turbulence and Combustion*, 113:519–534, 2024.
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- [46] Elias Trautner, Josef Hasslberger, Paolo Cifani, and Markus Klein. Enforcing accurate volume conservation in VOF-based long-term simulations of turbulent bubble-laden flows on coarse grids. *International Journal for Numerical Methods in Fluids*, 96:1057–1077, 2024.
- [47] Tony Di Fabbio, Karthick Rajkumar, Eike Tangermann, and Markus Klein. Towards the understanding of vortex breakdown for improved RANS turbulence modeling. *Aerospace Science and Technology*, 146:108973, 2024.
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- [52] K. Rajkumar, E. Tangermann, and M. Klein. Efficient scale-resolving simulations of open cavity flows for straight and sideslip conditions. *Fluids*, 8:227, 2023.
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- [54] M. Pfitzner, J. Shin, and M. Klein. A priori validation of a multidimensional turbulent premixed combustion model for high-pressure Bunsen flames. *Combustion Science and Technology*, 195:3262–3280, 2023.
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- [58] P. Wenig, S. Kelm, and M. Klein. CFD uncertainty quantification using stochastic spectral methods - exemplary application to a buoyancy-driven mixing process. *Nuclear Engineering and Design*, 409:112317, 2023.
- [59] O. Krzeczek, T. Trummler, E. Trautner, and M. Klein. Effect of the density ratio on emulsions and their segregation: A direct numerical simulation study. *Energies*, 16:3160, 2023.
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- [383] S. Ketterl and M. Klein. Towards large-eddy simulation of liquid jet atomization: DNS and a-priori subgrid analysis. In *13th Multiphase Flow Conference & Short Course*, Dresden, Germany, November 2015.
- [384] K. Amend and M. Klein. Influence of the contact angle model on gravity driven water films. In *13th Multiphase Flow Conference & Short Course*, Dresden, Germany, November 2015.
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- [389] Eike Tangermann, Markus Klein, and Michael Pfitzner. Large eddy simulation of flame flashback by combustion induced vortex breakdown. In *9th International Symposium on Turbulence and Shear Flow*, Melbourne, Australia, July 2015.
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## Invited Talks

- [442] M. Klein. Modelling multiphase flows across scales and physics. In *DLES 15 - ERCOFTAC workshop on Direct and Large Eddy Simulation*, Delft, Netherlands, May 2026.
- [443] M. Klein. Towards eulerian-lagrangian les of multiphase flows with moving interfaces. In *Department of Mechanical and Aerospace Engineering*, University of Turino, Italy, September 2025.
- [444] M. Klein. Towards les of liquid jet atomization using an eulerian-lagrangian multiscale approach. In *hpc.bw Seminar Series*, Helmut Schmitt Universität, Hamburg, March 2025.
- [445] M. Klein. Machine learning for (LES based) turbulence modelling. In *Division of Fluid Mechanics*, Lund University, Sweden, June 2023.
- [446] M. Klein. Towards gene expression programming for high fidelity LES closures. In *International Conference on Advanced Computational Engineering and Experimenting*, Florence, Italy, July 2022.
- [447] M. Klein. Part 1: Generation of synthetic turbulent inflow conditions; part 2: LES modeling using gene expression programming. In *Lecture: Innovative approaches to the simulation of turbulent flows in aerospace propulsion systems*, University of Turino, Italy, May 2022.
- [448] M. Klein. Recent efforts in LES modelling using traditional and machine learning techniques. In *Aerodynamics Seminar*, TU Delft, Netherlands, March 2022.
- [449] M. Klein. Towards LES of primary atomization. In *International Workshop on Clean Combustion: Principles and Applications*, Darmstadt, September 2019.
- [450] M. Klein. Towards LES of multiphase flows with moving interfaces. University of Groningen, July 2019.
- [451] M. Klein. Towards LES of multiphase flows with moving interfaces. Darmstadt, May 2019.
- [452] M. Klein. Towards LES of multiphase flows with moving interfaces. In *16th Multiphase Flow Conference and Short Course*, Dresden, November 2018.
- [453] M. Klein. Mathematische und physikalische Modellierung von turbulenten Zweiphasenströmungen. ITLR, University Stuttgart, March 2018.
- [454] M. Klein. Towards LES for two phase flows. Helmholtz-Zentrum Dresden-Rossendorf, July 2017.
- [455] M. Klein. Recent experiences with modelling of turbulence chemistry interaction in the context of LES using DNS of turbulent premixed generic planar flame configurations. Annual meeting of the UK Consortium on Turbulent Reacting Flows, September 2016.
- [456] M. Klein. Analysis of the combined modelling of subgrid transport and filtered flame propagation for premixed turbulent combustion. University of Duisburg, January 2015.
- [457] M. Klein. An attempt to assess the quality of les in the context of implicit filtering. University of Newcastle, November 2013.
- [458] M. Klein. Industrial CFD: Applications and challenges. Technical University of Munich, February 2013.
- [459] M. Klein. 3D CFD base engine development. University of Applied Science, Darmstadt, December 2010.

- [460] M. Klein. 3D CFD base engine development. University of Applied Science, Darmstadt, December 2009.
- [461] M. Klein. 3D CFD base engine development. University of Applied Science, Darmstadt, January 2008.
- [462] M. Klein. LES quality assessment. In *8th Workshop on Turbulent Nonpremixed Flames*, Heidelberg, August 2006.
- [463] M. Klein. Quality assessment of LES in the context of implicit filtering. In *Quality Assessment of Unsteady Methods for Turbulent Combustion Prediction and Validation*, Darmstadt, June 2005.
- [464] M. Klein. Numerical and experimental characterization of the turbulence structure in swirled flows. Cambridge University, November 2004.
- [465] M. Klein. How LES can be made an engineering tool. Cambridge University, July 2004.
- [466] M. Klein. Direkte numerische Simulation von ebenen ein- und zweiphasigen Freistrahlen. University of Zurich, Mai 2003.
- [467] M. Klein. On the artificial generation of inlet and initial data for unsteady turbulent flow simulation. In *17. TECFLAM-Seminar*, Stuttgart, Dezember 2003.

## Patent Applications

- [468] T. Hehn, M. Klein, F. Zimmer, and J. Holtmannspötter. Verfahren zur Impedanzreduzierung in additiv gefertigten Schaltungsträgern. *eingereicht*, 24.06.2025.
- [469] M. Klein und S. Kraft. Hydrostößel mit einer zweiten Ölzuführung. *DE102011101239*, 15.11.2012.
- [470] W. Schlidt, P. Seeger, S. Vogel, C. Tauscher, M. Klein, and R. Maucher. Zylinderkopf mit Flüssigkeitskühlung und Verfahren zur Kühlung des Zylinderkopfes. *DE102010052830*, 31.05.2012.
- [471] P. Seeger M. Klein, M. Janeck. Auslasssystem für einen Verbrennungsmotor. *DE102011116360*, 19.10.2011.