

# 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] V. Mohan, M. Herbert, M. Klein, and N. Chakraborty. A direct numerical simulation assessment of turbulent burning velocity parametrizations for non-unity Lewis numbers. *Energies*, 2023, accepted.
- [4] A. Begemann, T. Trummler, A. Doehring, M. Pfitzner, and M. Klein. Assessment of the thermodynamic and numerical modeling of LES of multi-component jet mixing at high pressure. *Energies*, 2023, accepted.
- [5] M. Bambauer, J. Hasslberger, G. Ozel-Erol, N. Chakraborty, and M. Klein. Surface topologies and self interactions in reactive and nonreactive Richtmyer-Meshkov instability. *Scientific Reports*, 2023, accepted.
- [6] M. Klein, N. Chakraborty, A. Kempf, and A. Sadiki. Development and validation of models for turbulent reacting flows. *Physics of Fluids*, 2022, accepted.
- [7] E. Trautner, J. Hasslberger, S. Ketterl, and M. Klein. Primary atomization of liquid jets: identification and investigation of droplets at the instant of their formation using direct numerical simulation. *International Journal of Multiphase Flow*, 2022, accepted.
- [8] M. B. Vocke, R. Kapulla, C. Morton, M. Klein, and R.J. Martinuzzi. Advection-based temporal reconstruction technique for turbulent velocity fields. *Physics of Fluids*, 2022, accepted.
- [9] R. Ji, P. Wenig, S. Kelm, and M. Klein. Epistemic uncertainty in URANS based CFD analysis of buoyancy driven flows - comparison of URANS and LES. *Annals of Nuclear Energy*, 2022, accepted.
- [10] T. Trummler, M. Glatzle, A. Doehring, N. Urban, and M. Klein. Thermodynamic modeling for numerical simulations based on the generalized cubic equation of state. *Physics of Fluids*, 2022, accepted.
- [11] T. Trummler, A. Begemann, E. Trautner, and M. Klein. Numerical investigation of the segregation of turbulent emulsions. *Physics of Fluids*, 2022, accepted.
- [12] G. Ozel-Erol, J. Hasslberger, N. Chakraborty, and M. Klein. Effects of water droplet injection on turbulent premixed flame propagation: A direct numerical simulation investigation. *Flow Turbulence and Combustion*, 2022, accepted.
- [13] S.K. Ghai, U. Ahmed, M. Klein, and N. Chakraborty. Turbulent kinetic energy evolution in turbulent boundary layers during head-on interaction of premixed flames with inert walls for different thermal boundary conditions. *Proc. Comb. Inst.*, 2022, accepted.

- [14] R. Concetti, J. Hasslberger, N. Chakraborty, and M. Klein. Analysis of water droplet interaction with turbulent premixed and spray flames using carrier phase direct numerical simulations. *Combustion Science and Technology*, 2022, accepted.
- [15] K. Rajkumar, E. Tangermann, M. Klein, S. Ketterl, and A. Winkler. Time-efficient simulations of fighter aircraft weapon bay. *CEAS Aeronautical Journal*, 2022, accepted.
- [16] E. Tangermann, G. Ercolani, and M. Klein. Aerodynamic behavior of a biomimetic wing in soaring flight - a numerical study. *Flow Turbulence and Combustion*, 2022.
- [17] N. Chakraborty, R. Rasool, U. Ahmed, and M. Klein. Relations between statistics of three-dimensional flame curvature and their two-dimensional counterpart in turbulent premixed flames. *Flow Turbulence and Combustion*, 2022.
- [18] M. Klein, T. Trummler, and J. Radtke. Multiscale analysis of the Reynolds stress, dissipation and subgrid-scale tensor in turbulent bubbly channel flows - characterisation of anisotropy and modelling implications. *Physics of Fluids*, 34:085122, 2022.
- [19] C. Kasten, J. Shin, M. Pfitzner, and M. Klein. Modelling filtered reaction rate in turbulent premixed flames using feature importance analysis, gene expression programming and tiny artificial neural networks. *International Journal of Heat and Fluid Flow*, 2022.
- [20] L. Engelmann, J. Laichter, P. Wollny, M. Klein, S.A. Kaiser, and A.M. Kempf. Cyclic variations in the flame propagation in an spark-ignited engine: multi cycle large eddy simulation supported by imaging diagnostics. *Flow Turbulence and Combustion*, 2022.
- [21] C. Kasten, J. Fahr, and M. Klein. An efficient way of introducing gender into evolutionary algorithms. *IEEE Transactions on Evolutionary Computation*, 2022.
- [22] C. Kasten, J. Shin, R.D. Sandberg, M. Pfitzner, N. Chakraborty, and M. Klein. Modelling subgrid-scale scalar dissipation rate in turbulent premixed flames using gene expression programming and deep artificial neural networks. *Physics of Fluids*, 34:085113, 2022.
- [23] S. Ghai, U. Ahmed, M. Klein, and N. Chakraborty. Energy integral equation for premixed flame-wall interaction in turbulent boundary layers and its application to turbulent burning velocity and wall flux evaluations. *International Journal of Heat and Mass Transfer*, 196:123230, 2022.
- [24] J. Hasslberger, R. Concetti, N. Chakraborty, and M. Klein. Inertial effects on the interaction of water droplets with turbulent premixed flames: a direct numerical simulation analysis. *Proc. Comb. Inst.*, 2022.
- [25] S. Ghai, N. Chakraborty, U. Ahmed, and M. Klein. Enstrophy evolution during head-on wall interaction of premixed flames within turbulent boundary layers. *Physics of Fluids*, 34:075124, 2022.
- [26] N. Chakraborty, U. Ahmed, M. Klein, and H.G. Im. Alignment statistics of pressure Hessian with strain rate tensor and reactive scalar gradient in turbulent premixed flames. *Physics of Fluids*, 34:065120, 2022.
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- [29] A. Begemann, T. Trummler, E. Trautner, J. Hasslberger, and M. Klein. Effect of turbulence intensity and surface tension on the emulsification process and its stationary state -A numerical study. *Canadian Journal of Chemical Engineering*, 2022.
- [30] L. Engelmann, J. Hasslberger, E. Inanc, M. Klein, and A. Kempf. A-posteriori assessment of Large-Eddy Simulation subgrid-closures for momentum and scalar fluxes in a turbulent premixed burner experiment. *Computers and Fluids*, 240:105441, 2022.
- [31] S. Ghai, U. Ahmed, N. Chakraborty, and M. Klein. Entropy generation during head-on interaction of premixed flames with inert walls within turbulent boundary layers. *Entropy*, 24(4):463, 2022.
- [32] M. Pfitzner, J. Shin, and M. Klein. A multidimensional combustion model for oblique, wrinkled premixed flames. *Combustion and Flame*, 241:112121, 2022.
- [33] M. Klein, T. Trummler, N. Urban, and N. Chakraborty. Multiscale analysis of anisotropy of Reynolds stresses, sub-grid stresses and dissipation in statistically planar turbulent premixed flames. *Applied Sciences*, 12(5):2275, 2022.
- [34] T. Di Fabbio, E. Tangermann, and M. Klein. Investigation of transonic aerodynamics on a triple-delta wing in side slip conditions. *CEAS Aeronautical Journal*, 2022.
- [35] N. Chakraborty, C. Kasten, U. Ahmed, and M. Klein. Evolutions of strain rate and dissipation rate of kinetic energy in turbulent premixed flames. *Physics of Fluids*, 33:125132, 2021.
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- [48] M. Bambauer, N. Chakraborty, M. Klein, and J. Hasslberger. Vortex dynamics and fractal structures in reactive and nonreactive Richtmyer-Meshkov instability. *Physics of Fluids*, 33 (4):044114, 2021.
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- [263] K. Amend and M. Klein. Modeling and simulation of water flow on containment walls with inhomogeneous contact angle distribution. In *48th Annual Meeting on Nuclear Technology*, Berlin, May 2017.
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- [269] E. Tangermann, T. Prigge, and M. Klein. Detached eddy simulation of an SD7003 airfoil. In *6th Symposium on Hybrid RANS-LES Methods*, Strasbourg, France, September 2016.
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- [280] 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.
- [281] N. Wegh, S. Bachschuster, D. Gaudlitz, and M. Klein. Multi-phase flow in porous media: 3d simulation of the impregnation stage of the RTM process. In *OpenFOAM User Meeting*, Darmstadt, Germany, August 2015.
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- [284] M. Klein, C. Wolff, and E. Tangermann. A-priori analysis of a LES model for scalar flux based on interscale energy transfer. In *9th International Symposium on Turbulence and Shear Flow*, Melbourne, Australia, July 2015.
- [285] 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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- [288] M. Klein, U. Allauddin, R. Keppeler, and M. Pfitzner. Towards uncertainty quantification and quality assessment for large eddy simulation of turbulent premixed combustion. In *Uncertainty Quantification in Computational Fluid Dynamics*, Paris, France, May 2015.
- [289] N. Wegh, S. Bachschuster, D. Gaudlitz, and M. Klein. Three-dimensional simulation of the impregnation stage of the RTM process considering the local structure of the fiber layup. In *8th International Conference on Computational and Experimental Methods in Multiphase and Complex Flow*, Valencia, Spain, April 2015.

- [290] M. Klein, C. Kasten, Y. Gao, and N. Chakraborty. A-priori assessment of sub-grid scale stress tensor closures for turbulent premixed combustion. In *7th European Combustion Meeting*, Budapest, Hungary, April 2015.
- [291] U. Allauddin, M. Klein, M. Pfitzner, and N. Chakraborty. A-priori and a-posteriori analysis of algebraic flame surface density modeling in the context of large eddy simulation of turbulent premixed combustion. In *SPEIC14 - Towards Sustainable Combustion*, Lisboa, Portugal, November 2014.
- [292] N. Chakraborty and M. Klein. A-priori direct numerical simulation assessment of the effects of lewis number on the performances of sub-grid scalar flux models for large eddy simulation of premixed flames. In *CONV-14: Int. Symp. on Convective Heat and Mass Transfer*, Turkey, June 2014.
- [293] M. Klein. Error quantification of passive scalar transport in the context of large eddy simulation using implicit filtering. In *Euromech 543, Quantification of uncertainties in modeling and predictive simulation of fluids*, pages 34–35, Munich, October 2013.
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- [295] T. Lauer, M. Heiss, S. Fischer, and M. Klein. Prediction of the wall film formation and performance of an engine operated with the ethanol blend e85. In *13th EAEC European automotive congress*, Valencia, June 2011.
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- [308] D. Goryntsev, M. Klein, and J. Janicka. Large Eddy Simulation of cycle-to-cycle variations in a realistic Direct Injection Engine. In *VIII. Tagung Motorische Verbrennung*, March 2007.
- [309] M. Fatali, M. Klein, T. Broeckhoven, C. Lacor, and M. Baelmans. Stochastic generation of velocity fluctuation for turbulent inflow and initial condition. In *Forth International Conference on Computational Fluid Dynamics*, Ghent, Belgium, July 2006.
- [310] I. Celik, M. Klein, and J. Janicka. Assessment measures for LES applications. In *Proceedings of the ASME 2006 Joint U.S. European Fluids Engineering Summer Meeting*, Miami, Florida, July 2006.
- [311] N. Chakraborty, M. Klein, and R.S. Cant. Effects of turbulence on self-sustained combustion in premixed flame kernels: A direct numerical simulation (DNS) study. In *11th International Conference on Numerical Combustion*, Granada, Spain, April 2006.
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- [313] M. Klein, M. Freitag, and J. Janicka. Numerical determination of the scaling exponent of the modelled subgrid stresses for eddy viscosity models. In *The Cyprus International Symposium on Complex Effects in Large Eddy Simulations*, September 2005.
- [314] D. Goryntsev, M. Klein, and J. Janicka. Charakterisierung der zyklischen Schwankungen in einem direkteinspritzenden Ottomotor mittels der Grobstruktursimulation. In *BMBF Workshop: Turbulenz in der Energietechnik*, Juni 2005.
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- [316] M. Freitag, M. Klein, and J. Janicka. Application of a LES quality assessment procedure to a swirling recirculating flow. In *Quality Assessment of Unsteady Methods for Turbulent Combustion Prediction and Validation*, Darmstadt, June 2005.
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- [319] N. Chakraborty, M. Klein, K.W. Jenkins, and R.S. Cant. Effects of strain rate and curvature on flame displacement speed in a spherical kernel in the thin reaction zones regime. In *European Combustion Meeting*, 2005.
- [320] D. Goryntsev, O. Stein, M. Klein, and J. Janicka. Charakterisierung zyklischer Schwankungen der Brennrauminnenströmung eines direkteinspritzenden Ottomotors mittels der Grobstruktursimulation. In *VII. Tagung Motorische Verbrennung*, März 2005.
- [321] M. Klein, J. Scholz, and J. Janicka. Development of an LES based model for the prediction of atomization. In *DFG-Schwerpunktprogramm Fluidzerstäubung und Sprühvorgänge*, Dortmund, March 2004.
- [322] M. Klein. An attempt to assess the quality of large eddy simulations in the context of implicit filtering. In *2nd International Workshop on Trends in Numerical and Physical Modelling for Turbulent Processes in Gas Turbine Combustors*, Heidelberg, 2004.
- [323] D. Goryntsev, M. Klein, and J. Janicka. LES der Strömung und Mischung in einem direkteinspritzenden Ottomotor. In *BMBF Workshop: Turbulenz in der Energietechnik*, Juli 2004.
- [324] M. Klein, A. Kempf, A. Sadiki, and J. Janicka. Mixing analysis of a plane jet using direct numerical simulation. In *Euromech 10th European Turbulence Conference*, Trondheim, Norway, July 2004.
- [325] M. Freitag, M. Klein, and J. Janicka. Direct numerical simulation of a recirculating, swirling flow. In *2nd International Workshop on Trends in Numerical and Physical Modelling for Turbulent Processes in Gas Turbine Combustors*, Heidelberg, 2004.
- [326] M. Klein and J. Janicka. Large-eddy-simulation of the primary breakup of a spatially developing liquid film. In *ICLASS 2003, International Conference on Atomization and Sprays*, Sorrento, July 2003.
- [327] A. Kempf, M. Klein, and J. Janicka. Transient inflow-data for LES:towards the generation of turbulent inflow conditions for combustion LES. In *Workshop on Direct and Large Eddy Simulation 5*, München, Germany, 2003.
- [328] M. Klein, A. Kempf, L. di Mare, and J. Janicka. On the artificial generation of inlet and initial data for unsteady turbulent flow simulation. In *17. TECFLAM-Seminar, ISBN 3926751274*, Stuttgart, Dezember 2003.
- [329] M. Klein, A. Sadiki, and J. Janicka. Direct numerical simulation of the primary breakup of a spatially developing liquid jet. In *TSFP3, 3rd International Symposium on Turbulence and Shear Flow Phenomena*, Sendai, Japan, June 2003.
- [330] M. Klein, A. Sadiki, and J. Janicka. Untersuchung des Primärzerfalls eines Flüssigkeitsfilms: Vergleich Direkte Numerische Simulation, Experiment und lineare Theorie. In *Spray 2002, 7. Workshop über Techniken der Fluidzerstäubung und Untersuchungen von Sprühvorgängen*, pages 63–72, Freiberg, 2002.
- [331] A. Kempf, M. Klein, R. Bauer, A. Sadiki, and J. Janicka. Towards the generation of turbulent inflow conditions for combustion LES. In *Proceedings of the Ninth International Conference on Numerical Combustion*, Sorrento, Italy, 2002.



- [332] M. Klein, A. Sadiki, and J. Janicka. Effects of the surface stretching or the surface deformation rate on the breakup of a viscous drop in simple shear flow: Numerical simulation. In *5th International Symposium on Engineering Turbulence Modelling and Measurements*, Mallorca, September 2002.
- [333] M. Klein, A. Sadiki, and J. Janicka. Influence of the inflow conditions on the direct numerical simulation of primary breakup of liquid jets. In *ILASS-Europe 2001, 17. Annual Conference on Liquid Atomization and Spray Systems*, pages 475–480, Zürich, September 2001.
- [334] M. Klein, A. Sadiki, and J. Janicka. Untersuchung des Einflusses der Düseninnenströmung auf den primären Zerfall eines Flüssigkeitsfilms mittels Direkter Numerischer Simulation. In *Spray 2001, 6. Workshop über Techniken der Fluidzerstäubung und Untersuchungen von Sprühvorgängen*, pages P.9–1 – P.9–8, Hamburg, 2001.
- [335] M. Klein, A. Sadiki, and J. Janicka. Influence of the boundary conditions on the direct numerical simulation of a plane turbulent jet. In *TSFP2, 2nd International Symposium on Turbulence and Shear Flow Phenomena*, volume I, pages 401–406, Stockholm, June 2001.
- [336] M. Klein, A. Sadiki, and J. Janicka. Direct numerical simulations of plane turbulent jets at moderate Reynolds numbers. In *20th IUTAM Congress, ICTAM 2000*, Chicago, September 2000.
- [337] M. Klein, A. Sadiki, and J. Janicka. Study of primary jet breakup using direct numerical simulation. In *ILASS-Europe 2000, 16. Annual Conference on Liquid Atomization and Spray Systems*, Darmstadt, September 2000.

## Invited Talks

- [338] M. Klein. Towards gene expression programming for high fidelity LES closures. In *International Conference on Advanced Computational Engineering and Experimenting*, Florence, Italy, July 2022.
- [339] M. Klein. Part 1: Generation of synthetic turbulent inflow conditions; part 2: LES modelling using gene expression programming. In *Lecture: Innovative approaches to the simulation of turbulent flows in aerospace propulsion systems*, University of Turino, Italy, May 2022.
- [340] M. Klein. Recent efforts in LES modelling using traditional and machine learning techniques. In *Aerodynamics Seminar*, TU Delft, Netherlands, March 2022.
- [341] M. Klein. Towards LES of primary atomization. In *International Workshop on Clean Combustion: Principles and Applications*, Darmstadt, September 2019.
- [342] M. Klein. Towards LES of multiphase flows with moving interfaces. University of Groningen, July 2019.
- [343] M. Klein. Towards LES of multiphase flows with moving interfaces. Darmstadt, May 2019.
- [344] M. Klein. Towards LES of multiphase flows with moving interfaces. In *16th Multiphase Flow Conference and Short Course*, Dresden, November 2018.
- [345] M. Klein. Mathematische und physikalische Modellierung von turbulenten Zweiphasenströmungen. ITLR, University Stuttgart, March 2018.
- [346] M. Klein. Towards LES for two phase flows. Helmholtz-Zentrum Dresden-Rossendorf, July 2017.
- [347] 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.
- [348] M. Klein. Analysis of the combined modelling of subgrid transport and filtered flame propagation for premixed turbulent combustion. University of Duisburg, January 2015.
- [349] M. Klein. An attempt to assess the quality of les in the context of implicit filtering. University of Newcastle, November 2013.
- [350] M. Klein. Industrial CFD: Applications and challenges. Technical University of Munich, February 2013.
- [351] M. Klein. 3D CFD base engine development. University of Applied Science, Darmstadt, December 2010.
- [352] M. Klein. 3D CFD base engine development. University of Applied Science, Darmstadt, December 2009.
- [353] M. Klein. 3D CFD base engine development. University of Applied Science, Darmstadt, January 2008.
- [354] M. Klein. LES quality assessment. In *8th Workshop on Turbulent Nonpremixed Flames*, Heidelberg, August 2006.
- [355] 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.

- [356] M. Klein. Numerical and experimental characterization of the turbulence structure in swirled flows. Cambridge University, November 2004.
- [357] M. Klein. How LES can be made an engineering tool. Cambridge University, July 2004.
- [358] M. Klein. Direkte numerische Simulation von ebenen ein- und zweiphasigen Freistrahlen. University of Zurich, Mai 2003.
- [359] M. Klein. On the artificial generation of inlet and initial data for unsteady turbulent flow simulation. In *17. TECFLAM-Seminar*, Stuttgart, Dezember 2003.