Ing. David Celný, Ph.D.

Curriculum Vitae

Ke Hřišti 177
Žalany, 417 63
Czech Republic
+420 266 052 030
✉ celny@it.cas.cz
www.it.cas.cz/en/davidcelny/

Research interests

- Phase interface
- Nucleation
- Molecular Dynamics
- Parallel programming on GPU
- Equations of State

Education

2010–2013 **B.Sc.**, *Mathematical Modeling*,
Faculty of Nuclear Sciences and engineering, Czech technical University, Prague

2013–2016 **M.Sc.**, *Mathematical Engineering*,
Faculty of Nuclear Sciences and engineering, Czech technical University, Prague

2016–2024 **Ph.D.**, *Mathematical Engineering*,
Faculty of Nuclear Sciences and engineering, Czech technical University, Prague

Academic exchanges

2018–2019 **ERASMUS+**, *Ruhr Univeristy in Bochum*, Germany

Extracurricular courses

2018–2019 **Parallel programming on GPU**,
Ruhr Univeristy in Bochum, Bochum

2019 **Parallel programming in CUDA and openACC**,
Nvidia DLI, IT4Inovation, Ostrava

Awards and Honors

- Award for best poster at ATCP 2016 Yokohama
- Award for education at FNSPE 2016, *Exercises of Mathematical analysis*

Research experience

2012–2013 **Research assistant**,
Department of Thermodynamics, Institute of Thermomechanics, Prague
Thesis: Mathematical modeling of phase interfaces for mixtures using the Cahn-Hilliard theory

2013–2016 **Research assistant**,
Department of Thermodynamics, Institute of Thermomechanics, Prague
Thesis: Mathematical modeling of planar and spherical phase interfaces for multicomponent fluids

2016–2017	**Researcher**,

2016–2017 **Researcher**,
Department of Thermodynamics, Institute of Thermomechanics, Prague
Topic: Investigation of curvature effects on phase interface for CCS relevant fluid mixtures

2017–2021 **Researcher**,
Department of Physical Chemistry, University of Chemistry and Technology, Prague
Thesis: Development of Paralell Algorithms for Molecular Dynamics Simulation of Heterogeneous Atomistic Systems

2018–2019 **Research assistant**,
Department of thermodynamics, Ruhr Univeristy in Bochum, Bochum
Topic: Investigation of metastable system properties with application in equation of state development.
Component of the ERASMUS+ stay.

2019–2024 **Researcher**,
Department of Thermodynamics, Institute of Thermomechanics, Prague
Topics: Investigation of metastable system properties and investigation of thermophysical properties of Hydrofluoroethers.

Teaching and supervising

2016–2018 **Mathematical Analysis Exercises**,
Department of Mathematics, Faculty of Nuclear Sciences and engineering, Prague
Part of certified course of Mathematical analysis

2020 **Introduction into MATLAB**,
Department of Thermodynamics, Institute of Thermomechanics, Prague
not certified series of courses

2021 **Parallel programming in CUDA**,
Department of Physical Chemistry, University of Chemistry and Technology, Prague
Certified course for master level students

2022 **Co-supervisor of B.Sc. student**,
Department of Thermodynamics, Institute of Thermomechanics, Prague
Topic: Parameter optimization of PC-SAFT equation of state for the modeling of thermophysical properties of fluids

Publications

As first author

2015: **Celný, David**, Václav Vinš, Barbora Planková, and Jan Hrubý. Mathematical Modeling of Planar and Spherical Vapor–Liquid Phase Interfaces for Multicomponent Fluids. Edited by P. Dančová and M. Veselý. *EPJ Web of Conferences*. 2015, **114**, 106-111.

- https://doi.org/10.1051/epjconf/201611402011
- cited(WoS 01.03.2024): 1

2019: **Celný, David**, Václav Vinš, and Jan Hrubý. Modelling of Planar and Spherical Phase Interfaces for Multicomponent Systems Using Density Gradient Theory. *Fluid Phase Equilibria*. 2019, **483**, 70–83.

- https://doi.org/10.1016/j.fluid.2018.10.014
- IF(WoS 2022): 2.6, cited(WoS 01.03.2024): 2
- Ranking (WoS): CHEMISTRY, PHYSICAL: Q3; ENGINEERING, CHEMICAL: Q3; THERMODYNAMICS: Q2

2021: **Celný, David**, Martin Klíma, and Jiří Kolafa. Molecular Dynamics of Heterogeneous Systems on GPUs and Their Application to Nucleation in Gas Expanding to a Vacuum. *Journal of Chemical Theory and Computation*. 2021, **17**(12), 7397-7405.

- https://doi.org/10.1021/acs.jctc.1c00736
- IF(WoS 2022): 5.5, cited(WoS 01.03.2024): 3
- Ranking (WoS): CHEMISTRY, PHYSICAL: Q2; PHYSICS, ATOMIC, MOLECULAR & CHEMICAL: Q1

2024: **Celný, David**, Sven Pohl, Monika Thol, Václav Vinš, Roland Span, and Jadran Vrabec. Thermodynamic Properties of Metastable Liquid and Vapor Phases by Molecular Dynamics with Grid Cluster Criteria, *Journal of Chemical Physics*

- (submitted for publication)

As co-author

2013: Vinš, Václav, Barbora Planková, Jan Hrubý, and **David Celný**. Density Gradient Theory Combined with the PC-SAFT Equation of State Used for Modeling the Surface Tension of Associating Systems. Edited by Tomáš Vít, Petra Dančová, and Petr Novotný. *EPJ Web of Conferences*. 2013, **67**, 767-772.

- https://doi.org/10.1051/epjconf/20146702129
- cited(WoS 01.03.2024): 5

2015: Planková, Barbora, Václav Vinš, Jan Hrubý, Michal Duška, Tomáš Němec, and **David Celný**. Molecular Simulation of Water Vapor–Liquid Phase Interfaces Using TIP4P/2005 Model. Edited by Petra Dančová and Tomáš Vít. *EPJ Web of Conferences*. 2015, **92**, 493-496.

- https://doi.org/10.1051/epjconf/20159202071
- cited(WoS 01.03.2024): 4

2015: Vinš, Václav, **David Celný**, Barbora Planková, Tomáš Němec, Michal Duška, and Jan Hrubý. Molecular Simulations of the Vapor–Liquid Phase Interfaces of Pure Water Modeled with the SPC/E and the TIP4P/2005 Molecular Models. Edited by P. Dančová and M. Veselý. *EPJ Web of Conferences*. 2015, **114**, 884-889.

- https://doi.org/10.1051/epjconf/201611402136
- cited(WoS 01.03.2024): 13

2020: Vinš, Václav, Jiří Hykl, Jan Hrubý, Aleš Blahut, **David Celný**, Miroslav Čenský, and Olga Prokopová. Possible Anomaly in the Surface Tension of Supercooled Water: New Experiments at Extreme Supercooling down to -31.4 C. *Journal of Physical Chemistry Letters*. 2020, **11**(11), 4443–4447.

- https://doi.org/10.1021/acs.jpclett.0c01163
- IF(WoS 2022): 5.7, cited(WoS 01.03.2024): 9
- Ranking (WoS): CHEMISTRY, PHYSICAL: Q2; MATERIALS SCIENCE, MULTIDISCIPLINARY: Q2; NANOSCIENCE & NANOTECHNOLOGY: Q2; PHYSICS, ATOMIC, MOLECULAR & CHEMICAL: Q1

2021: Vinš, Václav, Ali Aminian, **David Celný**, Monika Součková, Jaroslav Klomfar, Miroslav Čenský, and Olga Prokopová. Surface Tension and Density of Dielectric Heat Transfer Fluids of HFE Type-Experimental Data at 0.1 MPa and Modeling with PC-SAFT Equation of State and Density Gradient Theory. *International Journal of Refrigeration*. 2021, **131**, 956–969.

- https://doi.org/10.1016/j.ijrefrig.2021.06.029
- IF(WoS 2022): 3.9, cited(WoS 01.03.2024): 13
- Ranking (WoS): ENGINEERING, MECHANICAL: Q2; THERMODYNAMICS: Q2

2021: Fingerhut, Robin, Gabriela Guevara-Carrion, Isabel Nitzke, Denis Saric, Joshua Marx, Kai Langenbach, Sergei Prokopev, **David Celný**, Bernreuther Martin, Simon Stephan, Maximilian Kohns, Hans Hasse, and Jadran Vrabec. ms2: A Molecular Simulation Tool for Thermodynamic Properties, Release 4.0. *Computer Physics Communications*. 2021, **262**, 107860.

- https://doi.org/10.1016/j.cpc.2021.107860
- IF(WoS 2022): 6.2, cited(WoS 01.03.2024): 28
- Ranking (WoS): COMPUTER SCIENCE, INTERDISCIPLINARY APPLICATIONS: Q1; PHYSICS, MATHEMATICAL: Q1

2022: Aminian, Ali, **David Celný**, Erik Mickoleit, Andreas Jäger, and Václav Vinš. Ideal Gas Heat Capacity and Critical Properties of HFE-Type Engineering Fluids: Ab Initio Predictions of Cpig, Modeling of Phase Behavior and Thermodynamic Properties Using Peng–Robinson and Volume-Translated Peng–Robinson Equations of State. *International Journal of Thermophysics*. 2022, **43**(6), 87.

- https://doi.org/10.1007/s10765-022-03006-z
- IF(WoS 2022): 2.2, cited(WoS 01.03.2024): 3
- Ranking (WoS): CHEMISTRY, PHYSICAL: Q4; MECHANICS: Q3; PHYSICS, APPLIED: Q3; THERMODYNAMICS: Q3

2023: Klíma, Martin, **David Celný**, Jiří Janek, and Jiří Kolafa. Properties of Water and Argon Clusters Developed in Supersonic Expansions, *Journal of Chemical Physics*. 2023, **159**(12), 124302.

- https://doi.org/10.1063/5.0166912
- IF(WoS 2022): 4.4, cited(WoS 01.03.2024): 0
- Ranking (WoS): CHEMISTRY, PHYSICAL: Q2; PHYSICS, ATOMIC, MOLECULAR & CHEMICAL: Q1

Conference Presentations

EFM 2015: Experimental fluid mechanics *Prague*, presentation

- Mathematical modeling of planar and spherical vapor–liquid phase interfaces for multicomponent fluids

WSC 2016: Workshop on Scientific Computing at *Děčín*, presentation

- Mathematical modeling of phase interfaces of liquid mixtures using PC-SAFT equation of state.

ATPC 2016: Asian Thremophysical Properties Conference at *Yokohama*, poster

- Mathematical modeling of planar and spherical vapor-liquid phase interfaces for multicomponent fluids

DDNY 2017: Doctoral days at *FNSPE Prague*, presentation

- Model of planar and spherical phase interface geometries for multi-component mixtures

DDNY 2018: Doctoral days at *FNSPE Prague*, presentation

- Use of GPU for molecular simulations of nucleation and metastable state

DDNY 2019: Doctoral days at *FNSPE Prague*, presentation

- Runtime molecular simulation nucleation criterion for metastable states

Kolloquium 2019: Thermodynamik-Kolloquium at *Duisburg*, poster(DE)

- Laufzeit-Nukleation-Kriterium für Molekularsimulationen Metastabiler Zustände

JETC 2021: Joint European Thermodynamics Conference at *Prague*, poster

- Nucleation criteria detection as a mean to investigate metastable state

DDNY 2021: Doctoral days at *FNSPE Prague*, presentation

- Molecular dynamics of heterogeneous systems on GPUs and application to nucleation in gas expanding to a vacuum

Project participation

- "Research centre for low-carbon energy technologies", project No. CZ.02.1.01/0.0/0.0-/16_019/0000753, of the OP VVV program of the Ministry of Education, Youth and Sports of the Czech Republic

- "Thermal Energy Storage Materials: Thermophysical Characteristics for the Design of Thermal Batteries", No. GA17-08218S, of the Czech Science Foundation grant

- "Support of the Institute of Thermomechanics of the CAS, v. v. i.", project No. RVO:61388998, of the internal Grant agency of Institute of Thermomechanics

- "Application of analytical mathematical methods in study of physical and biological systems 2", project No. SGS18/189/OHK4/3T/14, of the Student Grant Agency of the Czech Technical University in Prague,

- "Application of rigorous mathematical methods in study of physical models", project No. SGS21/166/OHK4/3T/14, of the Student Grant Agency of the Czech Technical University in Prague

- "Investigation of non-equilibrium steam condensation: A new approach", project No. CEP16-GA0-GA-U/01:1, of the Czech Science Foundation grant

- "Phase behaviour in CCS systems", project No. 7F14466, of the Norwegian Financial Mechanism program of the Ministry of Education, Youth and Sports of the Czech

- "Surface tension of water and water mixtures in equilibrium and metastable state", project No. GJ15-07129Y, GA0/GJ, of the Junior Grant program of Czech Science Foundation grant