TECHNISCHE UNIVERSITÄT DARMSTADT

PhD position announcement

Simulation reaktiver Thermo-Fluid Systeme

Simulation of reactive Thermo-Fluid Systems

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The following four PhD researcher positions (First Stage Researcher R1) are to be filled in May to October 2025. They are part of European funded Doctoral Networks[1] and provide funding for 3 years. The home institution (place of employment) will be the Institute for Simulation of reactive Thermo-Fluids Systems (STFS) at Technical University of Darmstadt, Germany. As part of the doctoral training, two secondments at project partners are planned, see the description for the specific PhD positions for more details below. The Early Career Researchers (ECR) will obtain a dual PhD degree from TU Darmstadt and a second university, usually the location of the secondment.

In total four PhD positions are to be filled, two positions in two projects, more information on the specific position can be found on the following pages.

Project 1 – Decarbonising Energy-intenSIve industries with Renewable synthetic fuels (DESIRE)
Position #1: **Modelling and simulation of multi-regime turbulent combustion**
Position #2: **Modeling and simulation of turbulent combustion of liquid e-fuels**

Project 2 – Upscaling deep conversion routes for hard-to-reCYCLE biogenic waste (UPCYCLE)
Position #3: **CFD of thermal conversion of contaminated wooden biomass**
Position #4: **TEA/LCA for thermal conversion of contaminated wooden biomass**

More about the research philosophy at STFS can be found here: Link.

If you are interested, please contact Prof. Hasse directly and provide CV, transcript of records, and references. Clearly indicate which position you are interested in.

⚠ **Before sending your material**, please ensure that you are eligible according to section 1.3 of the *Horizon Europe - Work Programme 2023-2024 Marie Skłodowska-Curie Actions*. In particular, the mobility rule needs to be considered:
“Recruited researchers must not have resided or carried out their main activity (work, studies, etc.) in Germany for more than 12 months in the 36 months immediately before their recruitment date.”

[1] https://marie-sklodowska-curie-actions.ec.europa.eu/actions/doctoral-networks

DESIRE: Decarbonising Energy-intenSIve industries with REnewable synthetic fuels

PhD position #1 (Dual degree TU Darmstadt and Politecnico di Milano)

Modelling and simulation of multi-regime turbulent combustion and pollutant formation of carbon e-fuels and their blends with traditional fuels

Objectives: Develop a predictive multi-regime model for turbulent combustion and pollutant formation of carbon e-fuels (methanol, DME or OME) for future applications in IC engines and stationary power generation. The framework is based on detailed kinetic mechanisms and shall be validated against high-resolution experimental data.

Expected Results: The fully-coupled predictive model of multi-regime combustion and pollutant formation will be based on a comprehensive analysis of the underlying physical-chemical processes. The holistic model formulation will be implemented in a LES code. As an integral part of the model validation, the numerical simulation results will extensively be compared against reliable experimental data, which provide simultaneous information on combustion and pollutant formation. The modelling framework will be provided to other doctoral candidates for extension to multi-phase combustion and the application in engine applications. The expected results are: 1) a multi-regime model for prediction of turbulent combustion of carbon e-fuels and their blends with traditional fuels; 2) a model to predict pollutant formation under multi-regime conditions for e-fuels and their blends with traditional fuels; 3) the impact of kinetic uncertainties on the prediction of turbulent combustion and pollutant formation under engine-relevant conditions is quantified for carbon e-fuels and their blends with traditional fuels. Part of the experimental data for validation purposes will be provided from collaborators.

Secondments: Centre National de la Recherche Scientifique (Paris/France), to quantify the impact of kinetic parameter uncertainty on modelling of turbulent combustion and pollutant formation to carbon e-fuels and their blends with traditional fuels. Rolls-Royce Germany (Site: Berlin), to transfer the modelling approach for multi-regime combustion and pollutant formation of carbon e-fuels and their blends with traditional fuels.

PhD position #2 (Dual degree TU Darmstadt and Université Paris-Saclay)

Modeling and simulation of turbulent combustion of liquid e-fuels based on the Transported FDF approach

Objectives: Develop a novel Hybrid Eulerian-Lagrangian/Transported FDF framework combined with the stochastic field solution scheme for numerically describing turbulent spray combustion of liquid e-fuels. The approach extends an existing single phase Transported-FDF modelling to reacting sprays of liquid e-fuels.

Expected Results: The main expected results are: 1) Under consideration of detailed chemical reaction mechanisms and thermo-physical properties provided by project partners, a novel Hybrid Eulerian-Lagrangian/Transported FDF framework combined with the stochastic field solution scheme will be developed for numerically predicting turbulent spray combustion characteristics of liquid e-fuels; 2) Advanced Spray module for liquid e-fuels. Thereby, the challenging features of spray formation and evolution of liquid e-fuels (breakup, atomization, turbulent dispersion, multicomponent evaporation, mixture formation) will be incorporated; 3) Extended multi-regime combustion model for turbulent spray combustion; 4) Validated overall model. The overall model including well validated sub-models will be assessed using experimental data from the consortium and possible available data from the literature. The resulting overall validated model is the main outcome from this DC; 5) Analysis of impact of heat transfer and pressure on the flame evolution and pollutant formation in turbulent spray combustion of liquid e-fuels under subcritical flow conditions. Expected interactions: DC5 (detailed kinetics of e-fuels); DC6 (multi-regime modelling for single phase combustion); DC11 (advanced modelling of single droplets and sprays of carbon e-fuels); DC14 (validation and model comparison from the experimental and numerical investigations in an industrial internal combustion engine).

Secondments: Politecnico di Milano (Italy), to get deeper insight in the modelling of turbulence-particle-chemistry interactions; Rolls-Royce Germany (Site: Berlin), to transfer the multidimensional modelling approach for liquid e-fuels.

UPCYCLE: UPscaling deep conversion routes for hard-to-reCYCLE biogenic waste

PhD position #3 (Dual degree TU Darmstadt and Politecnico di Milano)

High-fidelity CFD simulations for pyrolysis/gasification reactors of contaminated lignocellulosic biomasses

Objectives: (1) Development of high-fidelity CFD models for deep conversion processes; (2) Coupling of advanced kinetic models from molecular scale research; (3) Integration of gas phase kinetics of complex fuel components; (4) consideration of morphological characteristics of feedstock

Expected results: (1) Validated software framework with predictive multi-scale and multi-physics CFD models for pyrolysis/gasification of contaminated lignocellulosic biomasses; (2) Hierarchical modeling approach and scientific understanding from single particle to turbulent reacting flow for biomasses explicitly considering the contaminants; (3) Particle models considering morphological characteristics from feedstock analyses; (4) Database and established interface for reducing 3-D CFD data to CRNs (DC4); (5) OpenFOAM-based simulation platform, which allows model integration and exchange with project partners and network of collaborators.

Secondments: Politecnico di Milano (Italy) to provide process boundary conditions for the determination of kinetics and product spectrum of biogenic waste streams; Vyncke (Belgium) to investigate and address technical challenges observed in reactor applications.

PhD position #4 (Dual degree TU Darmstadt and KU Leuven)

Techno-economic analysis (TEA) and life cycle assessment (LCA) of thermodynamic process modeling for pyrolysis/gasification of contaminated wooden biomass

Objectives: (1) LCA of pyrolysis/gasification processes of contaminated wooden biomass; (2) TEA considering carbon utilization (syngas/tars) and contaminant management; (3) Interfacing process assessment with thermodynamic modeling.

Expected results: (1) Energy and resource consumption by the overall deep conversion process; (2) LCIA addressing relevant environmental indicators (GHG, impact on air/soil/water, etc.); (3) Economic feasibility analysis for different technological options and system integrations with other energy or chemical processes; (4) Identification of key parameters and sensitivities controlling the economics of the deep conversion process; (5) Explorative technology assessment for a future, transformed economy utilizing forecasting methods (foreground and background system, prospective LCA); (6) Thermodynamic models for different process schemes including simplified reactor models and pre-/post-treatment steps for feedstock; (7) Flow chart analysis tracing contaminant streams.

Secondments: Katholieke Universiteit Leuven (Belgium) to collaboratively gain insight in contributing processes from thermodynamic perspective; Sulzer Management AG (Switzerland) to explore technological options for waste stream valorisation considering both, ecological and economical aspects