

**DIPARTIMENTO DI INGEGNERIA – UNIVERSITY OF PERUGIA
PHD COURSE IN INDUSTRIAL AND INFORMATION ENGINEERING -
38TH CYCLE**

Title of the research activity:	High Fidelity Simulations and experiments of Cryogenic Carbon capture Process
State of the art:	A novel process in post-combustion technology is the carbon capture using a cryogenic process. A CO ₂ -laden flue gas is cooled to desublimation temperatures (–100 to –135 °C) and separates CO ₂ in the solid form. A sprayed contact liquid can be used to condense the gas to a solid on liquid droplets so that a liquid CO ₂ stream can be recovered and separated. No equivalent industrial process exists and therefore there is no precedent operating experience with these systems [1-3]. The performance of the Cryogenic Carbon Capture (CCC) system depends on effective performance of the desublimation spray tower heat exchanger. The process design and optimization require insights from high-fidelity multi-dimensional simulations, validated against novel data. To this end, fundamental understanding of underlying physical and chemical processes is critical [4-6].
Short description and objectives of the research activity:	The proposed PhD project aims to enable and facilitate the CCC technology development by enhancing predictive capabilities through high-fidelity modeling validated against parallel novel experiments. Since capturing detailed phase interfaces is impossible at the device scale, a subgrid-scale (SGS) model for interface heat and mass transfers needs to be developed. The models will account for the desublimation of carbon dioxide from the flue gas on the drop surface and for the dissolution from the frost layer into the inner liquid core. The closure models will then be coupled to existing LES multi-phase frameworks [7-14]. These new spray model capabilities will be validated against experimental data, collected in spray chamber experiments by partners at the collaborating institutions, and then applied to assist the design and optimization of the contact liquid desublimating heat exchanger, a crucial component of the cryogenic carbon capture system. The PhD activity is part of a large project involving also KAUST and Cambridge universities. The research aims to develop a new two-phase flow solver for liquid sprays with cryogenic desublimation phase change model. The specific focus is on low-temperature conditions, multicomponent thermodynamics, sgs models for heat and mass transfer associated with the CO ₂ desublimation on cold spray droplets. The code will be developed in OpenFOAM.
Bibliography:	<ol style="list-style-type: none"> 1. Sayre, A., D. Frankman, A. Baxter, K. Stitt, and L. Baxter. Field Testing of Cryogenic Carbon Capture. in Carbon Management Technology Conference. 2017. Carbon Management Technology Conference. 2. Baxter, L., Method for forming consistently-sized and controllably-timed droplets. 2019, US Patent 10,443,838. 3. James, D. W. (2015). Falling Drop CO₂ Deposition (Desublimation) Heat Exchange for the Cryogenic Carbon Capture Process. Masters Thesis. Brigham Young University. Provo, UT. 4. Na, B., & Webb, R. L. (2003). A fundamental understanding of factors affecting frost nucleation. <i>International Journal of Heat and Mass Transfer</i>, 46(20), 3797–3808. doi: 10.1016/s0017-9310(03)00194-7 5. Na, B., & Webb, R. L. (2004). New model for frost growth rate. <i>International Journal of Heat and Mass Transfer</i>, 47(5), 925–936. doi: 10.1016/j.ijheatmasstransfer.2003.09.001 6. Na, B., & Webb, R. L. (2004). Mass transfer on and within a frost layer. <i>International Journal of Heat and Mass Transfer</i>, 47(5), 899–911. doi: 10.1016/j.ijheatmasstransfer.2003.08.023 7. Vukcevic, V., Jasak, H., Gatin, I. (2017). Implementation of the ghost fluid method for free surface flows in polyhedral finite volume framework. <i>Comput. Fluids</i>, 153, 1-19. 8. Hongyan Zhu, Michele Battistoni, Bittagowdanahalli Manjegowda Ningegowda, Faniry Nadia Zazaravaka Rahantamialisoa, Zongyu Yue, Hu Wang, Mingfa Yao,

	<p>Thermodynamic modeling of trans/supercritical fuel sprays in internal combustion engines based on a generalized cubic equation of state, <i>Fuel</i>, Volume 307, 2022, 121894, https://doi.org/10.1016/j.fuel.2021.121894.</p> <p>9. Xue Q., Battistoni M., Powell C.F., Longman D.E., Quan S.P., Pomraning E., Senecal P.K., Schmidt D.P., Som S. (2015). An Eulerian CFD model and X-ray radiography for coupled nozzle flow and spray in internal combustion engines. <i>Int. J. of Multiphase Flow</i>, 70, p. 77-88.</p> <p>10. Battistoni M., Xue Q., Som S. (2016). Large-Eddy Simulation (LES) of Spray Transients: Start and End of Injection Phenomena. <i>Oil & Gas Sc. and Tech.</i>, 71.</p> <p>11. Matheis J., Hickel S., (2018) Multi-component vapor-liquid equilibrium model for LES of high-pressure fuel injection and application to ECN Spray A, <i>Int. J. of Multiphase Flow</i>, 99, p. 294-311.</p> <p>12. A. Pandal, B.M. Ningegowda, F.N.Z. Rahantamialisoa, J. Zembí, H.G. Im, M. Battistoni, Development of a drift-flux velocity closure for a coupled Σ-Y spray atomization model, <i>International Journal of Multiphase Flow</i>, Volume 141, 2021, 103691, https://doi.org/10.1016/j.ijmultiphaseflow.2021.103691.</p> <p>13. Battistoni, M., Som, S., & Powell, C. F. (2019). Highly resolved Eulerian simulations of fuel spray transients in single and multi-hole injectors: Nozzle flow and near-exit dynamics. <i>Fuel</i>, 251, 709–729. doi: 10.1016/j.fuel.2019.04.076</p> <p>14. Keser, R., Vukčević, V., Battistoni, M., Im, H., & Jasak, H. (2019). Implicitly coupled phase fraction equations for the Eulerian multi-fluid model. <i>Computers & Fluids</i>, 192, 104277. doi: 10.1016/j.compfluid.2019.104277.</p>
Scientific coordinator (s)	Michele Battistoni
Contact (s)	michele.battistoni@unipg.it