

DIPARTIMENTO DI INGEGNERIA – UNIVERSITY OF PERUGIA
PHD COURSE IN INDUSTRIAL AND INFORMATION ENGINEERING –
41st CYCLE

Title of the research activity:	Multiscale modelling for the optimization of operative conditions in a microfluidic bioreactor for nano-particles generation
State of the Art:	Microfluidic technology is transforming the field of personalized drug delivery by providing unmatched precision and scalability in the synthesis of nanoparticles. However, numerous challenges persist. Problems such as droplet polydispersity and intricate fluid management must be resolved to guarantee consistency and dependability in nanoparticle manufacturing. Multiscale models can offer the necessary insights to enhance this process; nevertheless, they demand thorough experimental validation because of the intricate interactions of phenomena across various scales. An interdisciplinary strategy can facilitate the connection between experimental studies and numerical simulations.
Short description and objectives of the research activity:	The project is aimed at optimizing the control parameters of a reactor for the production of nanoparticles, based on flash nano-precipitation inside a continuous microfluidic mixer of a solvent, in which poly- ϵ -caprolactone and a so-called anti-solvent are dissolved. The control of the size of the nanoparticles generated in this way is difficult to control due to the speed of the process, therefore it is desirable to develop validated numerical models that allow to optimize the operating conditions of the reactor. The project aims to give a contribution in this direction through a multiscale approach in which molecular dynamics (MD) are combined at the nanoscale, population balance (PBM) for the meso-scale and computational fluid dynamics (CFD) for the macro-scale. The research activity will be carried out in close contact with the Department of Biotechnology for the experimental validation of the model.
Bibliography:	S. Tripathi, S. Verma, K. Dhingra, J. Knowl. Learn. Sci. Technol. 3 (2024) 213–223 P. Pico, K. Nathanael, A. D. Lavino, N. M. Kovalchuk, M. J.H. Simmons, O. K. Matar, Journal, Volume 474, 2023, 145692,
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