Proceedings of the 11th World Congress on New Technologies (NewTech'25)
Paris, France - August, 2025
Paper No. ICNFA 128
DOI: 10.11159/icnfa25.128

Thermal-Fluidic Coupled Vortex-Induced Shear Controllable Synthesis of Nanoparticles Using a Hybrid Rankine Vortex-Variable Through Flow Cross-Section Taylor-Couette Flow Reactor

Yanqing Guo[1], Luming Chen[2] Jiaying LU[1], Xiaogang Yang[1,*] Jie Yang[3]

[1]University of Nottingham Ningbo China, Ningbo 315100, PR China
Yanqing.guo2@nottingham.edu.cn,
Jiaying.lu@nottingham.edu.cn,
Xiaogang Yang@nottingham.edu.cn (Corresponding author),
[2]Zhejiang University of Technology, Hangzhou, 310014, PR China
lumingchen@zjut.edu.cn
[3]School of Natural Sciences, University of Hull, Hull HU6 7RX, UK

Extended Abstract

This study focuses on the dynamic process of thermal-fluidic coupled vortex-induced shear controllable synthesis of ZnO nanoparticles with a hybrid Rankine vortex-variable through-flow cross-section Taylor-Couette flow reactor. This type of novel hybrid reactor integrates a Rankine swirling vortex reactor with a variable through-flow cross section of Taylor-Couette flow reactor, effectively intensifying turbulence induced shear in the flow which can significantly affect the synthesis process of micro/nano particles. The generated local turbulence induced shear particularly affect the aggregation and breakage of particles. The important conclusions have been reached as the output from the present study:

(1) The role of intensified turbulence induced shear in controlling particle aggregation and breakage was analysed. We have developed large eddy simulations (LES) multiscale-based model to for prediction of particle properties under varying local shear rate conditions, and validated the effectiveness of adopting such reactor in hydrodynamic and thermodynamic interactions between fluid and solid-phase particles. The interplay between turbulent eddies and the thermal-fluidic coupling was found to have an impact on the synthesised nanoparticle characteristics. It has been demonstrated that key parameters in such thermal-fluidic coupled turbulence induced shear controllable synthesis include the eddy size based Reynolds number, reactant concentration, and reaction temperature inside the flow system in the reactor. To highlight this point, Eulerian-Lagrangian approach was adopted, where large eddy simulations were conducted for turbulence induced shear prediction while particle Lagrangian trajectories was used to obtain the statistics of the synthesised particle aggregation characteristics. In the numerical modelling, it was assumed that the synthesised particle diameter (d_p) is less than the Kolmogorov scale (η_κ) to approximate the influence of the existence of nanoparticles on the turbulence induced shear low in the reactor.

(2) As large eddy simulation modelling was performed, meso scale turbulence structures in the reactor has been identified, which allows for direct assessment of the impact of micro scale turbulent eddies on particle crystallisation and growth process.

(3) By correlating with particle morphology, such as size and aspect ratio. Simulation parameters and turbulence statistics included the Reynolds number (Re) based on the Kolmogorov microscale, the Prandtl number (Pr), and the Nusselt number (Nu). The findings reveal that the stretching and deformation behavior of vortices of different scales significantly influences the synthesis of ZnO nanoparticles, particularly in terms of thermal and hydrodynamic interactions with the particle phase. It has been demonstrated that the aspect ratio of ZnO nanoparticles correlates with the local turbulent eddy induced shear stress. The proposed LES multiscale model was found to be able to well predict nanoparticle aggregation and growth behaviour. In the study, the synthesised nanoparticle size and morphology were assessed using scanning electron

microscopy (SEM) and transmission electron microscopy (TEM). The stability of the ZnO nanoparticles was measured using Zeta Sizer and atomic force microscopy (AFM).

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