Scalable Liquid Phase Exfoliation of Layered and 2D Materials

Mariam Badawi, Muhammad Faizan, Yarjan Abdul Samad, Imran Afgan
Khalifa University, Shakhbout Bin Sultan St, Abu Dhabi, UAE
100063763@ku.ac.ae

Liquid phase exfoliation (LPE) methods are becoming increasingly significant in the exfoliation of graphene and other 2D materials due to their easiness and high production rates compared to other mechanical or chemical methods [1]. Inks produced by LPE are required in a wide range of applications including but not limited to flexible electronics [2], conductive coatings, and composite materials. The scalability of these processes is still a challenge, particularly due to limited flake sizes [1]. Current LPE methods that are widely investigated by researchers include sonication [2], shear mixing [3], and high-pressure homogenization [4]. Sonication is a cavitation-dominated process, while shear-mixing and high-pressure homogenization are shear-dominated forces accompanied with cavitation and collision effects. The cavitation and collision effects involved in these methods can induce significant defects in the resulting material, as well as the long process time for sonication limit the scalability of these methods [5]. In this work, a new LPE method is introduced, in which exfoliation occurs due to high shear forces developed among successive stationary and high-speed rotating discs. CFD simulations are performed for the device to evaluate the resulting shear forces acting on the fluid. A structured hexahedral mesh is employed in the simulations with k-ω SST turbulence model for accurate near-wall resolution. Simulations are performed in the transient regime with a timestep of $1*10^{-5}$ s. Mesh sensitivity study is conducted employing mesh size range from 0.5 to 9.5 million to obtain mesh independent results. In this work, a broad range of rotational speeds from 1,000 to 10,000 RPM is examined, and the impact of each speed on flow behavior and shear rate will be presented. A snap of the results is shown in Figure 1 which depicts the velocity and strain-rate contours for the flow domain at 5000 rpm with the strain rate reaching a maximum value of $4.5*10^{6}$ s^{-1} and an average value of $5.4*10^{4}$ s^{-1}, which exceeds the minimum shear-rate required for graphene exfoliation (10^{4} s^{-1}) [3]. Overall, this method has the potential to produce larger flakes with minimum defects due to shear force dominance, which facilitates the efficient scalable production of graphene and 2D materials inks to be used in different applications.

References

[1] F. Bonaccorso et al., Materials Today, 15 (2012) 564.
[2] K. Pan et al., Nature Communications, 9 (2018) 5197.
[3] KR Paton et al., Nature Materials, 13 (2014) 624.
[4] PG Karagiannidis et al., ACS Nano, 11 (2017) 2742.
[5] M. Yi, Z. Shen, RSC Advances, 6 (2016) 72525.

Figures

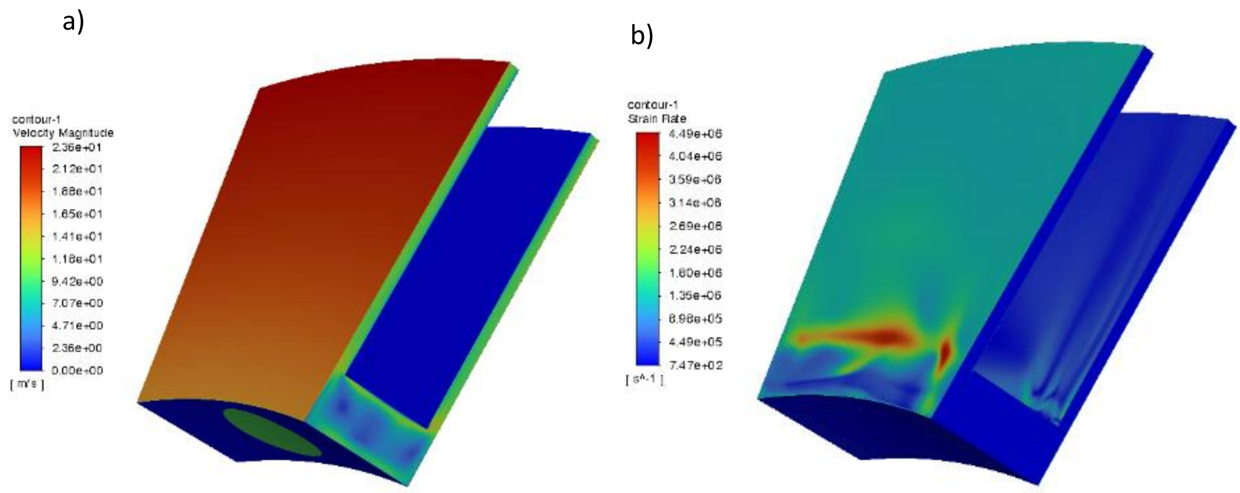

Figure 1: a) Velocity contour, and b) Strain rate contour.