Supplemental materials

Exfoliation of graphite into graphene by a rotor-stator in supercritical CO2: Experiment and simulation

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1. Grid-independent analysis

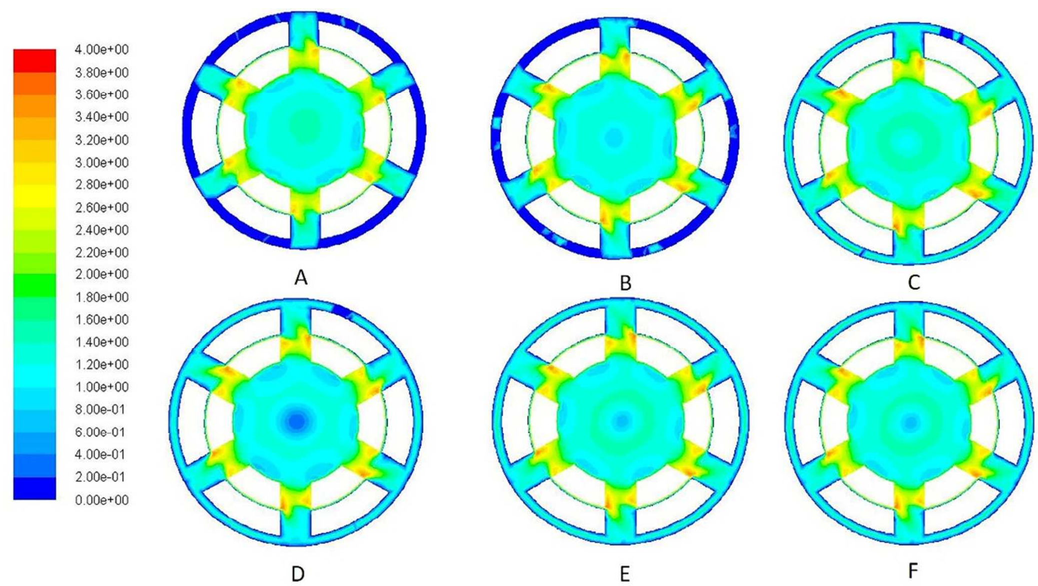

Figure S1. Velocity distribution in a rotor-stator mixer using (A) 20W cells, (B) 40W cells, (C) 57W cells, (D) 68W cells, (E) 80W cells, (F) 100W cells.

By using mesh refining technique, a 3D analysis was carried out to verify that the results were independent of the grid as the resolution increases. Fig. S1 displays the contours of the horizontal velocity at six mesh resolutions, respectively. The simulation was conducted with a steady-state at 3000 shearing speed, and the solution converged with residuals below 10^{-4}. The six mesh exploited grids discretizing the 3D flow domain into tetrahedral cells. Fig. S1 shows that the contours of the velocity are sensitive toward the grid resolution from 20W cells to 57W cells. There is no fluid-flow between the stator and the wall of the vessel using 20W and 57W cells. The shape of the contours changed slightly when the number of cells changed from 57W to 100W. The results of simulation show that the velocity distribution altered with the change of the grid resolution. Maximum velocity improved from 3.31m/s to 3.94m/s when the number of cells changed from 20W to 68W. However, the velocity distribution changed little from 80W cells to 100W cells. In conclusion, the fluid-flow can be predicted accurately using 80W cells. The minimum tetrahedral element is 0.5mm.

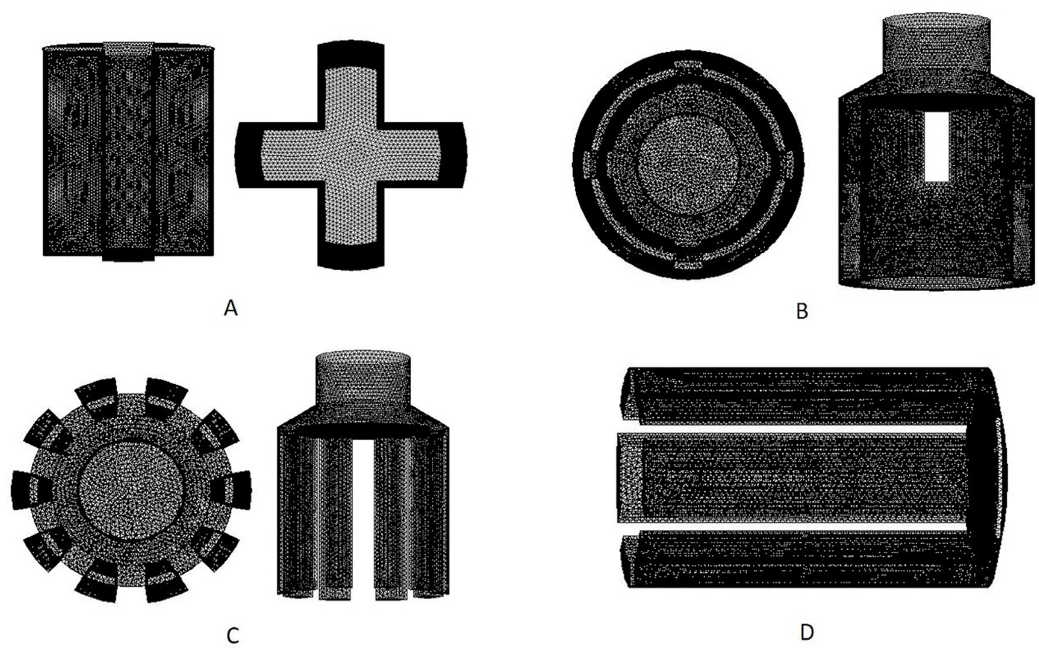

Figure S2. Computational domains of stators and rotors: (A) cross rotor, (B) more wall stator, (C) ten-tooth stator, (D) long stator.

Figure S3. A side view of the all-wall stator.

2. Structure of the stator-rotor and the exfoliation yield

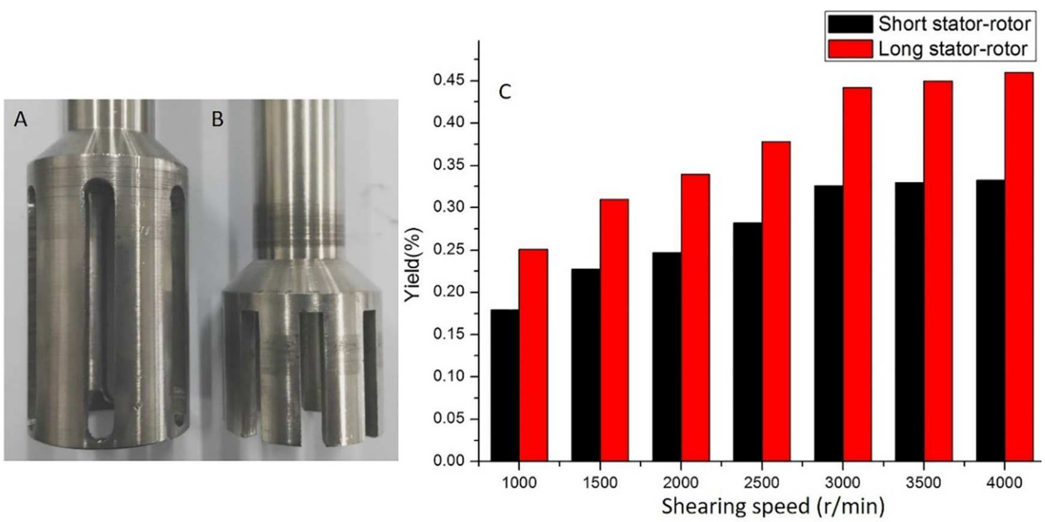

Figure S4. (A) a digital photo of the long stator and, (B) a digital picture of the short stator, (C) the yield of graphene for the short stator and extended stator at different shearing speed.

Fig. S4 A-B shows the digital pictures of the extended and the short stator. Both of them have the same diameter and the number of teeth. But the length of the extended stator is twice the short one. It means that the active region of the former is twice as the latter. The yield of the extended stator should be higher than the short stator. It was confirmed by the experimental results shown in Fig. S4B. The yield of the extended stator is around 1.3-1.4 times as much as that of the short stator at the fixed peeling time of 4 hours and different speeds. Therefore, when using the rotor-stator mixer to produce the graphene, the long stator is better than a short one. Also, the height of the rotor-stator and the vessel should be close to achieving the yield as much as possible.