Computational Fluid Dynamics modelling of a microwave plasma torch for the synthesis of graphene

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A steady state, two-dimensional (2D) two temperature (electrons and heavy particles) argon plasma model based on [1] with and extended calculation domain of the electromagnetic (EM) field is proposed to simulate the synthesis of graphene in a microwave torch, namely TIAGO. The technique of extending the EM domain outside the plasma discharge region has been used before to simplify the boundary conditions of the electric fields [2]. The model is implemented with the commercial Computational Fluid Dynamics (CFD) software Fluent Ansys [3] and the addition of Maxwell's equations as C language routines as well as the ionization-recombination reactions. Turbulence effects are considered and solved according to the k-epsilon model proposed in accordance with a parallel study [4]. The whole set of equations are solved for the 2D axisymmetric mesh structure of the TIAGO torch with dimensions and boundary conditions according to the experimental work of [5-6]. Modeling results show the temperature profiles of electrons and heavy particles, velocities, recirculation patterns and turbulence at every section of the reactor geometry. This work aims to complete the analysis of graphene formation of [5-6] by providing information about temperature and flow dynamics that cannot be observed with other techniques and are key to understand and control the process. It is the first time that a two-temperature model has been adapted to the commercial code Fluent for the TIAGO microwave plasma torch proving a practical tool for scientists and engineers to help the understanding, optimization, and scale-up of the graphene process without the trial error cost of experiments.

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