Temperature optimization in a gas reactor for the synthesis of carbon nanofibers: a numerical approach

Authors:

- Elena Castellanos, Universidad de Castilla- La Mancha (`elena.castellanos1@alu.uclm.es`)

- José Luis Valverde, Universidad de Castilla- La Mancha (`joseluis.valverde@uclm.es`)

- <u>María Cruz Navarro</u>, Universidad de Castilla- La Mancha (`mariacruz.navarro@uclm.es`)

Abstract: Carbon nanotubes (CNT) and Carbon nanofibers (CNF) have become materials with a great variety of applications: Information and Communication Technologies (ICT)[1], construction industry [2], medicine [3], among others.

The temperature at which the CNF synthesis process is carried out determines the final structure of the carbon nanofiber. At $873.15K$ the formation of the fishbone structure is favored, which is the most interesting industrially and the one with the best process performance [4].

In this work we address the modeling and numerical simulation of flow and temperature for a mixture of gases in a reactor to optimize the temperature inside it using COMSOL Multiphysics [5]. The study is focused on determining appropriate temperatures at the reactor shell, to assure optimal temperatures at the catalyst support device where the reaction of formation of CNF takes place. Different locations of the support device are considered.

References:

[1] Alhawat A et al. (2020) Investigation of magneto-electric effects in (PMN-PT) @ NiFe2O4 core shell nanostructures and nanocomposites for non volatile memory applications, *Materials Letters*, **261**, 127082.

[2] Tao S et al. (2019) Research progress on CNTs/CNFs-modified cement-based composites: A review, *Construction and Building Materials*, **202**, 290–307.

[3] Zihui L et al. (2020) The high luminescent polydopamine nanosphere-based ECL biosensor with steric effect for MUC1 detection, *Chemical Engineering Journal*, **385**, 123825.

[4] De Lucas A et al. (2006) Catalytic synthesis of carbon nanofibers with different graphene plane alignments using Ni deposited on iron pillared clays, *Applied Catalysis A: General*, **301**, 123–132.

[5] COMSOL Multiphysics v. 6.0 (2021). https://www.comsol.com