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COLLOQUIUM

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Lecture Hall (Αμφιθέατρο Φυσικής), Physics Building (Zografou Campus), National Technical University of Athens

"From aerosol synthesis of materials and devices to a new value for the mean free path of air"

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Recent advances in understanding of combustion and aerosol formation and growth through multiscale process design, allow now inexpensive synthesis of nanoparticles with sophisticated composition, size and morphology by flame spray combustion at kg/h even at an academic institution with such units now all over the world (UK, Spain, India etc.). These have led to synthesis of single noble atom heterogeneous catalysts, biomaterials and highly porous sensing films that led to commercial devices for detection of adulterated liquor as highlighted even by Greek Radio and Television (EPT).

These advances and community's keen interest on nanoscale phenomena have motivated a closer look to the fundamentals of aerosol dynamics in the free molecule regime. The mean free path (MFP) dictates when gas-phase nanoparticle transport takes place in the free molecule or continuum regime. This distinction is crucial in process design of gas phase processes (laser, plasma, hot wall, ultrasonic and flame) in synthesis of films and nanoparticles.

For eons, the kinetic theory of gases has been used to determine the MFP assuming elastic collisions between spherical gas molecules [1]. However, is this so with what we know about molecular shape and force fields today? Having reached a state of maturity now, molecular dynamics (MD) simulations can elucidate the fundamentals of basic gas-phase (aerosol) processes that lead to better understanding of natural phenomena and accelerating process scale-up [2]. Here the mechanics of gas collisions are elucidated for plain air at room temperature by thoroughly-validated atomistic MD treating O_2 and N_2 as true diatomic molecules accounting for their shape and force field, for the first time to our knowledge. So it is revealed that their trajectories are no longer straight, and collision frequencies were much higher due to the attractive part of the force field and the diatomic, thus more voluminous, shape of N_2 and O_2 as will be shown by the respective videos. Detailed analysis of the latter trajectories revealed that molecular collisions involve strong interactions between colliding molecules. Frequently, colliding molecules were split from each other but soon return to collide again and again without interacting with any other molecule in between resulting in orbiting collisions as had been envisioned 70 years ago [3]. A direct result of the enhanced interactions between air molecules when treated as true diatomic molecules is that their MFP comes out to be considerably smaller than that from the classic kinetic theory. The new MFP for air is 38.5 nm, almost 43% smaller than that in textbooks of 67.3 nm at 300 K and 1 atm. Aside from its fundamental value, such a result is significant in gas-phase synthesis of tiny (< 5 nm) nanoparticles where asymptotic (self-preserving) particle size distributions and (fractal-like) structure have not been attained yet to simplify the corresponding process design.

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2. Mavrantzas VG & Pratsinis SE, Curr. Opinion Chem. Eng., 23 (2019) 174.
3. Hirschfelder, JO, Curtiss, CF, Bird, RB, Molecular Theory of Gases & Liquids, Wiley, 1954.

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