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Opinion

Overcoming Frontiers of Chemical Reactions: Reactive Molecular Dynamics Simulations

Rene FB Gonçalves*

Department of Chemistry, Brazil

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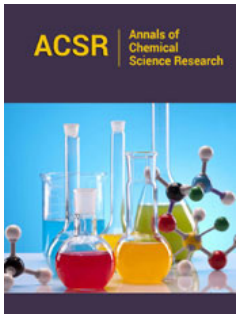

***[1]Corresponding author:** Rene FB Gonçalves, Department of Chemistry, Aeronautics Institute of Technology, São José dos Campos/SP, Brazil

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Opinion

Since the birth of chemistry, philosophers, researchers, scientists have spent their efforts in explaining transformations, elucidating reactions and discovering new methods and compounds. Over the centuries, the techniques and methodologies have evolved, so more and more explanations and findings were published. Besides the growth of scientific methodology, technology experienced an exponential evolution in the past decades. Computer simulations can now be used as a useful, trustful and fast tool to discover new reactions, processes and substances, then accelerating the development of chemistry.

Among the several models of simulations, the reactive molecular dynamics simulations are one of the state-of-the-art methodologies. Molecular dynamics simulations predict how every atom in a system will move over time, based on a general model of the physics governing interatomic interactions [1]. It has become an important and widely used theoretical tool that allows researchers in chemistry, physics, and biology to model the detailed microscopic dynamical behaviour of many different types of systems, including gases, liquids, solids, surfaces, and clusters [2].

The overall interactions, bonds and reactions occur according to a force field, which includes every possible interaction among the components of the system evaluated. Reactive force fields require potential energy expressions that are much more complex than fixed valence force fields and remain very difficult to parameterize accurately [3], however there are several research groups and companies which are now working actively in the development of such parameters in just a few months.

Therefore, with a trustful force field, chemical reactions can be analysed, as the atom/molecules in the system interact with each other and, with enough velocity or energy (temperature) the chemical reactions are observed. Among the reactions simulated by RMD one could cite pyrolysis, combustion, biochemical interactions (proteins, active ingredients), thermal decomposition etc. In the last couple of years, RMD simulations have also been used to predict the kinetic behaviour of the reactions. When simulating the same system in different temperatures, a first-order approximation can be applied and the Arrhenius parameters of the overall process (global reaction) may be calculated.

This approach is useful for fast reactions, which can be time-consuming and very costly to evaluate experimentally. Besides, this tool proves useful to save time and money on developments and research projects, as it can provide good starting points, i.e. in the case of formulations development, for example, RMD simulations can be used to narrow the possibilities of different compositions, thus optimizing the performance and reducing the time spent in the experiments.

RMD simulations can be quite expensive, depending on the size of the system and on the number of iterations (time) needed. As the computers and servers continue to develop, so does the simulations. Every year is possible to observe a significative improvement on the calculation speed and on the acuity of the results. For the near future, every project and development shall have an initial simulation phase to overcome possible difficulties and

challenges, to save money and time spent from the idea to the launch of the products and technologies.

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