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Computational modelling of the hydride generation reaction in a tubular reactor and hydride fragmentation in a dielectric barrier discharge atomizer

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Abstract

In this study, the hydride generation (HG) reaction in a helical tubular reactor and fragmentation of the generated hydride in a dielectric barrier discharge atomizer were investigated theoretically and experimental y. The aim was to interpret the optimal design condition towards adopting HG technique in producing an online, real time, fully automated instrumentation for heavy metals determination in wastewater. Expanded theoretical explorations were conducted, with aid of Matlab and Comsol Multiphysics software's, targeted the mechanism of arsenic hydride formation in a helical tubular reactor and the transported volatile hydride (VH) fragmentation in a rectangular DBD atomizer. Of two hypotheses reported in the literature, computation results showed that adopting the intermediate hydroboron species formation is more realistic for design purposes.

Accordingly, the optimal length of the tubular reactor was elucidated theoretically. Furthermore, computation results indicated that formation of intermediate species and free arsenic atoms is actual y initiated in the first section of DBD atomization channel before reaching the section between the electrodes, whilst the concentration of free arsenic atoms saturates to a maximum and does not vary thereafter along atomization channel. This finding is agreed with current understanding of atomization mechanism reported in literature, based on presence of abundance of hydrogen radicals along atomization channel which limits recombination reactions and ultimately maintains free atom life. This outcome suggests an approach for radial data acquisition from any position along DBD atomization channel with same sensitivity. Accordingly, the optimal length of DBD atomization channel has become able to be determined based on model results. The computation results of both HG mechanism and VH fragmentation were validated by applying experimental explorations, where a reasonable agreement was found from both approaches. To sum up, the theoretical and experimental investigations proved that DBD atomizer is appropriate for analytical purposes and competitive to other well known atomization tools such as a quartz cell atomizer.

Biography

Wameath Abdul-Majeed has completed his BSc & MSc studies in chemical engineering from the University of Technology/Baghdad. He has been awarded a PhD in chemical and process engineering from the University of Sheffield/UK. He is currently serving as a consulting engineer in a lead engineering company in Baghdad. He has published several articles in impacted journals and conference proceedings of reputable international conferences.