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We hope that this journal will provide a forum for the dissemination of high-quality research in Science and are open to any questions and suggestions.

The responsibility for the articles is exclusive to the authors.

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conversion of residual fatty acids to soaps through the saponification reaction or into esters through the esterification reaction with H2SO4 can be done observing the market of those products. The monitoring of the transesterification reaction in real time with laser spectroscopy allows the variation of the temperature during the reaction process without losing the reaction endpoint. The use of only one reaction vessel for the accomplishment of several unit operations aiming the reducing of the reaction time in the production process was well succeeded. The main resulting products are biodiesel, glycerol, fertilizer, and soaps. As expected the biodiesel can be used as a source of energy, the glycerol can be further refined but this process was not explored at this manuscript, the resulting salts can be used as fertilizers, and the soups can be sold and used as a soup.

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ARSENIC SPECIATION IN GROUNDWATER USING THE SOFTWARES PHREEQC, GWB AND GEODELING

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ABSTRACT

Geochemical modelling speciation is used to understand the interactions that occur in the groundwater. Thermodynamic data, kinetic parameters, numerical methods are factors that affect any geochemical modelling system. The conceptual formulation of geochemical modeling calculates the distribution of chemically reactive species for an aqueous solution. The mathematical formulation of the model results in a system of nonlinear algebraic equations that are solved using numerical methods. Most programs allow the user to estimate the speciation model. Activities of aqueous species are usually calculated using the Davies equation, Debye-Hückel equation, or the extended Debye-Hückel equation. We perform a comparative study of geochemical speciation using three different software: PHREEQC™, Geochemist's Workbench™ (GWB) and GEODELING. Details of each software take into account the distribution, mobility, and availability of chemical species in groundwater. We can observe very similar results in speciation when working with low-temperature systems (20 to 80°C). GWB™, PHREEQC™, and GEODELING employ an integrated system to define when to use Davies, Debye-Huckel or Bdot equation, according to the value of the solution ionic strength. The geochemical speciation aimed to compare the results of simulators able to predict the chemical species present in groundwater. The utilization of GEODELING allows comparing the results with software GWB™ and PHREEQC™ with a high degree of acceptance for low temperatures. The numerical methods used by GWB™, PHREEQC™, and GEODELING software are able to seek its own best set of numerical solutions to achieve the equilibrium. Users must be cautious when choosing geochemical modeling software, as an essential factor for choosing a simulator is to know the temperature range that will be used.

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TO AUTHORS