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EFFECT OF EXTERNAL ELECTRIC FIELDS ON THERMODYNAMIC PROPERTIES

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The efficient use of energy is one the biggest challenges our society faces at the moment and is one of the basic principles of modern chemical engineering. In the case of dielectric materials, microwave heating is known to be a faster and more selective way to transfer energy from a source to a recipient than conventional conduction-based heating. This is due to the volumetric and targeted character of microwave heating, meaning that all the material is heated simultaneously and only substances which respond to the microwave field will be affected. In contrast, conductive heating requires longer times for the energy to be transferred from the surface to the centre of the material.

Microwave technology has seen a significant growth in the last decades with applications such as food processing, pre-heating of rubber and plastics, and drying of different materials. More recently microwave heating has also been applied in organic synthesis, heterogeneous catalytic reactions, polymerization reactions and various separation processes [1]. In all these cases, important improvements have been reported with respect to conventional technologies. However, the physical mechanisms by which this enhancement occurs remain somehow unclear.

In this work, we propose the implementation of a multiscale modelling approach to develop a better understanding of the thermodynamics of systems under the influence of external electric fields. Modified equations of state are used to model the behaviour of such systems, and reproduce previously obtained experimental results. In addition, molecular simulations provide a deeper insight into the dielectric polarization mechanism, and are employed to study the influence of external electric fields on thermodynamic properties, with particular interest in free energies and chemical equilibrium. We start with the application of a static electric field on both one component systems and mixtures, with the goal of extending the analysis to alternating fields at microwave frequencies. In combination with previous work on dielectric spectroscopy of these materials, this study can provide a valuable tool for modelling dielectric heating processes.

References

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