عنوان مقاله:

Molecular Simulation of the Structure of Methane Hydrate Using the Wolf Method

محل انتشار:

هفتمین کنگره ملی مهندسی شیمی (سال: 1390)

تعداد صفحات اصل مقاله: 9

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خلاصه مقاله:

In this article, the structure of methane hydrate is predicted at the formation pressure and temperature using Monte Carlo molecular simulation. Electrostatic long-range interactions are calculated using the Wolf method. The most common method used for handling long-range interactions in simulating methane hydrates is the Ewald sum method. The Wolf method is less expensive than the Ewald sum in computational cost. The final equation is also much simplermathematically than the Ewald sum final equation. Simulation results show very good agreement with those .obtained by the Ewald method published in the open literature

کلمات کلیدی:

Methane Hydrate, Monte Carlo Simulation, Electrostatic Interactions, The Wolf Method