

مقاله به چاپ رسیده از رضا بلالی دهکردی در مجله های معتبر جهانی در زمینه پیشرفت های اخیر شرکت پایانه های نفتی ایران در ساخت نانوذرات بوده است.

بر اساس منشور نظام نامه پژوهش صنعت نفت؛



اسپادانا خبر | سیدفریور موسوی

شرکت پایانه های نفتی ایران به عنوان مسئول دریافت، ذخیره سازی و صادرات بیش از ۹۰ درصد نفت خام کشور انجام تمامی عملیات معاوضه نفت خام از کشورهای حوزه دریای خزر و صدور تمامی میعانات گازی کشور را بر عهده دارد.

این شرکت بر اساس منشور نظام نامه پژوهش صنعت نفت به منظور توسعه فعالیت های پژوهشی، افزایش همکاری های فی مابین صنعت و دانشگاه و بهره مندی از توانمندی های کارکنان متخصص شرکت پایانه های نفتی ایران همواره مشوق کارکنان برای تهیه مقالات و پژوهش های در مقاطع کارشناسی ارشد و دکتری بوده است.



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The effects of external force and electrical field on the agglomeration of Fe_3O_4 nanoparticles in electroosmotic flows in microchannels using molecular dynamics simulation

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ABSTRACT

Recent progress in nanoparticle construction can be seen as a breakthrough in increasing heat transfer methods. The small size of particles and low volume fraction of particles leads to solving agglomeration and pressure drop problems and reduce the cost of storing and transporting nanofluids. Molecular dynamics simulation is one of the essential branches of computational physics that can predict various structures' atomic behavior. In this study, the effects of external electrostatic force and external electrical field on the density, velocity, temperature of atomic structures, and agglomeration of Fe_3O_4 nanoparticles in a copper microchannel are investigated. The results of the physical properties of this structure are estimated using molecular dynamics simulation and LAMMPS software. The results show that with increasing the applied external electrostatic force the maximum velocity is converged to $0.0071 \text{ \AA/ps}$. Also, adding an external electrical field to the simulated nanofluid, the maximum values of density, velocity, and temperature are estimated to 1.32 g/cm^3 , $0.0078 \text{ \AA/ps}$, and 345 K , respectively. The external electrical field has a significant and essential role in the agglomeration process in atomic structures. Finally, it is observed that by increasing the external electrical field, the time required for the agglomeration process increases to 2.26 ns .

1. Introduction

Today, nanofluids are used in various fields [1–3]. The nanofluids application is divided into two parts: heat transfer and mass transfer [4–6]. Some exceptional properties like high stability, facile preparation, and acceptable viscosity have made nanofluids one of the most suitable and strong choices in both mass transfer and heat transfer fields. One of the basic needs in many industries and research projects is high-efficiency heat transfer [7–9]. Heat transfer environments are usually formed of fluids such as water, ethylene glycol, or oil. Compared to metals and even metal oxides, these fluids have a low thermal conductivity. Therefore, it is expected to show better thermal properties by adding nanoparticles to conventional fluids [10–13]. So far, most studies have focused on particles in millimeter or micrometer size. Particles on this scale cause severe problems in heat transfer equipment. These particles settle quickly in the system, and if the channel has a smaller diameter, the problem will be more serious. For instance, when flowing

through microchannels, they cause agglomeration and clogging of the path and finally resulting in a large pressure drop. Also, the collision of these particles with each other and the system's walls leads to abrasion [14–16]. Recent progress in nanoparticle construction can be seen as a breakthrough in increasing heat transfer methods. The small size and low volume fraction of nanoparticles lead to solving agglomeration and pressure drop problems and reduce the cost of storing and transporting nanofluids [17–19]. In recent decades, molecular dynamics (MD) simulations have been used to study the properties of nanofluids. MD method is one of the essential branches of computational physics that can predict the atomic behavior of various structures [20,21]. Because molecular systems generally contain large numbers of particles, the properties of complex systems cannot be obtained analytically. But molecular dynamics simulation solves this problem by applying computational methods and thus creates an interface between laboratory results and theoreticals [22–24].

In this computational study, the effect of external force and electrical

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پیشرفت های اخیر در ساخت نانوذرات را می توان به عنوان یک پیشرفت در افزایش روش های انتقال حرارت دید. اندازه کوچک ذرات و کسر حجمی کم ذرات منجر به حل مشکلات تجمع و افت فشار و کاهش هزینه های ذخیره سازی و انتقال نانوسیال می شود. شبیه سازی دینامیک مولکولی یکی از شاخه های اساسی فیزیک محاسباتی است که می تواند رفتار اتمی ساختارهای مختلف را پیش بینی کند. در این مطالعه، اثرات نیروی الکترواستاتیک خارجی و میدان الکتریکی خارجی بر چگالی، سرعت، دمای ساختارهای اتمی و تراکم نانوذرات Fe_3O_4 در یک میکروکانال مسی بررسی شده است

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