

STUDI PENGARUH FRAKSI KATION TERHADAP SIFAT TRANSPORT ION DAN STRUKTUR PADA CAIRAN IONIK GARAM GANDA [BMIM]/[EMIM][BF₄] MELALUI SIMULASI DINAMIKA MOLEKUL

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INTISARI

Pada penelitian ini dilakukan analisis terhadap pengaruh fraksi kation 1-butiril-3-metilimidazolium (BMIM⁺) dengan 1-etil-3-metilimidazolium (EMIM⁺) terhadap struktur dan sifat transport pada cairan ionik garam ganda (*Double-Salt Ionic Liquids*, DSILs) [BMIM]/[EMIM][BF₄] melalui simulasi dinamika molekul (*Molecular Dynamics*, MD). Penelitian yang dilakukan bertujuan untuk mengetahui pengaruh fraksi kation terhadap struktur sistem DSILs [BMIM]/[EMIM][BF₄] dan sifat transportnya.

Simulasi dinamika molekul (MD) dilakukan menggunakan medan gaya CL&P pada temperatur 300 K dan tekanan 1 bar melalui dua tahapan. Tahap pertama dimulai dengan simulasi produksi NPT untuk membentuk kotak simulasi sistem DSILs yang memiliki 320 jumlah molekul, dituliskan sebagai $X_{\text{BMIM}} + (1 - X)_{\text{EMIM}}$ menggunakan fraksi 0,00; 0,25; 0,50; 0,75; dan 1,00. Selanjutnya, kotak simulasi digunakan pada tahap produksi NVT untuk membentuk trajektori sistem. Trajektori yang terbentuk kemudian digunakan untuk menganalisis kerapatan massa, fungsi distribusi radial (*Radial Distribution Function*, RDF), koefisien difusi diri (D), dan konduktivitas ionik (σ) sistem DSILs [BMIM]/[EMIM][BF₄].

Berdasarkan penelitian yang telah dilakukan, peningkatan fraksi [BMIM]⁺ dan penurunan [EMIM]⁺ dalam sistem DSILs [BMIM]/[EMIM][BF₄] tidak menunjukkan perubahan signifikan pada struktur lokal. Analisis fungsi distribusi radial (RDF) berbasis perhitungan pusat masa (*Center of Mass*, COM) menunjukkan bahwa posisi puncak RDF yang relatif tetap pada pasangan kation-anion dan kation-kation. Karakteristik puncak RDF juga sesuai dengan literatur sistem [BMIM]/[EMIM][BF₄], di mana posisi puncak pertama pasangan kation-anion lebih dekat dan tajam dibandingkan pasangan ion lainnya. Pengecualian ditemukan pada pasangan anion-anion yang menunjukkan pergeseran puncak RDF ke jarak yang lebih jauh seiring dengan peningkatan fraksi ion [BMIM]⁺. Sementara itu, perubahan fraksi kation memengaruhi sifat transport secara signifikan, diindikasikan dengan penurunan koefisien difusi diri dan konduktivitas ionik.

Kata kunci: cairan ionik garam ganda, CL&P, dinamika molekul.

STUDY OF THE EFFECT OF CATION FRACTION ON THE TRANSPORT AND STRUCTURAL PROPERTIES OF [BMIM]/[EMIM][BF₄] DOUBLE-SALT IONIC LIQUIDS THROUGH MOLECULAR DYNAMICS SIMULATION

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ABSTRACT

In this research, an analysis of the effect of cation fraction between 1-butyl-3-methylimidazolium (BMIM⁺) and 1-ethyl-3-methylimidazolium (EMIM⁺) on the structural and transport properties of the [BMIM]/[EMIM][BF₄] double-salt ionic liquids (DSILs) system was conducted using molecular dynamics (MD) simulation. This study was aimed at understanding the effect of cation fraction on the structural and transport properties of [BMIM]/[EMIM][BF₄] DSILs.

The molecular dynamics (MD) simulations were performed using the CL&P force field at a temperature of 300 K and a pressure of 1 bar through two steps. The first step involved an NPT production simulation to construct the simulation box of the DSILs system with 320 total molecules, denoted by $X_{\text{BMIM}} + (1-X)_{\text{EMIM}}$ using mole fractions of 0.00, 0.25, 0.50, 0.75, and 1.00. Furthermore, the simulation box was used at the NVT production step to form the trajectory of the system. The resulting trajectory was then used to analyse density, radial distribution function (RDF), self-diffusion coefficient (D), and ionic conductivity of the [BMIM]/[EMIM][BF₄] DSILs system.

Based on the research conducted, no significant changes in the local structure were observed with increasing [BMIM]⁺ fraction and decreasing [EMIM]⁺ in the [BMIM]/[EMIM][BF₄] DSILs system. Through radial distribution function (RDF) analysis based on center of mass (COM) calculations, it was found that the RDF peak positions were remained relatively unchanged for cation-anion and cation-cation pairs. These RDF characteristics were consistent with those reported in the literature for the [BMIM]/[EMIM][BF₄] system, where the first peak of the cation-anion pair was located at a closer distance and showed a sharper profile than those of other ion pairs. An exception was observed in the anion-anion pair, for which a shift of the RDF peak toward a larger distance was detected with increasing [BMIM]⁺ fraction. Meanwhile, significant effects of cation composition on transport properties were observed, as indicated by decreases in the self-diffusion coefficients and ionic conductivity.

Keywords: CL&P, double-salt ionic liquids, molecular dynamics.