# Numerical Studies of Transport Properties in Heterogeneous Food Systems

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**Abstract:**
The current computer simulation based study aims to elucidate the complex role that the state of aggregation and morphology of the food materials plays in determining their transport behaviour. Using Brownian dynamic simulations, applied to colloidal systems, we simulate the compression of two different dense layers of nanoparticles (with reversible and irreversible bonds), at interface, at three different compression rates. We determine the desired transport coefficient for these structures using a novel technique, originally proposed by Torquato and Kim (1990). This method allows us to consider complex structures in our study, for which calculations of effective transport coefficients using conventional methods, like finite elements and finite difference, would be relatively difficult. We first validate our algorithm by comparing its results with those of exact calculations, for different regular lattices. Our results are in excellent agreement with the theory. The variation in the transport coefficient of nano-particle monolayers during the compression, are also correlated with the build up of stress and changes in the structure of the films.

**Zusammenfassung:**
Die vorliegende Computersimulations-Studie verfolgt das Ziel, die komplexe Beziehung zwischen Aggregations-Zustand und der Morphologie von Lebensmitteln sowie ihren Fliesseigenschaften zu erhellen. Wir simulieren die Kompression zweier verschieden dichter Schichten von Nanopartikeln (mit reversiblen und irreversiblen Bindungen) an der Grenzfläche, unter Einsatz von Brownscher Molekulardynamik. Wir bestimmen die relevanten Transportkoeffizienten für diese Strukturen anhand einer Methode, die von Torquato und Kim (1990) vorgeschlagen wurde. Diese Methode erlaubt es uns, komplexe Strukturen zu berücksichtigen, für die die Berechnung von effektivenTransportkoeffizienten mit gewöhnlichen Methoden wie etwa Finite Elemente und finite Differenzenverfahren sehr aufwendig wäre. In einem ersten Schritt validieren wir unseren Algorithmus für verschiedene reguläre Gitter, indem wir die Resultate mit denen exakter Lösungen vergleichen. Unserer Resultate sind in sehr guter Übereinstimmung mit den theoretischen Ergebnissen. Die Variation der Transportkoeffizienten der Nanoteilchen-Monolagen unter dem Einfluss der Kompression werden zudem mit dem Spannungszustand und strukturellen Änderungen des Films korreliert.

**Résumé:**
Le présent papier vise à élucider le rôle complexe que la structure des matériaux alimentaires joue sur leur coefficient de transport. En utilisant une simulation dynamique Brownienne, appliquée aux systèmes colloïdaux, nous simulons la compression de couches denses de nanoparticules situées à l'interface de deux media, pour trois vitesses différentes, et ceci pour deux différents types de liaisons inter particules (réversible and irréversible). Nous déterminons le coefficient de transport recherché pour ces structures, utilisant une nouvelle technique, originairement proposée par Torquato and Kim (1990). Cette méthode nous permet de considérer des structures complexes, pour lesquelles le calcul du coefficient de transport effectif, utilisant des méthodes conventionnelles telles que les méthodes des éléments finis et différences finies, seraient difficilement applicable. Nos résultats sont en très bon accord avec ceux théoriques. Les variations du coefficient de transport des couches de nanoparticules sous compression, sont corrélées à celles du stress et aux changements de structures des couches.

**Key words:** Transport properties, Brownian motion, heterogeneous system, aggregation





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faces. Two different systems involving reversible and irreversible bond forming particles are considered. In both systems, the dielectric constants are correlated to the mechanical properties of the monolayers. The variation of both properties shows the same general trend under compression, i.e. a higher rate of increase after the onset of the particle desorbsion process. The structure of the monolayers, undergoing fast compressions, are rougher and much more disordered than those obtained under slower compressions, for both systems with reversible and irreversible bonds. The higher dielectric constants attained for more rapidly compressed films are attributed to such increased roughness. Comparing the reversible and irreversible bond forming systems under the same compression rate, higher dielectric values are obtained when the bonds are reversible and particle rearrangement is possible. The reversible nature of bonds means that, once derobed, a particle can break the old bonds and form new ones with the particles still at the interface. In time this allows a secondary particle layer on top of the original monolayer to developed, giving the film a higher dielectric constant. The same process is also responsible for the higher surface area covered by the particles at the interface for the reversible bond forming particles. The values for the reversible and irreversible bond forming particles are 80% and 70%, respectively. Similarly, the coordinate number for particles at the interfacial layers are 4.5 for the film with the reversible bonds, as oppose to 3.5 for the irreversible case.

We have demonstrated differences in the variation of the dielectric constant of the film during compression, at various rates of compression. It is shown that the same trends are also closely reflected in the manner in which the stress builds up in such systems. These variations are in turn related to the ways in which the particles rearrange or are expelled from the interface, at different rates of surface compression.

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