Charge Transport At Liquid/Liquid Interface

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Abstract

Charge transfer (CT) at liquid/liquid interfaces are described theoretically depending on the quantum theory .A model that derived used to calculate the rate constant of transport at liquid/liquid interfaces. The calculation of the rate constant of charge transfer depends on the calculation of the reorganization energy, driving force ,and the coupling coefficient . Large reorganization energies and large rate constant for charge transfer ,indicate that the transitions involve more energy to happen . The system have large $E_0\,(eV)$ refers that type of liquid is more reactive media than other liquid types with same donor. Driving force energy to drive the charge increases with the increase of absorption energy and decrease of in wave length. Height barrier at liquid/liquid interface that decreasing with decreasing the driving force energy and increasing the absorption energies .Charge transfer is so much small as a barrier of large values but in the low values of barrier ,the transfer is most probable. The large height barrier exclusion transfers across liquid/liquid system and the charger suffers from much resistant to transfer . However, this excluded transfer could be significantly large for high barrier and small concentrations .The theoretical values of rate constant of charge transfer show a good agreement with some of the experimental studies.

Key Word: Charge Transfer, Liquid/Liquid interface.

Introduction

Charge transfer (CT) reaction is one of the most important processes in chemistry and biology. It has been the subject of lively investigation recently. In the past 30 years, both experiment and theory of charge transfer have made tremendous progress [1] . In simple terms, an electron transfer reaction involves the transfer of an electron from a 'donor'$|D>$ to an 'acceptor'$|A>$ state .[2].Since no chemical bonds are broken or formed in the transfer and further more the changes in the bond lengths and angles are rather small .As a result ,the donor becomes oxidized and the acceptor will be reduced to the redox reactions .Redox reactions play an important role in everyday life, for example, the sequence of reactions which sustain the metabolism in plants and animals consists entirely of redox reactions[3] . Since the late 1940 s, the field of (CT) processes have grown enormously, both in chemistry and biology. The development of the field of the (CT) is experimental and theoretical, as will as its relation to the study of other kinds of chemical reactions [4].

The charge transfer is of highly importance in bioenergetics and is an active field of research. Much attention has been devoted to study the charge transfer at liquid /liquid interface and molecular transport reaction processes [5] The classical transfer theory was initially generalized for the liquid |liquid interface considered the charge transfer reaction as asides of steps, where the formation of a precursor complex of the reactants is followed by reorganization of the precursor, charge transfer and dissociation of the products [6]. liquid/liquid system theoretically uses quantum mechanics ;this will be atransfer rate constant which is calculated.

Theoretical Framework

For the system liquid-liquid interface, we can suppose two localized quantum states $|\Phi_{DL}>$,and $|\Phi_{AL}>$, donor and acceptor liquid state .The time dependent wave function at one dimensional quantum system is [7].

$$|\Phi_{(r,t)}>=\sum_0^\infty |\Phi_{(r)}> e^{\frac{-i}{\hbar}ET} \text{...... .... (1).}$$

Where$|\Phi_{(r)}>$is the basis of the state vector in a Hilbert space. The model Hamiltonians used to describe the electron transfer dynamics comprise of several parts that have well defined physical origins. The full Hamiltonian ,H, is spilt into the donor liquid,H_{DL},acceptor liquid, H_{AL} and time dependent term which describes the interaction H_{DAL} [8].

$$H = H_{DL} + H_{AL} + H_{DLAL} = H_0 + H_{DLAL} \text{ ....(2)}$$

Where H_0 is the time independent of the unperturbed system, the condition on the perturbation H_{DLAL} is relaxed to permit it to vary in time.

In terms of orthonormal set $\Phi_k(r)$ which satisfies [9].

$$H_0\Phi_k(r)=E_k\Phi_k(r) \text{ ....(3)}$$

Then the probability of electron transition from donor liquid state to acceptor liquid state is given by [10].

$$W_{DLAL} = \frac{2\pi}{\hbar}|T_{DLAL}|2\delta(E_{DL} - E_{AL} - \hbar\omega) \text{ ....(4).}$$

Then the rate constant is given by with density [11].

$$K_{\mathrm{ET}}^{L/L} = \frac{2\pi}{\hbar}|T_{DA}|^2 \rho(E_A - E_D) \text{ ....(5)}$$

Rate transfer Eq. (5) with density becomes.

$$K_{\mathrm{ET}}^{L/L} =\frac{2\pi}{\hbar}|T_{DA}|^2 \mathrm{N}\ e^{\frac{-(E_0+\Delta G_0)^2}{4E_0k_BT}} \text{ .... (6)}$$

But

$$\mathrm{N}(\frac{\pi}{\beta})^{\frac{1}{2}} = 1 \Rightarrow \mathrm{N} = (\frac{\beta}{\pi})^{\frac{1}{2}}=(\frac{1}{4\pi E_0k_BT})^{\frac{1}{2}} \text{ ....(7)}$$

Eq. (6) with Eq. (7) is written

$$K_{\mathrm{ET}}^{L/L} = \frac{2\pi}{\hbar} \; |\mathrm{T_{DA}}|^2 \quad \left(\frac{1}{4\pi E_0 K_B T}\right)^{\frac{1}{2}} exp^{\frac{-(E_0+\Delta G_0)^2}{4E_0 k_B T}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(8).}$$

Where $\hbar = \frac{h}{2\pi}$ is the h Planck constant,k_B is the Boltzmann constant, T is the absolute temperature and T_{DA} is the coupling matrix element. When the liquid/liquid system absorption photon light to excite according to expression [12].

$$\Delta G_{\,o} = h\nu - E_0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\text{(9)}$$

Where ΔG_0 is the effective free energy (driving force) is given by [13] .$\Delta G_{\,o} = h\left(\frac{c}{\lambda}\right) - E_0$ ……………………………………………….(10)

Where ν is the frequency, c is the velocity of light and λ is the wave length .Also E_0 is contribution of the reorganization energy due to reaction, can be written as [14] .

$$E_0 = \frac{(\Delta e)^2}{4\pi\epsilon_0}\left[\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R}\right]\left(\frac{1}{\epsilon_1^{op}+\epsilon_2^{op}} - \frac{1}{\epsilon_1^{S}+\epsilon_2^{S}}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\text{(11)}$$

Where $R = a_1 + a_2$ is the separation distance between the two reactants and a_1, a_2 are the radii of ions,ϵ_{op} *and* ϵ_s refers to the optical and static dielectric constant of two liquid .The radii of donor and acceptor can be estimated from the apparent molar volume using spherical approach[15].

$$a_i = \left(\frac{3MW}{4\pi N_A \rho}\right)^{\frac{1}{3}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\text{(12)}$$

Where a_i is the radius of donor or acceptor, Avogadro's number construes NA, MW is the molecular weight , and ρ is the mass density of liquid.

Results

A quantum theory have been used to study and calculate the transitions of electron rate constant at liquid/liquid system . The calculation of the rate constant of electron transfer is dependent on the calculation of the reorganization energy , the electronic coupling, and the driving force energy . One first step to calculate the reorganization energy . $E_0(eV)$ that can be calculated theoretically using Eq.(11).To calculate the reorganization energies $E_0(eV)$ for water/liquid system, one can estimate the radius for donor (water) and acceptor liquid using Eq.(12) , substation the values of Avogadro's construes $NA = 6.02 \times 10^{23} \frac{Molecule}{mol}$ molecular weight MW ,and Density mass ρ for all liquids from table (1) in Eq.(12),result are listed in table (2) . Inserting in Eq. (11) the values of radii of donor and accepter , dielectric constant ϵ_s optical dielectric constant ϵ_{op} from table (1) and assume the distance $R = a_D + a_A$ between center to center for donor and acceptor, knowing that $\frac{e^2}{4\pi\epsilon} = 14.4\; eV$ the results of reorganization free energy have been summarized in table (3) .

On the otherhand, we can calculate the driving force energy (free energy) term at the liquid/liquid interface as a function of the reorganization energy ,and the absorption energy using Eq.(10). The absorption energy in Eq.(9) can be roughly taking from the wave length in visible spectrum(4000A°-7000 A°) and transform energy equation $E = h\nu = \frac{hc}{\lambda}$ Where h is Planck constant ,c is the velocity of light ,and λ is the wave length .

Since we have considered that the absorbed visible light is directed to the aqueous phase .we evaluated the driving force energy for liquid/liquid system by inserting the values of the reorganization energy from table(3),and absorption energy from spectrum in Eq.(8),results are listed in table(4).Next ,we calculate the rate constant using Eq.(7), by feedback in a Math lab program the results of both reorganization energy are from table(3), driving force energy is in table (4), and using the coupling coefficient (200 ,400)cm^{-1}[5],results are summarized in tables (5) to (6).

Discussion

First-order perturbation theory and quantum theory treatment have been used to drive an expression to the transitions of electron rate constant at liquid/liquid system .Rate constant of charge transfer depends on many parameters such that :the reorganization energy, driving force energy ,height barrier ,and coupling coefficient. In this paper we will calculate the rate constant for charge transfer at liquid/liquid interface system depending on the results of the reorganization energies and the driving free energy (driving force). The exponential in Eq.(8) have tested the probability of the transfer of charge from donor water to liquid acceptor state. The reorganization of free energies is calculated depending on the semi classical model for charge transfer at liquid/liquid interface system using a two spherical model based on the Marcus theory of charge transfer (CT) . Table(3) shows that the reorganization energy for charge transfer at liquid-liquid system indicates that is in general whenever there is an increase in the dielectric constant for acceptor, there is increase in the reorganization energies lead to an increases in rate of charge in tables (5) and (6) respectively and vice versa , similarly whenever, there is an increase in the interface index for acceptor liquid leads to a decrease in the reorganization energies for system with the same refractive index and dielectric constant for the donor resulted to decrease in rate of charge transfer .

This indicates that the reorganization energy as a function of the polarity $f(n,\epsilon)=\left(\frac{1}{\epsilon_{op}}-\frac{1}{\epsilon_s}\right)$ for system, this means that a small polarity function results to a decrease in the reorganization energy and vice versa. Comparison of the results of calculation of the reorganization energy E_0 are in table (3) and the rate of charge transfer is in table(5)and(6),indicates that the charge transfer is more probable in liquid-liquid system have more polarity parameter for example water/formic acid have $f(n,\epsilon)\cong 0.2657$ leads to large reorganization energy $E_0\approx 0.898\ eV$. Notably the charge transfer in the system that have large dielectric constant is stronger than the system have that a small dielectric constant. Our results showed agreement with experimental value for E_O [16].

Next the results of driving force showed that table(4) gives the results of the driving force energy for charge transfer take term accounting for the attractive interactions between the tails of the donor state wave function and acceptor state wave function. Results in table (4) of driving force ΔG_0(eV), show that energy that is taken to bring the donor and acceptor together and is the part of the work broken to derive the charge to transfer from donor to acceptor. The driving force energy to drive the charge increases with the increase of absorption energy and decreases in wave length. The exponential in rate describing the barrier height is the function of both reorganization energy and driving force .Decreasing barrier leads to increase the transfer of charge cross liquid/liquid interface with a decrease of the driving force energy and increase the absorption energies .This indicates the absorption energy is divided into reorientation of the system to transfer and the other enables to drive the charge to transfer due to potential barrier height from donor to acceptor. Again, the transition is so much small as a barrier large values but in the low values of barrier ,the transfer is most probable the large height barrier exclusion transfer across liquid/liquid system and the electron suffering much resistant to transfer . However, this excluded transfer could be significantly lower for high barrier and small concentrations of charge because of the hard (large height) barrier overlapping effect .The theoretical result as well as with the other results[2].

Conclusions

In this study ,it can be concluded depending on our results of calculation that the rate of charge transfer is more probable happen and stronger depends on the reorganization and driving force energies . The reorganization energy depends on three parameter dielectric constant, optical properties (refractive index n)and polarity .It has shown that all donor molecular have large dielectric constant ,have large reorganization energies and large rate constant for charge transfer ,indicates that the transitions involve more energy to happen . On the otherhand the system have large $E_0\,(eV)$ refers that type of liquid is more a reactive media than other liquid type with the same donor. The driving force energy for charge transfer takes term accounting for the attractive interactions between the tails of the donor state wave function and acceptor state wave function and depends on the reorganization energy and the absorption energy visible spectrum. Its energy that is taken to bring the donor and acceptor together and drive the charge increases with the increase of absorption energy and decrease in wave length .Height barrier at liquid/liquid interface that decreases with the decrease of the driving force energy and increases the absorption energies .

This indicates that the absorption energy is divided into reformation the system to transfer and the other enables to drive the charge to transfer due to potential barrier height from donor to acceptor. It can be concluded that the transition is so much small as barrier large values but in the low values of barrier ,the transfer is most probable the large height barrier exclusion transfer across liquid/liquid system and the charger suffers much resistant to transfer . However, this excluded transfer could be significantly lower for high barrier and small concentrations of charge because of the hard (large height) barrier overlapping effect .

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Table No.(1):Characteristic of liquid material

Liquid Type	**Molecule weight (MW) $g.mol^{-1}$ [17,18,19]**	**Density (ρ) $g.cm^{-3}$ [17,18,19]**	**Dielectric Constant ϵ_s [20,21]**	**Refractive index (n) [20,21]**
Water	18	1	80	1.333
Acetone	58.08	0.791	20.493	1.3588
Formic acid	46.03	1.22	51.1	1.3714
Bromoform	252.73	2.889	4.2488	1.6005
Chloroform	119.38	1.483	4.7113	1.4459
N-methylformamide	59.07	1.003	181.59	1.4319
N,N dimethylformamide	73.09	0.944	37.219	1.4305
Ethanol	46.0414	0.790	24.852	1.3611
n-hexadecane	226.44	0.733	2.0402	1.4345
Haxanic acid	116.16	0.93	2.6	1.4163
1,2 ethanediol	63	1.1151	40.245	1.4318

Table No.(2):The theoretical calculation values of radii $a_i(A°)$ for donor and acceptor liquid

Liquid Type	Molecule weight $g.mol^{-1}$ [17,18,19]	density $g.cm^{-3}$ [17,18,19]	radii$a_i(A^0)$
Water	18	1	1.92520792
Acetone	58.08	0.791	3.076121696
Formic acid	46.03	1.22	2.463847665
Bromoform	252.73	2.889	3.261043233
Chloroform	119.38	1.483	3.171881441
N-methylformamide	59.07	1.003	2.858087259
N,N dimethylformamide	73.09	0.944	3.13099322
Ethanol	46.0414	0.790	2.848135287
n-hexadecane	226.44	0.733	4.96595975
Haxanic acid	116.16	0.93	3.672073423
1,2 ethanediol	63	1.1151	2.818787796

Table No.(3):Our calculation results of reorganization free energy $E_0\ (eV)$ for change transfer at Water\Liquid interface system.

System	Dielectric constant for acceptor ϵ_s [20,21]	Optical dielectric constant for acceptor ϵ_{op}	Reorganization free energy $E_0\ (eV)$
Water/Acetone	20.493	1.84633744	0.8516752339
WaterFformic acid	51.1	1.88073796	0.8986405084
Water/Bromoform	4.2488	2.56160025	0.6932973949
Water/Chloroform	4.7113	2.09062681	0.7858438989
Water/N,Methylformamide	181.59	2.05033761	0.8363805396
Water/N,Ndimeethylformamide	37.219	2.04633025	0.8075301745
Water/Ethanol	24.852	1.85259321	0.8635918533
Water/n-hexadecane	2.0402	2.05779025	0.8246426859
Water/Hexanic acid	2.6	2.00590569	0.8118435171
Water/1,2 ethanediol	40.245	2.05005124	0.8244227082

Table No. (4):The result of our calculation of driving force energy $\Delta G_o(eV)$for charge transport in Water/Liquid system.

	Driving force energy $\Delta G_o(eV)$									
Wave length λ (A^o)	Water-bromoform	Water-n-hexadecane	Water-chloroform	Water-N,Ndimethylformamide	Water-haxanic acid	Water-1,2ethanediol	Water-n-methylformamide	Water-Acetone	Water-ethanol	Water-Formic acid
4000	2.4127	2.2813	2.3201	2.2984	2..2941	2.2815	2.2696	2.2543	2.2424	2.2073
4500	2.0676	1.9362	1.9750	1.9533	1.9490	1.9364	1.9245	1.9092	1.8973	1.8622
5000	1.7915	1.6601	1.6989	1.6772	1.6729	1.6603	1.6484	1.6331	1.6212	1.5861
5500	1.5656	1.4342	1.4730	1.4513	1.4470	1.4344	1.4225	1.4072	1.3953	1.3602
6000	1.3774	1.2460	1.2848	1.2631	1.2588	1.2462	1.2343	1.2190	1.2071	1,1720
6500	1.2181	1.0867	1.1255	1.1038	1.0995	1.0869	1.0750	1.0597	1.0478	1.0127
7000	1.0816	0.9502	0.9890	0.9673	0.9630	0.9504	0.9673	0.9232	0.9113	0.8762

Table No.(5):Results of the electron transfer rate constant at Water/Liquid interface system with coupling coefficient $T_{DA} = \frac{200}{8065.52} = 0.0247969$ (eV).

Wave length λ (A^o)	Rate constant $K_{\mathrm{ET}}^{L/L}$ (sec^{-1})									
	Water-bromoform	Water-n-hexadecane	water-chloroform	Water-N,N dimethylformamide	Water-haxanic acid	Water-1,2 ethanediol	Water-N,methylformamide	Water-Acetone	Water-ethanol	Water-Formic acid
4000	4.562 $\times10^{-48}$	1.788 $\times10^{-38}$	3.807 $\times10^{-41}$	1.530 $\times10^{-39}$	2.871 $\times10^{-39}$	1.751 $\times10^{-38}$	9.183 $\times10^{-38}$	7.343 $\times10^{-37}$	3.428 $\times10^{-36}$	2.641 $\times10^{-34}$
4500	2.20 8×10^{-35}	8.226 $\times10^{-28}$	8.845 $\times10^{-30}$	1.184 $\times10^{-28}$	1.947 $\times10^{-28}$	8.123 $\times10^{-28}$	3.007 $\times10^{-27}$	1.548 $\times10^{-26}$	5.209 $\times10^{-26}$	1.605 $\times10^{-24}$
5000	2.614 $\times10^{-26}$	3.492 $\times10^{-20}$	8.946 $\times10^{-22}$	7.293 $\times10^{-21}$	1.089 $\times10^{-20}$	3.462 $\times10^{-20}$	9.963 $\times10^{-20}$	3.755 $\times10^{-19}$	1.001 $\times10^{-18}$	1.603 $\times10^{-17}$
5500	1.353 $\times10^{-19}$	1.539 $\times10^{-14}$	7.476 $\times10^{-16}$	4.218 $\times10^{-15}$	5.887 $\times10^{-15}$	1.525 $\times10^{-14}$	3.652 $\times10^{-14}$	1.091 $\times10^{-13}$	2.461 $\times10^{-13}$	2.426 $\times10^{-12}$
6000	1.719 $\times10^{-14}$	3.006 $\times10^{-10}$	2.379 $\times10^{-11}$	1.018 $\times10^{-10}$	1.344 $\times10^{-10}$	2.992 $\times10^{-10}$	6.227 $\times10^{-10}$	1.561 $\times10^{-9}$	3.084 $\times10^{-9}$	2.104 $\times10^{-8}$
6500	1.621 $\times10^{-10}$	6.586 $\times10^{-7}$	7.621 $\times10^{-8}$	2.629 $\times10^{-7}$	3.333 $\times10^{-7}$	6.582 $\times10^{-7}$	1.224 $\times10^{-6}$	2.679 $\times10^{-6}$	4.771 $\times10^{-6}$	2.440 $\times10^{-5}$
7000	2.297 $\times10^{-7}$	2.948 $\times10^{-4}$	4.605 $\times10^{-5}$	1.343 $\times10^{-4}$	1.636 $\times10^{-4}$	2.935 $\times10^{-4}$	5.020 $\times10^{-4}$	9.859 $\times10^{-4}$	1.640 $\times10^{-3}$	6.599 $\times10^{-3}$

Table No.(6):Results of the electron transfer rate constant at Water/Liquid interface system with coupling coefficient $T_{DA} = \frac{400}{8065.52} = 0.0495938$(eV).

Wave length λ (A°)	Rate constant $K_{\mathrm{ET}}^{L/L}$ (sec^{-1})									
	Water-bromoform	Water-n-hexadecane	water-chloroform	Water-N,N dimethylformamide	Water-haxanic acid	Water-1,2 ethanediol	Water-N,methylformamide	Water-Acetone	Water-ethanol	Water-Formic acid
4000	1.839×10^{-47}	7.209×10^{-38}	1.535×10^{-40}	6.125×10^{-39}	1.149×10^{-38}	7.010×10^{-38}	3.675×10^{-37}	2.938×10^{-36}	1.372×10^{-35}	1.057×10^{-33}
4500	8.902×10^{-35}	3.316×10^{-27}	3.540×10^{-29}	4.739×10^{-28}	7.793×10^{-28}	3.251×10^{-27}	1.203×10^{-26}	6.197×10^{-26}	2.084×10^{-25}	6.424×10^{-24}
5000	1.053×10^{-25}	1.408×10^{-19}	3.580×10^{-21}	2.919×10^{-20}	4.360×10^{-20}	1.385×10^{-19}	3.987×10^{-19}	1.5030×10^{-18}	4.009×10^{-18}	6.437×10^{-17}
5500	5.457×10^{-19}	6.204×10^{-14}	2.992×10^{-15}	1.688×10^{-14}	2.356×10^{-14}	6.106×10^{-14}	1.461×10^{-13}	4.3692×10^{-13}	9.851×10^{-13}	9.709×10^{-12}
6000	6.931×10^{-14}	1.212×10^{-9}	9.522×10^{-11}	4.077×10^{-10}	5.380×10^{-10}	1.197×10^{-9}	2.492×10^{-9}	6.247×10^{-9}	1.234×10^{-8}	8.421×10^{-8}
6500	6.538×10^{-10}	2.655×10^{-6}	3.050×10^{-7}	1.052×10^{-6}	1.334×10^{-6}	2.634×10^{-6}	4.901×10^{-6}	1.072×10^{-5}	1.909×10^{-5}	9.767×10^{-5}
7000	9.262×10^{-7}	1.188×10^{-3}	1.843×10^{-4}	5.375×10^{-4}	6.548×10^{-4}	1.174×10^{-3}	2.009×10^{-3}	3.946×10^{-3}	6.565×10^{-3}	0.0264

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الخلاصة

انتقال الشحنة لسطح سائل/سائل وصفت نظريا اعتمادا على النظرية الكمية.الآنموذج المشتق استعمل لحساب ثابت معدل الأنتقال لسطح سائل/سائل. حساب ثابت معدل الأنتقال للشحنة اعتمد على حساب طاقة اعادة التنظيم، والقوة المساقة، ومعامل الترابط. طاقة الكبيرة لاعادة التنظيم والمعدل العالي لثابت الأنتقال لشحنة يشير الى ان الأنتقالات تتضمن مزيدا من الطاقة لتحدث. النظام الذي يملك $E_0\ (eV)$ (طاقة اعادة التنظيم المقاسة باالكترون فولت) عالية يشير الى نوعية السائل الذي يتفاعل بالوسط اكثر من السوائل الأخرى للواهب(المانح) نفسه.طاقة القوة المساقة والتي تسوق الشحنة تتزايد مع زيادة الطاقة الممتصة وبتناقص الأطوال الموجية .ارتفاع البئر لسطح سائل/سائل يتناقص مع تناقص القوة المساقة مع زيادة الطاقة الممتصة . والشحنة المنتقلة تكون قليلة الكمية لقيم عالية في بئر ما ولكن القيم واطئة لبئر فأن العبور يكون اكثر احتمالا منه.ارتفاع العالي للبئر يحجب الانتقال عبر نظام السائل والشحنة تعاني ممانعة الأنتقال .وعلى اي حال فأن احتجاب العبور يكون ملحوظا لبئر عالي الأرتفاع وبتركيز قليل. القيم النظرية لثابت معدل الانتقال للشحنة اظهرت تطابقا مع بعض الدراسات التجريبية.

الكلمات المفتاحية:أنتقال الشحنة، سطح سائل/سائل.