出國報告(出國類別:學術研討會)

赴日本參加
2017 ICFD- 14th International Conference Fluid Dynamic
返國報告

服 務 機 關 ：海軍軍官學校
姓 名 職 稱 ：戴中傑助理教授

派 赴 國 家 ：日本
出 國 期 間 ：106 年 10 月 28 日－11 月 5 日
報 告 日 期 ：106 年 11 月 8 日

摘要

計畫主持人於 2017 年 10 月 28 日研討會當日赴高雄小港機場坐一早班機飛往日本成田機場，並於 2017 年 11 月 1 日抵達本次在日本仙台東北大學開會的國際會議中心(Tohoku Unversity)進行報到和註冊，並領取大會資料和議程相關資料。11 月 1 日上午發表論文，題目為”Numerical Study to investigate proton transport in Proton Exchange Membrane Fuel Cell”。主要內容是報告數值研究質子交換膜燃料電池中質子的傳遞。利用分子動力學研究質子在高分子膜中的傳遞機制是本研究的重點，探討質子的傳遞機制可瞭解燃料電池核心質子交換膜的性能，也就是交換膜的導電度，是該研究計畫的重點。本計畫重點研究了分子之間的交互作用及質子在交換膜中傳遞的路徑。成功的將氫質子在膜中靠著水分子的載運機制及在水分子之間跳躍機制實現了傳遞機制，從陽極往陰極方向前進，最終與陰極的氧原子結合，形成水分子，提出高分子的模擬方法，最後運用 GRB 法完成了分子動力模擬；本研究計畫提出的方法除了可應用於高分子的分子動力模擬運算，更可運用於生物化學方面的模擬，可預測計算出交換膜的導電度及燃料電池的性能。報告後多人發問與發表建言，討論熱烈。

會議期間，主持人亦與一些研究學者討論有關氣體動力、再生能源以及計算模擬在產業上應用的知識與技術。

目次

出席國際會議心得報告

一、目的：

出席國際大型研討會，可與國際著名學者討論與交流有關燃料電池的分子動力模擬及新能源的發展與應用，並發表個人論文，參與討論以增加個人於本研究領域廣度及深度。

二、會議概況：

國際計算流體力學研討會（ICFD）為每年舉辦一次的國際學術研討會，今年為第 14 屆於 2017 年 11 月 1 日至 11 月 3 日在日本仙台的國際會議中心(Sendai International Center)舉行，這是日本原子能及工程計算科學學會(Computational Science and Engineering Division, Atomic Energy Society of Japan)等數個學會，每年所舉辦的其中一場關於計算流體力學頗具盛名的國際研討會，依照慣例，均在日本仙台舉辦，今年日本由東北大學 (Tohoku Unversity) 主辦。本次研討內容主要為複雜流場的模擬運算技術探討。會議邀請了許多重量級的學者與會演講，參加的學者以亞洲及歐美洲地區為最多數，每場演講後的討論正是各個學者意見互相交流的時間，可以相互激發思慮。本次研討會學術交流分為三個部份，包括：(一)專題演講(keynote speakers)及(二)口頭報告(presentations)。大會安排於 11 月 1 日至 3 日每天一場的專題演講、將近 480 篇的口頭報告，分為 19 個場次發表。本次研討會共計錄取 480 篇論文，每一篇均需要口頭報告，。本次大會三天共排進 20 個議程，每一個議程平均 3~6 場的報告；本人此次發表的研討會論文於 11 月 1 日下午於複雜計算流體力學議程中發表。由於專題演講、口頭發表與海報論文發表於同一時段進行，三天下來，研討會之論文發表與專題發表場次可選擇有興趣的參加，且與國外學者共同討論研究心得獲益良多。此外本次會議議程相當緊湊，除了下午的論文發表外，還有專題講演。連續三天早出晚歸，相當辛苦，不過也過得相當充實。除在學術專業與各國學者交流外，對異國風情文化亦略有體會與感受。

三、過程與心得：

計畫主持人參與會議經過，如下所述：

主持人於 2017 年 10 月 28 日研討會赴高雄小港機場坐一早班機飛往日本成田機場，適逢週末假日及日本萬聖節慶典，交通繁忙，於 10 月 29 日抵達日本仙台，於 11 月 1 日在仙台國際會議中心(Sendai International Center)進行報到和註冊，並領取大會資料和議程相關資料。此次大會的主要學術議程有邀請演講、口頭報告二種方式。主持人於會議期間 11 月 1 日下午

3 點 20 分發表一篇口頭論文報告，題目為" Numerical Study to investigate proton transport in Proton Exchange Membrane Fuel Cell "。主要內容是報告質子交換膜燃料電池中，質子的傳遞機制及演算方法。本研究重點在於使用分子動力學及 GRB 演算法。將高分子膜內含有的水分子與氫質子經過分子動力模擬計算後，擷取出氫質子與水分子的移動路徑及其分子間的交互作用，並展現氫質子與水分子之間的相對位置，演示出氫質子是依靠水分子的載運機制及擴散原理及在水分子間的跳躍運動。報告後多人發問與發表建言，討論熱烈。其中有學者對於論文提問有關影像來源及窒礙難行處理情形的解決方案；另有學者則是詢問論文的模擬參數設計以及與結果的比對驗證。顯示此一領域的國際學者在研究上是理論與實驗技術並重的。另外本次研討會當有其它研究領域的場次，研討會論文報告共計 480 篇：流場計算與燃燒、電漿流體動力及未來應用、渦動流體力學、紊流流體力學等各方面都有，並有各個論文作者分別在現場說明。

此外，聽了國防大學機航系的羅明忠教授討論有關極音速光窗冷卻的模擬計算演講，其中介紹了平行計算化的 DSMC 模擬及展示運用 DSMC 計算三維高速流場的光窗冷卻效應、溫度分布及模擬原理及運用，最後可以運用相關的模擬來設計高速導引飛彈的光窗附近的流場。而他的研究領域包含了太空衛星的流場計算及稀薄氣體的氣體動力計算，另在會議現場亦展示了相關三維模擬流場的相關物理量的分布，課題相當重要且有趣；加拿大麥克馬斯特大學數學及統計學系的 Bartosz Protas 教授發表了旋度加強與極端渦流的流體力學極限問題，提出了一個變化的框架來分析螺旋性對極端的結構和性質的影響，在粘性不可壓縮流動中的渦旋狀態呈現出系統動力學最大的增長所允許的一些強制約束下的自我保護，因此與可能的奇點形成的問題有關。讓不同領域的研究者對強烈極端的渦流流場有了基本的認識。此外，與日本東北大學的 Toru Sugita 教授討論有關燃燒的技術，它利用光學的原理控制甲烷混合二甲醚的微弱火焰在微反應器的溫度控制問題，教授在演講時發表了他與他的團隊使用雷射光測量燃燒溫度及控制反應器的加熱溫度的解決方法；讓我們與會者受益良多。這場研討會所邀請之專家學者演講之主題與流體力學及計算流體力學有濃厚的關係，而與本人未來的研究相當有關連，參加本次研討會，雖然只有短短三天，但所學習的新知，卻是需要花費大量研讀時間才可獲得的，因此也激發了個人在相關研究上的靈感。

研討會最後一天(11 月 3 日)無與本人相關論文發表以及學術議程，因此本人並無參加，11 月 4 日返回東京市，於隔日 11 月 5 日由東京成田機場搭機返台，結束本次受益良多的研討會。

四、論文發表：

Numerical Study to investigate proton transport in Proton Exchange Membrane Fuel Cell

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[2]Department of Chemistry, National Sun Yat Sen University, Kaoshiung 80424, Taiwan, R.O.C.

ABSTRACT

Proton exchange membrane is most important components in fuel cell. The study focus on Nafion 117(Dupont) membrane at hydration level λ=4. We investigate the mechanism of transport of proton at 298K from MD simulation. Mean square displacement, radial distribution function, and movement trajectories of protons from MD simulation were analyzed. We observed that protons were coordinated to their neighboring water molecules. The result suggested the proton transfer in such nafion polymer system belongs to Grotthuss and vehicle mechanisms.

1. Introduction

Proton-exchange membrane fuel cell (PEMFC) is a promising type for clean and efficient power generation in this century. The polymer membrane is a key component of fuel cell systems that separates the fuel and the oxidants and transports protons from the anode side to the cathode side[1].Many studies of such systems were focused on the proton conductivity and its dependence on temperature and humidity. J. Benzigr et al. [2] found the rate of limiting water self-diffusivity increases exponentially at water content λ =1~ 4. Urata et al. [3] theoretically modeled such system of hydrated Nafion at λ = 2.8, 5.9,13.3 and 35.4. They concluded that the sulfonic groups are the only sits of the polymer to which water molecules bind in the pendant chain. Jang et al.[4] used MD simulation to investigate hydrated Nafion at λ = 16. The result showed n water transport depending on the structure of Nafion chain. Lei Chen et al. [5] carried out MD calculation for Nafion 117 Membrane with different water content at 300K and 353K. They found that, at the same temperature, the diffusion coefficients of both water molecules and hydroniums increase with the water content. In spite of these valuable experimental and theoretical studies, the detailed mechanism of proton transport in hydrated nafion is still unclear. Literature suggested mechanisms for proton transport including vehicular and Grotthuss. However, these mechanisms are still not verified.

2. Method

In the present study, Molecular Dynamics simulation with NVT ensemble was carried out. The time step was set at 1.0 fs and the system temperature was 298K. In order to construct a reasonable simulated system, the gradually-reduce-box (GRB) method was applied[6]. The initial cell size dimensions were 100Å×100Å×100Å and the corresponding density was 0.1g/cm^3, which is much smaller than the experimental value of Nafion membranes. The large space allows molecules to move freely and have very weak inter-molecular interactions. This membrane consists of a copolymer of fluorocarbon (CF_2) and sulfonic acid (SO_3). The number of water molecules is determined by the water content λ , which is defined as

$$\lambda = \frac{N_{water}}{N_{sulfur}} \qquad (1)$$

Where N_{water} is the number of water molecules and N_{sulfer} is the number of sulfonate groups in the Nafion chain. In this study, the membrane water content parameter was set at λ=4.

To analyze the inter-molecular distance, the radial distribution functions (RDF) between molecules were calculated. An RDF is defined as a measure of the probability of finding an atom B at a distance r from a reference atom A, which can be calculated as

$$g_{A-B}(r) = \frac{n_B V}{N_B 4\pi r^2 dr} \qquad (2)$$

where n_B is the number of *B* particles situated at a distance r in a shell of thickness *dr* from particle *A*, and *B* and *V* are the total number of *B* particles and the total volume of the system, respectively[7].

3. Results and Discussion

Figure 1 shows RDF between hydronium ions and oxygen atom of sulfonate, the first peak appears at 5.8 Å. This indicates that the most probable distance between hydronium ion and sulfonate oxygen is 5.8 Å. Figure 2 shows RDF between hydronium ions and oxygen atom of water molecular. The first peak appears at 2.3 Å with very high peak value. Since 2.3 Å is within the range of hydrogen-bonding distance, therefore this indicates that hydronium ion was strongly coordinated to water oxygen due to hydrogen bonding. Figure 3 shows that RDF between oxygen atom of water and oxygen atoms of sulfonate. The first peak appears at 3.5 Å. It indicates that the closet distance between sulfonate and water molecule is approximately 3.5 Å. The positions of first peaks in pair correlation functions are given in Table 1. The RDF analysis showed that the hydronium ion was bonded to the oxygen of water molecule but not oxygen at sulfonate group. Therefore the mechanism of proton transport in this system corresponds to the reported vehicle mechanism. Since the hydronium ion was away from the sulfonate group, therefore the guessed jumping mechanism in between sulfonate groups of nafion was not appeared here. Figure 4 shows the trajectories of distances for a selected proton to oxygen atoms of the neighboring waters. In the figure, we found that originally, the proton was closed to an oxygen atoms (marked by red and green). As time went, the red colored oxygen atom moved away and blue colored oxygen came close to the proton. In the end, the proton was only close to the blue colored oxygen. The figure indicates that the proton was solvated by these water molecules and the proton transport is similar to the proposed vehicular and Grotthuss mechanism.

4. Concluding Remarks

Molecular Dynamics simulation has been used to investigate the mechanism of proton transport in nafion fuel-cell membrane. The analysis of pair correlation functions shows that the water molecules surrounded protons and spaced out the sulfonic acid groups and protons. From the trajectories of protons, we showed that protons moving in cluster-network of nafion membrane. In addition, we found that the proton transport between water molecules was similar to the proposed vehicular and Grotthuss mechanism.

Acknowledgements

The study was partially supported by the Ministry of Science and Technology through Grants MOST 106-2221-E-012-003.

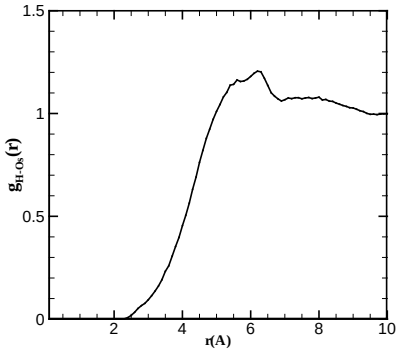

Figure1. RDF between proton and oxygen atoms of sulfonate

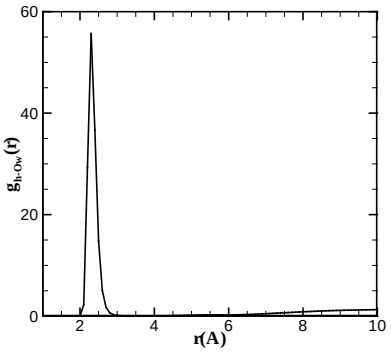

Figure 2. RDF between proton and oxygen atom of water molecule

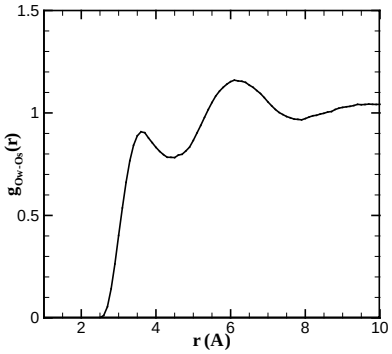

Figure 3. RDF between oxygen of water and sulfur atoms of sulfonate

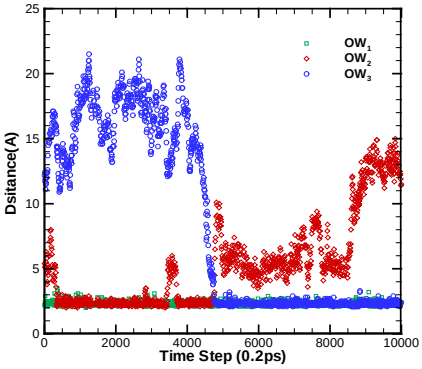

Figure 4. The trajectories of distances of a selected proton and oxygen atoms of neighboring water molecules.

Table 1.Distances of the first peaks in RDF's

RDF $g_{A-B}(r)$	First peak appearance distance
$g_{H-O_S}(r)$	5.8 Å
$g_{H-O_w}(r)$	2.3 Å
$g_{O_w-O_s}(r)$	3.5 Å

References

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五、建議事項：

本次研討會給我的感覺是學術交流與國際視野開拓的重要性。國際間，針對各種專業領域不乏會有知名學者。在交流的過程中，可從問答之間，感受高手過招之樂；亦可在私下討論時，了解每位學者間所關注的焦點，能使我們對整體研究趨勢有些了解，有助我們掌握新的研究方向。因此，教育部或科技部往後應盡量補助國內年輕學者或博士生，早日參與國際學術會議，開拓其國際視野並邁向國際；同時，也希望能多多補助支持國內大專院校，承辦一些大型國際會議，使無法獲得出國補助的學生及國內年輕老師，也能參與國際會議，增加與國外學者進行交流與見習的機會，亦可提升台灣在國際上的知名度。總結此次學術之旅，共可歸結出幾點重要結論與建議：

(1)每參與一次會議就有一次的體認與感觸，此次會議即已警覺近年來日韓等國一些科技研究多為先進技術的理論問題。這顯示了尖端技術的發展，還是要有透徹的理論基礎，這或許是我們國家必須反思的課題。

(2)不少論文乃頗有前瞻性的議題，例如光學的運用、電腦運算與理論模擬等研究；甚有參考價值。但範圍頗廣，個人收穫者有限，台灣近年來學界亦逐漸重視此領域，希望能夠及時追趕國際腳步，使台灣的資訊科技在國際上一直走在最前端。

(3)建議政府針對有潛力以及具未來性的研究議題能擇項支援，不但可嘉惠師生，又可領先世界。另日本政府補助當地教授級教師與會與國際研究學者的交流，可作為國內借境。

附錄一：活動照片

本人於 ICFD 研討會會場註冊

本人於研討會會場發表研究論文

附錄二：大會議程截錄

PRECISE **Wednesday, November 1, 2017**

		14:00-14:20 OS2-4 Radiative and Environmental Characteristics of Cylindrical Infrared Burners *A. Maznov, A. Kirdyashkin, S. Minaev*	13:30-13:50 OS10-3 Feasibility Study of Laser-propelled Launch Demonstration *K. Mori* 13:50-14:10 OS10-4 Development of High-Performance Multi-Rotor Drone *K. Tonezawa, H. Matzumoto, K. Sugiyama, H. Tokutake, Y. Tanabe, S. Sunada* 14:10-14:30 OS10-5 Transient Flight Aerodynamic Parameters Estimation of Quadrotor Helicopter *N. D. Hung, Y. Liu, K. Mori*	13:40-14:00 OS19-3 Direct Observation of Reaction Distribution in a Porous Composite Positive Electrode for Li Ion Batteries by Using Two-Dimensional X-ray Absorption Spectroscopy *Y. Kimura, K. Chiba, T. Watanabe, T. Nakamura, K. Amezawa, H. Tanida, Y. Uchimoto, Z. Ogumi* 14:00-14:20 OS19-4 Location Related Variability of Permeability Characteristics in Cancellous Bone *M. Ito, S. Tupin, H. Anzai, A. Suzuki, M. Ohta*			13:50-14:10 OS16-2 A Signal Separation Method for Hybrid PECT/EMAT Nondestructive Testing Method Based on Wavelet Analysis *S. Xie, M. Tian, Z. Chen, T. Uchimoto, T. Takagi* 14:10-14:30 OS16-3 Coupled Computing of Hydrogen Leakage with Crack Propagation Using Hybrid Particle and Euler Method *J. Ishimoto, T. Sato, A. Combescure*	13:53-14:06 OS13-4 Design and Balance of a Membrane Dehumidification System *S.-M. Li, C.-C. Wang* 14:06-14:19 OS13-5 The Experimental Analysis of Heat Transfer Enhancement Techniques by Combining Electrostatic Vibration and Corona Wind *T.-K. Wei, H.-H. Chin, Y.-X. Huang, Y.-Y. Tsui, C.-C. Wang* 14:19-14:32 OS13-6 The Transient Analysis of Two-Phase Flow in a Parallel Rectangular Channel under Vibration Conditions *Y.-H. Chang, S.-W. Chen, M.-L. Chat, H.-J. Lin, J.-D. Lee, J.-R. Wang, C. Shih*
14:30	BREAK							14:30
14:40	Exhibition Bldg. MEETING ROOM 1	Exhibition Bldg. MEETING ROOM 2	Exhibition Bldg. MEETING ROOM 3	Exhibition Bldg. MEETING ROOM 4-B	Conference Bldg. MEETING ROOM 1	Conference Bldg. MEETING ROOM 2	Conference Bldg. TACHIBANA	Conference Bldg. SHIRAKASHI 2	14:40
	OS17:The 13th International Students / Young Birds Seminar on Multi-scale Flow Dynamics	**OS7: The 19th International Symposium on Innovative Energy Research II** **International Workshop on Combustion Technology and Fundamentals** OSII-2 *Chair: H. Im*	**OS9: New Dimensions of Magnetic Suspension and Balance System** *Chair: K. Asai*	**OS19: Porous Media** Gas Transport *Chairs: S. Togaraj & A. Suzuki*	**GS1: General Session** Heat Transfer *Chair: J. Okajima*	**OS14: Vortex Motion: Stability, Nonlinear Dynamics, and Turbulence** Vortex Dynamics *Chair: Y. Fukumoto*	**OS16: Fourth International Symposium on Smart Layered Materials and Structures for Energy Saving** Composite *Chair: F. Kajima*	**OS13: Complex Thermofluid System** Complex Fluids *Chair: H.-Y. Wang*	
	13:30- (15:00) OS17-1 - OS17-25 *Short Oral Presentation* (15:00- 16:30) OS17-1 - OS17-25 *Poster Presentation*	14:40-15:00 OS2-5 Dual Effect of Potassium-Containing Compounds on Combustion Processes *V. I. Babushok* 15:00-15:20 OS2-6 Application of Molecular Beam Mass Spectrometry for Studying Laminar Premixed Burner-Stabilized Flames at 1-5 atm *D. Knyazkov, A. Dmitriev, T. Bolshova, V. Shvartzberg, K. Ozipova, A. Shmakov, O. Korobeinichev*	14:40-15:20 OS9-1 *Invited* Unsteady Aerodynamics Simulation for Automobile in Real World Conditions *M. Tsubokura, T. Nakashima* 15:20-15:40 OS9-2 Improvements of 1 m Magnetic Suspension and Balance System for Wind Tunnel Tests at High Angles of Attack *H. Senda, H. Sawada, H. Okuizumi, Y. Konishi, S. Obayashi*	14:40-15:00 OS19-5 Numerical Study on Gas Flow in Micro-/Nanoscale Porous Media by Direct Simulation Monte Carlo Method *Y. Kawaguc, S. Tonemura* 15:00-15:20 OS19-6 Construction of Theoretical Expression for Gas Transport in Micro-/Nanoscale Porous Media *Y. Kawaguc, S. Tonemura*	14:40-15:00 GS1-4 Advanced Exergy Analysis of Waste Heat Powered Combined Power Generation and Refrigeration System *A. Ustaoglu, M. Alptekin* 15:00-15:20 GS1-5 Effect of Laser Annealing on Pencil Drown Paper *Y. Motoizumi, H. Ito, C. Kato, S. Tanaka, T. Rachi, K. Satoh, R. Sudo, S. Tazuhara, M. Can, S. Shawuti, T. Tokumasu, S. Kaneko*	14:40-15:20 OS14-4 *Invited* Helicity-Enhanced Extreme Vortex States and the Hydrodynamic Blow-Up Problem *D. Tun, R. Protaz* 15:20-15:40 OS14-5 One-dimensional Hydrodynamic PDE Model for Turbulence with Cascade and Singular Solutions *T. Matzumoto, T. Sakajo*	14:40-15:00 OS16-4 Interlaminar Electrical Resistance and its Influence on Eddy Currents in CFRP Composites *X. Xu, H. Ji, J. Qiu, T. Takagi* 15:00-15:20 OS16-5 Advanced Maintenance Technique on CFRP - Eddy Current Testing and Functionalization in Mechanical/electromagnetic Properties - *H. Kosukegawa, T. Uchimoto, T. Takagi, G. Dobmann*	14:40-15:00 OS13-7 *Invited* Electrical Conductivity of Nanofluids - Theory and Experiment *U. Lei, L.-P. Xu* 15:00-15:20 OS13-8 *Invited* Liquid Crystal Measurement of Heat Transfer in a Rotating Cooling Channel with Partial Pin-fins *C.-C. Wang, S.-C. Huang, Y.-H. Liu* 15:20-15:33 OS13-9 Numerical Study to Investigate Proton Transport in Proton Exchange Membrane Fuel Cell *C. C. Tai, C. L. Chen*	