Date: Tue, 17 Nov 2009 13:40:20 -0500
To: Kerry Rowe <rowek@queensu.ca>
From: Mort Shirkhanzadeh <shirkhan@queensu.ca>
Subject: Allegations of scientific misconduct - Re: Solute mass diffusion coefficient: Comparison of microgravity experiments with molecular dynamic simulation and Enskog hard sphere corrected estimates [Scott and Smith, J. Appl. Phys. 104, 043706 (2008)].
Cc: Marie.Emond@nserc-crsng.gc.ca
Bcc: shirkhan@queensu.ca

Dear Dr. Rowe,

Re: Solute mass diffusion coefficient: Comparison of microgravity experiments with molecular dynamic simulation and Enskog hard sphere corrected estimates [Scott and Smith, J. Appl. Phys. 104, 043706 (2008)].

As shown below, there are a number of ethical problems with the above referenced paper (attached). The source of funding is not given in the paper. But the source is likely to be NSERC.

Erroneous Abstract:

The microgravity data used in the above article were obtained from the liquid diffusion experiments that were conducted on US shuttles in the early 1990s. The abstract of the article gives the false impression that the experiments were carried out in an"Earth orbiting space station laboratories" or a "space platform". The authors do not refer to the US shuttle experiments and have eliminated the primary source of data (Zhu's Ph.D. thesis, 1996, see attached page 73 of Zhu's thesis which gives the data) that describes the shuttle experiments. Thus, the readers are led to believe that the data presented by Scott and Smith are relatively new and different from those reported almost 11 years ago by Zhu and Smith in Adv. Space Res.22, 1253 (1998). It is true that Smith et al have performed experiments on a space platform (MIR space station) in the past, but the experimental data used in J. Appl. Phys. 104, 043706 (2008) are all coming from space shuttle experiments in 1990s and not from a space platform. The abstract of the paper by Scott and Smith is erroneous; an accurate account of the research performed has not been presented.

Erroneous Introduction:

In the introduction section of their paper, the authors give the impression that the experimental data were obtained using the Canadian Space Agency microgravity isolation mount (MIM) to reduce g-jitter effects. This is misleading; data reported by Scott and Smith in the referenced paper were obtained without using MIM. Nowhere in the article the authors explicitly refer to the fact that experiments were conducted onboard US shuttles and without using MIM. The introduction section is misleading; an accurate account of the research performed has not been presented in the introduction section.

Relevant Sources are eliminated:

The data presented by Scott and Smith in the referenced paper were compared in 1998 with the theoretical diffusion coefficient derived from Enskog hard sphere model and molecular dynamic calculation (Adv. Space Res.22, 1253 (1998)). Despite its similarity and relevance, the authors have eliminated this reference.This givies the impression that the data are new.

Erroneous Conclusions:

In the referenced paper (J. Appl. Phys. 104, 043706 (2008)), the authors conclude that the theoretical diffusion coefficients derived from molecular dynamic simulations are consistent with the experimental measurements. The authors suggest that the measured diffusion coefficients fit a linear relationship with a slope slightly greater than that predicted by the molecular dynamic simulations. This conclusion is erroneous since according to Smith and Smith et al (1-9) the experimental data in fact fit a non-linear relationship rather than a linear relationship. As claimed previously by Smith (5-9), experimentaldata fit the fluctuation theory ($D \sim T^2$) and this model is inconsistent with a linear model predicted by the molecular dynamics calculations. Furthermore, according to Smith and Smith et al (5-9), a linear dependence should only emerge if MIM is used to suppress the transient g-perturbations resulting from vibration of the space vehicle. Scott and Smith's data in J. Appl. Phys. 104, 043706 (2008) are coming from the shuttle experiments in 1990's without using MIM.

References:

1. X. Zhu and R.W. Smith " Diffusion in Liquid Pb-Au Binary System", Materials Science Forum 215-216, 113-118 (1996).

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6. R.W. Smith, "Results of Microgravity Experiments", Final Report. PW& GS File No. 9F007-4-6028/01-ST " Diffusion in Liquid"-QUELD Project 4-0028", Canadian Space Agency (2000).

7. R.W. Smith, X. Zhu, M.C. Tunnicliffe, T.J.N. Smith, L. Misener, and J. Admson, Ann. N.Y. Acad. Sci. 974:56-67 (2002).

8. R.A. Herring, W. M. B. Duval, R.W. Smith, K.S. Rezkellah, S. Varma, R.F. Redden, and B.V. Tryggvason, " Recent Measurements of Experiment Sensitivity to g-jitter and their Significance to ISS Facility Development", J. Jpn. Soc. Microgravity Appl., Vol.16, 234-244 (1999).

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Sincerely,

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