

Date: Mon, 26 Oct 2009 13:02:31 -0500

To: rowek@queensu.ca, Marie.Emond@nserc-crsng.qc.ca

From: Mort Shirkhanzadeh <shirkhan@queensu.ca>

Subject: Allegations of Academic Misconduct- Canadian Journal of Physics, 87: 933-944 (2009)- Scott and Smith (Funding Source: NSERC)

Bcc: shirkhan@queensu.ca

Dear Dr. Rowe,

Allegations of Academic Misconduct- Canadian Journal of Physics, 87: 933-944 (2009)- Scott and Smith (Funding Source: NSERC)

Background:

Throughout 2005, I raised serious concerns about a large number of papers authored by Smith and Smith et al dating back to 1996. Allegations included deceptive selective reporting of findings, omission of conflicting data, falsification and fabrication of data, bogus authorship, and intentional republication of numerous papers under different titles and under different authorship.

In all cases, allegations that were sent to your office and to NSERC were accompanied by significant documentations. Unfortunately in 2005, there was no transparent process for investigating the allegations in accordance with the Tri-Council Policy Statement. As a result, the investigation conducted by the university was superficial and incomplete and most allegations were left unanswered. In 2006, after receiving the university report, Council officials felt the university's "remedial action" was "rather minor in light of the many breaches of publication practices." Following a review by the CPSI, NSERC's integrity committee recommended the council reprimand the University for conducting an investigation that "was found to lack thoroughness."

There is now considerable evidence showing that the remedial action taken by the university in 2006 was ineffective in preventing the reoccurrence of academic misconduct. The university administration should take responsibility for the re-emergence of this problem. Below, I present you with the allegations of academic misconduct concerning a paper which has been very recently published in the Canadian Journal of Physics. Allegations concerning other papers published between 2006 -2009 will follow shortly after the funding source for each case is confirmed.

Canadian Journal of Physics, 87: 933-944 (2009)- Scott and Smith (Funding Source: NSERC)

There are a significant number of ethical problems with the experimental data presented in Can.J.Phys.87: 933-944 (2009) (attached). These problems undermine the validity of the conclusion presented in the paper. The conclusion of the paper is based on a set of experimental data that are fabricated. The conclusion of the paper misleads the scientific community.

Temperature values shown in Figs. 14 and 15 for samples processed in the MIR space station are not real measured values

Temperature values given in Figures 14 and 15 for samples processed in the MIR space station ("smith 1" data points) are not real measured values. Real measured temperatures were required for accurately calculating diffusion coefficients, but according to Smith (FINAL REPORT) (1) (attached) these temperatures could not be measured because of the problems associated with the thermocouples and mechanical failure during the space experiments. It is important to note that in the past, this "Final Report" has been used as a reference in a number of publications by Smith et al. The Final Report is included here in support of the allegations made in accordance with NSERC policy.

According to the Final Report, the astronaut that performed the experiments on MIR noted that a

large number of samples were not fully inserted into the furnace while they were being heated (see page 92). According to the Final Report, only 11 of the 37 samples were fully inserted into the furnace and so could be processed as desired (1). According to the Final Report, lead - gold samples processed on MIR in isolated mode (samples no. 1, 2, 3, 4, and 5 in Table VI-3, page 88) were among those samples that were only partially inserted into the furnace. The results obtained from sample # 2, 3, 4, and 5 are used in Figures 14 and 15 in the referenced paper. According to the Final Report, these samples did not experience the desired processing temperatures. According to the Final Report (page 92), it was hoped that the oxide film on the tubes would provide specific information about the furnace temperature, the treatment time, and the degree of container insertion into the furnace. According to the Final Report, the processing time and temperature for the above samples were deduced from the color of an oxide film that formed on the container tubes (page 94, 1st paragraph).

The subjective procedure that has been used to deduce the processing time and temperatures is not disclosed in Canadian Journal of Physics. An accurate account of the research performed is not presented. The scientific community has been led to believe that temperatures given in Can. J. Phys (Figures 14 and 15) are real temperatures of samples and were scientifically measured in the MIR space station. But, according to Smith in the Final Report, these temperatures are only “probable processing temperatures” (see Table VI-3, page 88) that were deduced by subjectively inspecting the samples tubes after the samples were returned to earth. What are the real processing temperatures that readers need to have in order to calculate the real diffusion coefficients (D) and to find the true relationship between D and T? According to Tri-Council Policy Statement, the councils hold researchers receiving council funds responsible for “using scholarly and scientific rigour and integrity in obtaining, recording and analyzing data, and in reporting and publishing results;”

In the Final Report, Smith states that the experimental results from lead-gold diffusion couples (sample # 1, 2,3, and 4) should be of “particular concern” (see the conclusions drawn on page 101). But this serious concern is not disclosed in the referenced paper.

Despite the fact that temperatures and diffusion coefficients could not be scientifically determined and despite the fact that the author himself has expressed concerns about the validity of his own experimental results in the report, the data presented in the referenced paper show a remarkably perfect linear relationship for these samples!

The reliability of the experimental data presented in Figs. 14 and 15 is in question. The conclusion of the paper that the theoretical models are in close agreement with the space results is erroneous. The theoretical models presented are only in close agreement with a set of experimental data that are fabricated. This matter needs to be appropriately redressed for the scientific community so that it can draw its own conclusion about reliability of the theoretical results.

Selective reporting of data in Figs 14 and 15

Conflicting data have been eliminated from figures 14 and 15. The omitted data are shown in Acta Astronautica 64, 256-263 (2009). When one includes the omitted data in the analysis, a non-linear relationship emerges. This problem is in addition to the problem discussed above and brings into question the overall integrity of the results and conclusions in the referenced paper.

Most relevant references are eliminated

One can also see that the most relevant references, including Acta Astronautica 64, 256-263 (2009), which sheds light on the omitted data and questions the reliability of the space results, are carefully excluded from the referenced paper.

In the introduction section, the authors claim that the diffusion results obtained in space by Smith remain the only g-jitter free results available for analysis. But the authors avoid stating that these results were in fact recently analyzed by Shirkhazadeh in Acta Astronautica 64, 256-263 (2009). It is clear that the referees that reviewed the paper needed this relevant reference during the review

process so that the paper could be objectively evaluated. The omission of the relevant reference in this case is an obvious violation of NRC publishing policy.

I have presented you with convincing evidence that the substance and conclusions of the published paper are erroneous. NSERC policy on integrity in research has been clearly violated.

An exact copy of this letter is sent to NSERC.

Please let me know if you have any question or if you need further supporting materials.

Sincerely,

M.Shirkhanzadeh

M.Shirkhanzadeh
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TEL: [\(613\) 533-2748](tel:6135332748)

Date: Mon, 09 Nov 2009 14:24:13 -0500

To: rowek@queensu.ca

From: Mort Shirkhanzadeh <shirkhan@queensu.ca>

Subject: Allegations of academic misconduct- The effects of buoyancy convection on measured solute diffusion coefficients in dilute metallic liquids"[J. Appl.Phys.96, 6213 (2004)]- Huang, Yang, and R.W.Smith.

Cc: Marie.Emond@nserc-crsng.gc.ca

Bcc: shirkhan@queensu.ca

Dear Dr. Rowe,

As shown below, there are significant ethical problems with this published paper (a copy of the paper is attached):

1. _____ An accurate account of the research performed has not been presented :

In the introduction section, the authors claim that "Queen's University Experiments in Liquid Diffusion (QUELDII) operated on MIR for more than two years and processed 121 diffusion samples". **An accurate and complete account of the research performed has not been presented.** According to Ref.#8 in the paper (R.W. Smith, Results of Microgravity Experiments-Final Report. PW&GS File No 9F007 -4- 6028-01-ST "Diffusion in Liquid"- QUELD project 4-0026 (2000)), "of samples prepared and shipped to MIR, only 63 provided data of sufficient quality to permit the derivation of accurate diffusion coefficients". a copy of

Ref. #8 is attached here.

2. Problems with the data shown in Table I:

As stated in the final report, the long capillary diffusion couples processed on the MIR space station encountered some difficulties due to the malfunction of the QUELD II furnace that made it impossible to accurately measure the processing times and temperatures. According to the final report, the astronaut performing the experiments on MIR noted that a large number of samples were not fully inserted into the furnace while they were being heated. Apparently, one of the sample's mounting arms became bent and "the tube containing the sample was entering the furnace at an angle and were catching on the furnace walls". As shown in Table VI-3 of the report (page 88) (attached), all samples used in Table I of J. Appl.Phys.96, 6213 (2004) were partially inserted into the furnace (see sample # 1-5 in Table VI-3) and, therefore, did not experience the desired processing times and temperatures. According to the final report, the experimental results from lead-gold diffusion couples "should be of particular concern". But this concern was not disclosed in J. Appl.Phys.96, 6213 (2004). In the final report, it is stated that" it was hoped that the oxide film on the tubes would provide specific information about the furnace temperature, the treatment time, and the degree of container insertion into the furnace". The processing time and temperatures were deduced by visually examining an oxide film that formed on the sample containers. In Table VI-3 of the report, only the "Probable Processing Temperatures" of samples are given. The arbitrary procedure that was employed for deducing time and temperature has not been described in J. Appl.Phys.96, 6213 (2004) or in any other paper. Temperatures presented in Table I and Table II of J. Appl.Phys.96, 6213 (2004) are in fact the altered version of the " probable processing temperatures" reported in Table VI-3 and those given in Microgravity Sci. Technol. XI (2) 78-84 (1998). It is difficult to understand how the temperatures shown in Table I could be determined from the " probable processing temperatures".

3. Selective reporting of data in Table I and II:

The authors have eliminated the conflicting data from Table I and II. This problem is discussed in detail in Acta Astronautica 48, 59-70 (2001). If the eliminated data are added to Table I and II, it will cast doubt on the reliability of the conclusions that were drawn based on the few selected data.

4. Astronauts onboard MIR did not run the microgravity experiments reported in Table II.

Diffusion coefficients that are reported in Table II are questionable. Data reported correspond to samples # 61, 62,63, 64, and 65. New documents from the Canadian Space Agency (CSA) confirm that crewmembers onboard MIR did not do these experiments under isolation condition. The conclusions drawn based on these results are erroneous.

5. Radial temperature gradients given in Fig.7 are not calculated. They appear to be hand drawn without using any data:

Despite the impression given in the paper, the authors present no evidence to support the claim that the radial temperature gradients given in Fig.7 of the paper were derived from a numerical model. It is seen in Fig.7 that while temperatures are given to the second decimal place, the radial temperature profiles appear to be hand-drawn without using any numerical model or calculation. Similarly, no evidence is given to support the claim that the temperature variations shown in Fig.5 and Fig.6 are derived from a numerical model. In fact, Fig. 6 appears to be basically the same as Fig.5 except that the temperature variations are given in a graphical form.

Sincerely,

M.Shirkhazadeh

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Date: Mon, 09 Nov 2009 15:01:37 -0500

To: rowek@queensu.ca

From: Mort Shirkhanzadeh <shirkhan@queensu.ca>

Subject: Allegations of academic misconduct- [J. Appl.Phys.102, 086103 (2007)- Author: R.W.Smith.

Cc: Marie.Emond@nserc-crsng.gc.ca

Dear Vice-Principal Rowe,

The affiliation given in the referenced paper is false and misleading. There is no "Materials Science and Microgravity Applications Group" recognized by Queen's University.

In the referenced paper, the single author (R.W.Smith) states: " In conclusion we reject the assertion of correspondent that results are seriously contaminated....."

In reality the paper is written by a single author (R.W. Smith) and the conclusion in the paper is not the view of a group of researchers at Queen's university. The single author is trying to gain credibility for his view by faking a Group name that is not recognized by the university.

The idea that Queen's University has an official research Group rejecting my findings published in JAP conveys a significant misrepresentation. The false affiliation should be corrected.

Sincerely,

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Date: Thu, 12 Nov 2009 12:23:47 -0500

To: rowek@queensu.ca

From: Mort Shirkhazadeh <shirkhan@queensu.ca>

Subject: Allegation of academic misconduct- " The Vibration Environment on the International Space Station: Its Significance to Fluid-Based Experiments", Acta Astronautica 48, 59-70 (2001). Smith et al.

Cc: Marie.Emond@nserc-crsng.gc.ca

Bcc: shirkhan@queensu.ca

Dear Dr. Rowe,

There are a significant number of data points in Fig.7 of this paper that are fabricated. The data points representing "3 mm dia. specimens" (QUELD II, MIM isolating) in Fig.7 do not correspond to any diffusion couples assembled and tested by Queen's University.

A list of the samples assembled and tested by Queen's University is given on page 80- 85 of a final report that was submitted to the Canadian Space Agency (CSA) in 2000 (attached). The list gives the sample number, date of delivery to NASA, type of diffusion couple, and the MIM mode for each sample delivered to NASA. The '3mm dia. specimens (MIM isolating)' have not been delivered to NASA for testing on MIR. Documents obtained through access to information act show various samples being tested on MIR but there is no information about "3 mm dia. specimens" (QUELD II, MIM isolating). Furthermore, CSA is unable to find the sample numbers or the date of delivery to NASA for these specimens. The fabricated data in Fig.7 of Acta Astronautica 48, 59-70 (2001) are misleading to the microgravity community. The fabricated data are also relevant to research and publications funded by NSERC.

In addition, the data points labeled "QUELDI & QUESTS (MIM not isolating)" in Fig. 7 of the above article are all altered version of the data presented on p. 73 by Zhu in his Ph.D. thesis (X. Zhu, " Diffusion in Liquid Binary alloys", Ph.D. Thesis, Queen's University, Canada, 1996). Using statistical analyses, Zhu concluded in 1996 that the measured diffusion coefficients derived from space experiments fit the Arrhenius law ($D \sim \exp. (A/T)$). In Acta Astronautica 48, 59-70 (2001), however, Zhu's original temperatures have been altered to obtain a non-linear relationship that fits the fluctuation theory ($D \sim T^2$). No reference is given to Zhu's original work. The measured temperatures have been changed in such a way that the relationship between D and T changed from a $D \sim \exp. (A/T)$ to a $D \sim T^2$.

The original data reported by Zhu in his thesis were based on two sets of space experiments that were sponsored by the Canadian Space Agency (CSA). These experiments were QUEST (Queen's University Experiments in Space Transportation Systems) and QUELD (Queen's University Experiments in Liquid Diffusion). The QUELD experiments were performed on the U.S. Space Shuttle Columbia mission STS-52, CANEX-2 in October 1992. According to Zhu, all diffusion experiments in mission STS-52 were performed manually by the Canadian Payload Specialist Dr. Steve MacLean. Dr. MacLean is now the president of the Canadian Space Agency. The results of the diffusion experiments performed by Dr. Steve MacLean in 1992 onboard the Space Shuttle Columbia, mission STS-52 is misrepresented in Acta Astronautica 48, 59-70 (2001).

Sincerely,

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Date: Mon, 16 Nov 2009 13:47:18 -0500

To: rowek@queensu.ca

From: Mort Shirkhazadeh <shirkhan@queensu.ca>

Subject: Fwd: Affiliation misrepresentation/ Bing-Jian Yang et al 2003 J. Phys.: Condens. Matter 15 3855-3865

Cc: Marie.Emond@nserc-crsng.gc.ca

Bcc: shirkhan@queensu.ca

Dear Dr. Rowe,

Allegation of scientific misconduct

Numerical modelling of transport in a liquid diffusion couple shear cell

Bing-Jian Yang et al 2003 J. Phys.: Condens. Matter 15 3855-3865

Materials Science and Microgravity Applications Group, Nicol Hall, Queen's University, Kingston, ON, K7L 3N6, Canada

The authors' affiliation in the above referenced paper is erroneous. "Materials Science and Microgravity Application Group" is not among the entities recognized by Queen's University. The misleading affiliation needs to be corrected. A more realistic affiliation for authors is given in the duplicated papers that were published around 2003-2004. These papers are attached.

Sincerely,

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3 Attachments

Date: Tue, 17 Nov 2009 13:40:20 -0500
To: Kerry Rowe <rowek@queensu.ca>
From: Mort ShirkHzadeh <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-crsnq.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 gives 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), experimental data 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).
2. X. Zhu, M. Kaya, and R.W. Smith, pp. 1-4, 7th International Symposium on Experimental Methods for Microgravity Materials Science, Edited by R. A. Schiffman (1995).
3. X. Zhu and R.W. Smith, Adv. Space Res., 22, 1253 (1998).
4. X. Zhu, " Diffusion in Liquid Binary Alloys", Ph.D. Thesis, Queen's University, Canada (1996).
5. R.W. Smith, " The influence of g-jitter on liquid diffusion- the QEULD/MIM/MIR Programme" Microgravity Sci. Technol. XI (2) 78-84 (1998).
6. R.W. Smith, "Results of Microgravity Experiments", Final Report. PW& GS File No. 9F007-4- 6028/01-ST " Diffusion in Liquid"-QEULD 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. Rezkallah, 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).
9. B.V. Tryggvason, R.F. Redden, R.A. Herring, W.M.B. Duval, R.W. Smith, K.S. Rezkallah and S.Varma, " The Vibration Environment on the International Space Station: Its Significance to Fluid-Based Experiments", Acta Astronautica 48, 59-70 (2001).

Sincerely,

M.Shirkhanzadeh

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2 Attachments

Date: Sat, 12 Dec 2009 15:16:45 -0500
To: Kerry Rowe <rowek@queensu.ca>
From: Mort Shirkhanzadeh <shirkhan@queensu.ca>
Subject: Allegations of data fabrication / J. Appl. Phys. (2004) 6213-6219
Cc: Marie.Emond@nserc-crsng.gc.ca
Bcc: shirkhan@queensu.ca

Dear Dr. Rowe,

Allegations of data fabrication against Dr. Smith and his co-authors were brought to your attention in my letter dated March 22, 2005 (attached) but these allegations were not investigated.

According to records, the scope of the investigation undertaken by the external expert in 2005 was only limited to data falsification. The external expert did not consider "other allegations of academic misconduct or questions concerning the scientific results and the analyses." This is confirmed by the external expert's statement in the investigation records.

According to your letter of December 22, 2005, Dr. McLatchie was selected to receive all of material, including responses from the external expert and render a final opinion on the file.

Dr. McLatchie's overall assessment in 2005 was as follows:

1. No evidence of data falsification
2. No evidence of plagiarism
3. Copyright agreements may not have been observed.

It is clear that Dr. McLatchie's assessment does not exclude the possibility of data fabrication.

The records also show that the allegations that I brought forward in 2005 were not accurately presented in the report. My allegations were presented as (a) data falsification, (b) plagiarism, and (c) republication of earlier work. The more serious allegations including data fabrication were completely eliminated from the list and, therefore, were not investigated. I should also note that both the external expert and Dr. McLatchie were selected with the approval of Dr. Smith. Furthermore, Dr. McLatchie had a clear conflict of interest in this case that should have been declared in the report.

According to the Tri-Council Policy Statement, "It is the responsibility of the institution to investigate all possible instances of misconduct in research and scholarship". In the present case, the allegations of data fabrication that I brought to your attention in 2005 were not investigated and the university did not determine whether or not a breach of integrity took place. It is clear that in this case, the University is in non-compliance with the Agency policy. The criteria for compliance are determined "by the responsibilities described in the *Tri-Council Policy Statement: Integrity in Research and Scholarship*."

Now that the case of non-compliance has been discovered, I am sending the original allegations of data fabrication with the request that the allegations be investigated in accordance with Tri-Council Policy Statement.

Please note that as I stated in my letter of March 22, 2005, the data used to generate the temperature plots in Fig. 7 (a), 7(b), and 7(c)) are all fabricated. Contrary to the author's claim in the paper, it is not possible to generate the temperature profiles from the results shown in Fig. 5 and Fig.6 of the referenced paper. These plots have been hand drawn without using any real data (like the temperature profiles shown in Fig.1).

The data used to plot the temperature profile in Fig.6 are also fabricated. It is not possible to calculate the data points for this graph from the heat input ($Q = 9230 \text{ W/m}^2$) and the temperature difference between the two ends of the sample. The temperature profile presented in Figs. 6 is hand drawn like the temperature profiles shown in Fig.1. Data presented in Fig.6 are fabricated.

Sincerely,

M.Shirkhanzadeh

Date: Mon, 04 Jan 2010 10:08:53 -0500
To: Kerry Rowe <rowek@queensu.ca>
From: Mort Shirkhanzadeh <shirkhan@queensu.ca>
Subject: Allegation of Data Fabrication and Deceptive Data Selection
Cc: Marie.Emond@nserc-crsng.gc.ca
Bcc: shirkhan@queensu.ca

Dera Dr. Rowe,

Re: Allegation of Data Fabrication and Deceptive Data Selection
Solute Diffusion in Nonionic Liquids Effects of Gravity,
Reginald W. Smith, Paul J. Scott, and Barbara Szpunar
Ann. N.Y. Acad. Sci. 1161: 526–536 (2009) (Research supported by NSERC)

There are a significant number of ethical problems with the experimental data presented in this recently published paper by Smith et al (a copy of the paper is attached). These problems undermine the validity of the conclusions presented in the paper. The conclusion of the paper is based on a set of experimental data that are fabricated. The research appears to be funded by NSERC.

Temperature values shown in Fig. 1 for the lead - gold samples processed in the MIR space station under isolated mode are not real measured values

Temperature values given in Figure 1 for samples processed under isolation mode in the MIR space station are fabricated. Real measured temperatures were required for accurately calculating diffusion coefficients, but according to Smith (FINAL REPORT) (attached), these temperatures could not be measured due to the problems associated with the thermocouples and mechanical failure during the space experiments.

According to the Final Report by Smith, the astronaut that performed the experiments on MIR noted that a large number of samples were not fully inserted into the furnace while they were being heated (see page 92). According to the Final Report, only 11 of the 37 samples were fully inserted into the furnace and so could be processed as desired. According to the Final Report, lead - gold samples processed on MIR in isolated mode (samples no. 1, 2, 3, 4, and 5 in Table VI-3, page 88) were among those samples that were only partially inserted into the furnace. The results obtained from sample # 2, 3, 4, and 5 are used in Figure 1 in the published paper (Ann. N.Y. Acad. Sci. 1161: 526–536 (2009)). According to the Final Report, these samples did not experience the desired processing temperatures. According to the Final Report (page 92), it was hoped that the oxide film on the tubes would provide specific information about the furnace temperature, the treatment time, and the degree of container insertion into the furnace. How was it possible to scientifically find these three parameters from the color of an oxide film?

The subjective procedure that was used to deduce the processing time and temperatures is not disclosed in the published paper (Ann. N.Y. Acad. Sci. 1161: 526–536 (2009)). An accurate account of the research performed is not presented. The scientific community has been led to believe that temperatures given in the published paper are real temperatures of samples and were scientifically measured in the MIR space station. But, according to Smith, these temperatures are only “probable processing temperatures” (see Table VI-3, page 88) that were deduced by subjectively inspecting the samples tubes after the samples were returned to earth. What are the real processing temperatures that readers need to have in order to calculate the real diffusion coefficients (D) and to find the true relationship between D and T?

In the Final Report , Smith states that the experimental results from lead-gold diffusion couples (sample # 1, 2,3, and 4) should be of “particular concern” (see the conclusions drawn on page 101). But this serious concern is not disclosed in the published paper ((Ann. N.Y. Acad. Sci. 1161: 526–536 (2009)). In fact, this concern is not disclosed in any papers or thesis (supervised by Dr.Smith) that are available to the scientific community.

Despite the fact that temperatures and diffusion coefficients could not be scientifically determined and despite the fact that the author himself has expressed concerns about the validity of his own experimental results in the Final Report, the data presented in Fig.1 of the published paper show a remarkably perfect linear relationship for these samples! The conclusion of the paper that the theoretical models are in close agreement with the space results is erroneous. The theoretical models presented are only in close agreement with a set of experimental data that are fabricated.

Selective reporting of data in Figs 1 and 2

Conflicting data have been eliminated from figures 1 and 2 in order to claim a linear relationship between D and T. As I have discussed in Acta Astronautica 64, 256-263 (2009), when one includes the omitted data in the analysis, a non-linear relationship emerges that undermines the conclusions.

The supporting document needed to investigate this allegation is Acta Astronautica 64, 256-263 (2009) (attached) and all relevant references given in that paper, including the Final Report on the Queen's University Experiments in Liquid Diffusion (QUELD) that was submitted to the Canadian Space Agency (CSA) (attached) and the Master thesis by Josee Robert that was sent to you before. The problem of selective reporting of data is in addition to the problem discussed in the previous section and brings into question the overall integrity of the results and conclusions the published paper.

Copyrights issue: The results shown in Fig.8 of the published paper (Ann. N.Y. Acad. Sci. 1161: 526–536 (2009)) are not Smith's results. These results come from “Hildebrand, J.L. , Viscosity and Diffusivity (1977), John Wiley & Sons. New York”. One would think that permission for republication of these results should be obtained from the real author (Hildebrand) and the publisher (John Wiley & Sons, New York), and not from Smith et al (1)! Furthermore, reference 1 (Smith et al) has been officially retracted from the Annals of New York Academy of Sciences. The results shown in Fig. 10 also are not Smith's results. One would expect that permission should be obtained from the real author(s) to republish these results.

I expect a thorough investigation of these allegations. Please let me know if you need any other supporting documents.

Sincerely,

M. Shirkhanzadeh

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Date: Mon, 04 Jan 2010 11:45:01 -0500
To: Kerry Rowe <rowek@queensu.ca>
From: Mort Shirkhanzadeh <shirkhan@queensu.ca>
Subject: Allegation of data fabrication and deceptive data selection- Josee Robert, MSc. Thesis (Queen's University) (1999).
Cc: Marie.Emond@nserc-crsng.gc.ca
Bcc: shirkhan@queensu.ca

Dear Dr. Rowe,

Re: Allegation of data fabrication and deceptive data selection -
Josee Robert, MSc. Thesis (Queen's University) (1999) (ATTACHED)

The research described in this thesis appears to be funded by NSERC. There are a significant number of ethical problems with the experimental data presented in the thesis. These problems undermine the validity of the conclusions. The conclusions of the thesis based on a set of experimental data that are fabricated.

Temperature values shown in Fig. 14 (page 41) for the lead - gold samples processed under isolated mode are not real measured values

Temperature values given in Figure 14 for the samples processed under isolation mode are fabricated. Real measured temperatures were required for accurately calculating diffusion coefficients, but according to Smith (FINAL REPORT), these temperatures could not be measured due to the problems associated with the thermocouples and mechanical failure during the space experiments. A copy of the Final Report was sent to you earlier.

According to the Final Report by Smith, the astronaut that performed the experiments on MIR noted that a large number of samples were not fully inserted into the furnace while they were being heated (see page 92 of the report). According to the Final Report, only 11 of the 37 samples were fully inserted into the furnace and so could be processed as desired. According to the Final Report, lead - gold samples processed on MIR in isolated mode (samples no. 1, 2, 3, 4, and 5 in Table VI-3, page 88) were among those samples that were only partially inserted into the furnace. The results obtained from sample # 2, 3, 4, and 5 are used in Figure 14 in the thesis. According to the Final Report, these samples did not experience the desired processing temperatures. According to the Final Report (page 92), it was hoped that the oxide film on the tubes would provide specific information about the furnace temperature, the treatment time, and the degree of container insertion into the furnace.

The subjective procedure that was used to deduce the processing time and temperatures is not disclosed in the thesis. An accurate account of the research performed is not presented. The

scientific community has been led to believe that temperatures given in the thesis are real temperatures of samples and were scientifically measured in the MIR space station. But, according to Smith, these temperatures are only “probable processing temperatures” (see Table VI-3, page 88 (Final Report)) that were deduced by visually inspecting the samples tubes after the samples were returned to earth. What are the real processing temperatures that readers need to have in order to calculate the real diffusion coefficients (D) and to find the true relationship between D and T?

In the Final Report , Smith states that the experimental results from lead-gold diffusion couples (sample # 1, 2,3, and 4) should be of “particular concern” (see the conclusions drawn on page 101). But this serious concern is not disclosed by Josee Robert in the thesis.

Despite the fact that temperatures and diffusion coefficients could not be scientifically determined, the data presented in Fig. 14 of the thesis show a remarkably perfect linear relationship for these samples! Given the fact that serious problems were encountered during experiments, the precision in Fig.14 is unrealistic. The conclusion of the thesis that D varies linearly with T under isolation mode is erroneous. Furthermore, the author of thesis has eliminated her own data (sample # 67, Table IV-1, page 99) from Fig. 14 because it does not fall on the straight line. The conclusion of the thesis appears to be based on a set of experimental data that were made up to fall on a straight line.

In addition, conflicting data have also been eliminated from figure 15 (page 43) in the thesis. The omitted data are shown in Acta Astronautica 64, 256-263 (2009). When one includes the omitted data in the analysis, a non-linear relationship emerges that again seriously undermines the validity of the conclusion in the thesis. A more detailed description of the ethical problems in the thesis and in the relevant publications is given in Acta Astronautica 64, 256-263 (2009) which is attached here. This paper and the references cited therein are relevant documents for investigating the allegations.

Please let me know if you need a copy of any other papers or documents.

Sincerely,

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Date: Mon, 04 Jan 2010 14:36:41 -0500
To: Kerry Rowe <rowek@queensu.ca>
From: Mort Shirkhanzadeh <shirkhan@queensu.ca>
Subject: Allegation of data fabrication- Scott and Smith (JPCM 21 (2009) 335104) (attached)
Cc: Marie.Emond@nserc-crsng.gc.ca
Bcc: shirkhan@queensu.ca

Dear Dr. Rowe

Re: Allegation of data fabrication- Scott and Smith (JPCM 21 (2009) 335104) (attached)

This very recent paper does not mention the name of the sponsor but it is likely that NSERC funding was involved. Your office probably can verify this.

Temperature values shown in Figs. 1 and 11 for samples processed in the MIR space station are not real measured values

Temperature values given in Figures 1 and 11 for samples processed in the MIR space station ("QUELD-II MIM" data points) are not real measured values. These data are coming from Reference #1 in the paper which is now officially retracted. Real measured temperatures were required for accurately calculating diffusion coefficients that are reported, but according to Smith (FINAL REPORT) (1), these temperatures could not be measured because of the problems associated with the thermocouples and mechanical failure during the experiments in space. According to Smith (1), the astronaut that performed the experiments on MIR noted that a large number of samples were not fully inserted into the furnace while they were being heated (see page 92).

According to Smith, only 11 of the 37 samples were fully inserted into the furnace and so could be processed as desired (1). According to Smith (1), the lead - gold samples processed on MIR in isolated mode (samples no. 1, 2, 3, 4, and 5 in Table VI-3, page 88) were among those samples that were only partially inserted into the furnace. The results obtained from sample # 2, 3, 4, and 5 are used in Figures 1 and 11 in the JPCM paper. According to Smith (1), these samples did not experience the desired processing temperatures (1). According to Smith (1) (page 92), "it was hoped that the oxide film on the tubes would provide specific information about the furnace temperature, the treatment time, and the degree of container insertion into the furnace".

According to Smith (1), the processing time and temperature for the above samples were deduced from the color of an oxide film that formed on the container tubes! (See page 94, 1st paragraph). The subjective procedure that was used to deduce the processing time and temperatures is not disclosed in JPCM. How was it possible to scientifically figure out the processing temperature and time from the color of an oxide film that formed on the container tubes? The community has been led to believe that temperatures given in JPCM (Figures 1 and 11) are real temperatures of samples and were scientifically measured in the MIR space station. But, according to Smith (1), these temperatures are only "probable processing temperatures" (see Table VI-3, page 88) that

were deduced by subjectively inspecting the sample's tubes after the samples were returned to earth. What are the real processing temperatures that readers need to have in order to calculate the real diffusion coefficients (D) and to find the true relationship between D and T?

In the Final Report (1), Smith states that the experimental results from lead-gold diffusion couples (sample # 1, 2,3, and 4) "should be of particular concern" (see the conclusions drawn on page 101). But this serious concern that was expressed by the author himself in the report is not disclosed in JPCM . In the JPCM, the authors refer to the same results as "high quality microgravity capillary experiment results" (see last page of the JPCM paper). .

Despite the fact that temperatures and diffusion coefficients could not be scientifically determined and despite the fact that the author himself has expressed concerns about the validity of his own experimental results in the report, the data presented in JPCM show a remarkably perfect linear relationship for these samples! (see Fig.1, "QUELD-II MIM" data points). The experimental data are fabricated. The goal of the paper was "to seek an independent theoretical verification of the high quality experimental estimates of mass diffusion coefficient.....". But the theoretical models presented in the paper agree only with a set of experimental data that are made up. The credibility of the theoretical models is in question.

Selective reporting of data in Figs 1 and 11

Conflicting data have been eliminated from figures 1 and 11. When one includes the omitted data in the analysis, a non-linear relationship emerges. This problem is in addition to the problem discussed above and brings into question the overall integrity of the results and conclusions. See Acta Astronautica 64, 256-263 (2009) for details.

The most recent and most relevant references, including Acta Astronautica 64, 256-263 (2009), which sheds light on the omitted data and questions the reliability of the results, are carefully excluded from the JPCM paper . According to the IOP ethical policy, authors should strive to be unbiased in all aspects of their work. It is clear that the referees that reviewed the JPCM paper needed these relevant references during the review process to see the omitted data and to make an intelligent decision. The IOP ethical policy has been clearly breached.

Please let me know if you have any question or if you need further supporting materials.

Sincerely,

M. Shirkhazadeh

1. R.W. Smith, "Results of Microgravity Experiments-Final Report. PW&GS File No 9F007 -4-6028-01-ST "Diffusion in Liquid"- QUELD project 4-0026 (2000) (attached).

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