Reply to "Comment on 'A Critique of Some Recent Suggestions to Correct the Kirkwood–Buff Integrals'"

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It is quite unfortunate that after so many exchanges of e-mails with the authors, trying to point out and explain to them their errors, I feel they still do not understand the meaning of the Kirkwood Buff integral (KBI).

This misunderstanding is also shared by those who have used the "correction" to the KBI as suggested by Matteoli.

Regarding the comments of Matteoli and Lepori, my paper contains all of the answers to these comments, but I would like to add the following points:

(1) My critique in my article is both relevant and well founded. I shall leave that to the scientific community to judge the merits of the critique.

(2) Most of their line of "defense" is latched on arguments of "not having meant this and that".

As I explained to them in writing and as a reply to the reviewer of my article, my criticism was not directed toward their thought, or on what they meant, but to what they actually published.

Their thoughts and intentions are irrelevant. What they wrote and published is flawed, logically, mathematically, and thermodynamically; sadly, it did cause a lot of damage to the field.

(3) As they admit in their comments, some relations are only approximate, not exact. However, in the original paper, they wrote them as exact equalities, not as approximate equalities.

(4) All of the experimental data that they presented are irrelevant to the criticism, which was aimed at the theory they published, not at the experimental data.

(5) They write "We have suggested to get rid of the volume difference..." when in fact they did not. Therefore, their claim is void.

(6) They say that some quantities are "much friendlier"; I do not know what that means.

I showed that their quantities have obscure meaning at best. Perhaps, they are friendly, but this should have been explained.

(7) Every student of Mathematics and Physics knows that in order to refute a theorem or a theory, it is sufficient to give one counterexample.

That is what I did in my paper (by the way, the second virial approximation becomes exact in the region of very low densities).

To prove a theorem, one example is not sufficient, and certainly not approximate examples.

(8) Finally, the authors conclude "the contested approach can therefore still be used". Of course, anyone is free to use the "corrected" quantities (to which they refer to as the contested approach). My critique is addressed to those who choose not to waste their time on meaningless quantities, and also to explain the correct interpretation of the KBI, which needs not be "corrected".

This is further explained in my recent monograph.[2]

References and Notes

(1) Matteoli, E.; Lepori, L. *J. Phys. Chem. B* **2007**, *111*, 3069.

(2) Ben-Naim, A. *Molecular Theory of Solutions*; Oxford University Press: Oxford, U.K., 2006.