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EDITORIAL

Concerns about images and rate laws

Gábor Lente[1]

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This issue of Reaction Kinetics, Mechanisms and Catalysis is not simply the first issue in 2024. This is the venue where the first ever editorial expression of concern is published in this journal [1]. In my 15 years as an associate editor and editor-in-chief, we have had a very small number of retractions, but no expressions of concern.

In this special case, it was the author of the original publication [2] who contacted the editorial office first saying that some images in the published paper were erroneous. Springer staff have analyzed the remarks and found that there were already two Pubpeer comments on possible image manipulation in this paper [3, 4]. The author provided new images from a current replication of the work, but including them as a correction is against the principles of scientific publishing because the inconsistences seem to have gone far beyond simply mixing up some images and the 'corrected' images, even by the admission of the author, did not exist at the time of publication. The Springer team first recommended the retraction of the paper.

However, as an editor, I had different views: a retraction makes the impression that the entire work is unreliable. The paper [2] is essentially about the synthesis of a solid and its use in a catalytic process. Neither of these two main points have anything to do with electron microscope images and have not been questioned by anyone. Would the article have been accepted without the images? For me, the answer is yes. Even if the authors are correct that the origin of the error is an honest data handling mistake, does this lower trust in their scientific integrity? For me, the answer is yes again. So I felt that an editorial expression of concern would be more appropriate in this case. Both the Springer staff and the authors have agreed to this.

My opinion was not formed in response to this special case. In fact, in my entire career as a scientific editor, I have nurtured reservations against the large number of electron microscope images used in this field of chemistry. It is true that my original training was in homogeneous reaction kinetics [5–7], so I am by no means an expert in heterogeneous processes, but still, the issue seems fundamental to me. The first thing I note is that imaging seems to be a routine part of solid characterization and

✉ Gábor Lente
reac@gamma.ttk.pte.hu

[1] Editorial Office, Reaction Kinetics, Mechanisms and Catalysis, Department of Physical Chemistry and Materials Science, University of Pécs, Pécs, Hungary

reviewers are bent on requiring it even if the images do not contribute anything to understanding. It is very rare that information obtained from an electron microscope image is directly correlated to catalytic usefulness. Images are sometimes used to determine particle sizes: in these cases, the particle size distribution is the primary information, which warrants a place for the image in the Supplementary Information, but maybe not in the main text of the article. Electron microscopes are pricy pieces of instrumentation and need substantial expertise to operate, but neither of these facts mean that the information they provide is valuable in every case.

But it becomes worse. Most of my work is on labile solution equilibria. There is one pivotal point that I frequently have to explain to chemist who are not familiar with these studies: this is the highly limited selection of experimental methods that give useful information on such reactions. For example, the use of chromatographic separation methods is usually out of question in a system that changes in response to external disturbance on a subsecond time scale. The reason why I explained this here is that recording electron microscope images is similar in an important way: it typically needs sample preparation under aggressive conditions. For example, noble metals are deposited on the surface in high vacuum to make it conductive. Why do a lot of experts still believe that this process leaves the surface unchanged? There are some works that consider this question [8], but I feel that this is a fundamental issue that would need to be addressed much better before anyone draws a conclusion form a scanning or transmission electron microscope image.

I would like to use this editorial to share some very similar reservations in a completely different field as well. These notes have not led to retractions or editorial expressions of concern, yet they have been constantly on my mind for the last 15 years of editing a scientific journal. This issue is the automatic use of the formulas obtained in chemical kinetics in photochemical processes. Even in this journal, describing heterogeneous photochemical processes by pseudo-first order (exponential) curves, is a very common practice [9–11]. No doubt, this has its origins in the fact that in non-photochemical kinetics, the use of the method of flooding typically leads to a first order rate equation [5–7, 12]. However, this is by no means true for processes induced by light: there light intensity, and the full form of Beer's law make the *a priori* description very different [13–17], the first order rate law does not have the same central role at all. One could make the argument that still, exponential curves fit the observations reasonably well in many cases. Yet, even if it is true, finding a detailed theoretical basis for this observations is long overdue.

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