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One of my favorite Chinese proverbs says: "Were I to await perfection, my book would never be finished". I find the comment of G. Lente strongly connected to this quote.

Any research field has several layers from where a project can be devised. In our realm of catalysis, we can study from the engineering of a reactor to the quantum dynamical reasons for the occurrence of a specific transition state.[1] In the middle, two fundamental layers appear: the measure of the TOF (the layer that Lente finds questionable) and the analysis of the rate law (the proposed substitute to the TOF). The rate law is clearly more informative, since it contains inside a function all the rate constants instead of just the TOF (which tells nothing of the elementary steps). But then, a thorough study of the mechanism is more informative than the rate law; exactly as the rate law intrinsically contains the TOF, the knowledge of the full mechanism intrinsically contains the rate law. And the calculation of the potential energy surface of the complete cycle contains, in principle, the reaction mechanism. This argument can continue ad infinitum. In the end, each research group is usually focused on a limited number of these layers, for if they were expecting to provide all of them "their book would never be finished".

In any case, the final objective in catalytic science is (quite obviously) to obtain an efficient catalyst; and probably the most important measure of efficiency is the TOF (even though the TON, the selectivity, and even the price of the catalyst are also quantities that must not be overlooked). It can be argued that the purpose of obtaining the rate law is nothing more than having a tool to calculate this TOF, so disregarding the use of this "bare number" means disregarding the reason to study the rate law in the first place. In his comment, Lente argues that "it is difficult to understand why the researcher should make a futile attempt to condense the information content of these measurements into a single physical quantity instead of reporting the rate law and the rate constants directly". The answer is simple: obtaining the rate law entails a lot of work and time that can also be exploited in other useful ways to improve a catalyst. Eventually, these improvements have to be evaluated by a standard measure and not by an equation, and why not use the TOF for this?

Another of my favorite quotes, this time from Einstein, says: "It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience". This passage is called "Einstein's razor", akin to the famous "Occam's razor". The comment by Lente appears to be driven by this quote, when saying "The Eyring equation should be used only for giving the temperature dependence of the rate constants of elementary reactions, but not directly for other kinetic quantities ... it cannot be used for combinations of rate constants or rates in its original form ... It is impossible to condense the information content of several pairs of physical quantities into a single pair".

This position is understandable when looking at the rate law from a rate constants perspective (the *k* representation), since the rate law is a complex equation formed by intermingled constants (the Michaelis–Menten model being the simplest example). However, when translating all these rate constants to energies through the transition state theory (obtaining the *E* representation), the rate law is simplified. From there, it can be seen that using an "Eyring-shaped" approximation actually makes sense.[2] This "energetic span approximation" does not require more "faith" than believing that there can be a rate-determining step (more than that, it corrects the rate-determining *step* concept in favor of the rate-determining *states*[3]).

Simply put, for simple catalytic cycles, it is certainly possible to condense the information content of several pairs of physical quantities into a single pair, as long as there is a determining intermediate and a determining transition state (usually a valid assumption).

Despite these disagreements, all this debate is by no means unproductive. One important point raised here is the lack of understanding between the groups that work in different layers of catalysis. Some researchers are, indeed, building bridges and forming a "coherent" field, with better communication among researchers.[4,5] For this, I am grateful to have received Lente's comment on the Viewpoint article.

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Notes

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