

Review of: "Reaction rate view on autocatalysis"

Jesús Ágreda¹

¹ Universidad Nacional de Colombia

Potential competing interests: The author(s) declared that no potential competing interests exist.

The work about autocatalysis presented in the manuscript is, as the author mention, not so commonly presented in the related literature. Now, some aspects can be improved as presented below:

In the introduction, the phrase:

"The modeling results demonstrated accelerated product formation when the product's initial concentration was non-zero and increased progressively. Consequently, the product served as a catalyst in the given reaction system, which was thus used to refine the definition of autocatalysis (and of autocatalyst)."

is disconnected from the previous idea and confused. A better redaction can improve the way that the ideas are presented.

Also, the phrase:

"Modeling was performed with the Chemical Reaction Engineering Module of the COMSOL Multiphysics package, version 5.6; the model of a batch reactor was used."

can be improved.

In results and discussion, figure 1 must be after the first mention in the text, not before. Same for table 1.

In the legend of figure 2:

"Figure 2. The product formation rate versus the product concentration calculated with the set Nr. 4 in Table 1. The arrow shows the course of time. Inset shows the concentration-time profile."

There is no inset.

The presentation from the point of view of the reaction rate complements the concentration point of view of Horváth.

However, the most general approach must be a set of values of rate constants where autocatalysis is possible (and evident at some time) because when concentrations or rates are considered, the evidence of autocatalysis always depends on the extent of reaction and the form of the concentration or reaction rates versus time (or concentration) will depend of that "extent." The latter means that depending on time (or concentration), and not only on reaction rate, the autocatalysis will be evident or not, in terms of increase or decrease of concentration or reaction rate. Instead, when considering the possibility of autocatalysis, no matter at what time (or concentration), the adequate set of rate constants will guarantee to observe autocatalysis in a complex mechanism (at some time or concentrations), where it is not easy to detect a couple of reactions that together produce autocatalysis behavior.