Review of: "Reaction rate view on autocatalysis"

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

I will not judge the novelty of this manuscript but will focus on whether concepts and data are processed correctly and described clearly.

Kinetics is of course very important for telling whether autocatalysis exists and whether it can be observed. The author correctly captures this point and tries to analyze the role of kinetic parameters in autocatalysis. However, there are some non-negligible problems in the manuscript.

First, the author states that "*It is noteworthy that, being proportional to the concentration of the product, the rate still fulfills the above textbook autocatalysis definition by Berry et al. which is thus seen to be insufficient.*" Berry et al.'s definition of autocatalysis is of course somehow problematic, because for an autocatalytic and elementary reaction 2A+B→3A, its reaction rate is k[A]^2[B], which is NOT proportional to the concentration of [A] but proportional to the square of [A], given that [B] is held constant. However, this does not mean that the statement made by the author is correct. For the first reaction step, the author states that the formation rate of C is $r_C = k_1(c_A^0 - c_C)(c_B^0 - c_C)$, and it is very clear that this rate is also the reaction rate of this step. Therefore, the reaction rate is NOT proportional to the concentration of the product, and therefore it does NOT match Berry et al.'s definition. It is the derivative of this reaction rate that takes a form of a linear function of the concentration of C; but that function's intercept with the vertical axis is not zero, so the derivative of the reaction rate still cannot be described as being proportional to the concentration of C.

Second, the way in which the author represents the rate of C production, the concentration of C, and time can be misleading. These simulations are run with the assumption that the reactor is closed, and that is why the relationship between the rate of C production and the concentration of C can be mapped as curves shown in the figures. However, many readers tend to interpret a curve as a representation of a function, so this manuscript runs into the risk that many readers may interpret those figure as representations of functions where the rate of C production is a dependent variable and the concentration of C is an independent variable. Such an interpretation is wrong, because the concentration of C shown in these figures (as the x-axis) is NOT an **independent variable** – once the rate constants and the initial concentrations of A and B are set, all x-coordinates on a figure are fixed. Therefore, if the author does want to make claims on how the concentration of a product of a reaction pathway affects the rate of that pathway, the appropriate practice had better be something like this: first, the y-axis represents rate of C production immediately after or within a short time interval after the reaction system starts to run, and the x-axis represent the concentration of C when the reaction starts (i.e., the initial concentration of C); second, the initial concentrations of A and B should be held constant for different initial concentrations of C; third, plot "the rate of C production immediately after or within a short interval after the reaction system starts to run" as a function of "the concentration of C when the reaction starts."

Third, the author seems to link a J-shape or S-shape concentration-versus-time curve to autocatalysis, which is implied by sentences like "*The increase of the rate (in the first half) is evident and can be accepted as a strong indicator of autocatalysis in the sense of a product accelerating, i.e. catalyzing, its formation.*" However, just as what was mentioned in the reference [3], "*Sometimes, this feature results in a characteristic sigmoidal concentration–time profile, though it is* ***neither necessary nor sufficient*** *to attribute a system as being autocatalytic, thus a sigmoidal concentration–time profile is just a possible but not a unique fingerprint of autocatalysis.*" A simple example is that if an autocatalytic reaction A+B→2A is started with a very high concentration of A and a very low concentration of B, the concentration-time curve is neither J-shape not S-shape but the reaction is nonetheless still autocatalytic. This is also why plotting "the concentration of C when the reaction starts" as an independent variable is important: we need to take a look at a wide range of initial concentrations of C to infer its effects on the reaction rate(s).

A minor issue is that chemical reactions are reversible in principle, so if the author could also discuss the cases where these reaction steps are reversible, the manuscript would be improved. However, this revision is not necessary and much less critical than the three big problems mentioned above.

If the manuscript is still in its current shape, I would not view it as appropriate for publication. The current manuscript should either be rejected or significantly revised.