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LETTER TO THE EDITOR

Comment on "identifiability of chemical reaction networks" by G. Craciun and C. Pantea

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Abstract An illustrative example is given in this comment for demonstrating that two different reaction networks with mass action kinetics may have the same differential equation description even if the source complexes are not the same in the reaction systems. This presents a possibility of a special case that was not taken into consideration in Theorem 4.4 in J Math Chem 44:244–259, 2008.

Keywords Chemical reaction networks · Mass action kinetics · Identifiability

The authors in the interesting article [1] examine the identifiability of chemical reaction networks with mass action kinetics. Valuable results are presented in the paper, in particular, necessary and sufficient condition is given for the unique identifiability of rate constants in reaction networks that is very easy to check. However, it seems that the authors did not take into consideration a special case in **Theorem 4.4**, when the monomials corresponding to certain source complexes are cancelled out in the differential equations of the reaction network. The definitions and notations used in this comment are the same as in [1].

In [1], two reaction networks are called *confoundable* "if they produce the same mass-action differential equations for some choice of the rate constants" Furthermore, **Theorem 4.4** says: *Under the mass-action kinetics assumption, two chemical reaction networks* $(\mathcal{S}, \mathcal{C}', \mathcal{R}')$ *and* $(\mathcal{S}, \mathcal{C}'', \mathcal{R}'')$ *are confoundable if and only if they have the same source complexes and* $Cone_{\mathcal{R}'}(y) \cap Cone_{\mathcal{R}''}(y)$ *is nonempty for every source complex* y.

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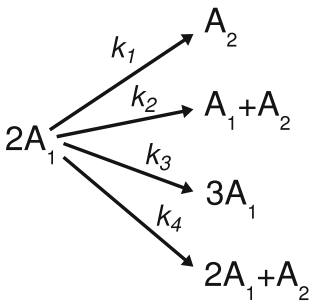
Fig. 1 Reaction network R_1



The possibility of the above mentioned monomial cancellation is illustrated in the following example. Consider the reaction network denoted by R_1 shown in Fig. 1 with the following parameters:

$$k_i = 1, \quad i = 1, 2, 3, 4$$

The differential equations of R_1 can be computed as

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = k_1 x_1^2 \begin{bmatrix} -2 \\ 1 \end{bmatrix} + k_2 x_1^2 \begin{bmatrix} -1 \\ 1 \end{bmatrix} + k_3 x_1^2 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + k_4 x_1^2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -2x_1^2 \\ 3x_1^2 \end{bmatrix} \tag{1}$$

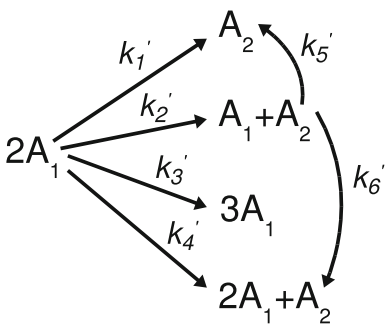
Now, take the reaction system R_1' depicted in Fig. 2 with the parameters:

$$k_1' = 1, \; k_2' = k_3' = k_5' = k_6' = 0.1, \; k_4' = 1.9$$

The equations of R_1' are

$$\begin{aligned} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} &= 1 \cdot x_1^2 \begin{bmatrix} -2 \\ 1 \end{bmatrix} + 0.1 x_1^2 \begin{bmatrix} -1 \\ 1 \end{bmatrix} + 0.1 x_1^2 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 1.9 x_1^2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ &\quad + 0.1 x_1 x_2 \begin{bmatrix} -1 \\ 0 \end{bmatrix} + 0.1 x_1 x_2 \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -2x_1^2 \\ 3x_1^2 \end{bmatrix} \end{aligned} \tag{2}$$

Fig. 2 Reaction network R_1'



It is clear from Eqs. 1–2 that R_1 and R_1' are confoundable in the sense of the original definition given in [1]. However, the source complexes in the two networks are not identical, since $A_1 + A_2$ is a source complex in R_1' but not in R_1.

It is remarked that the above example is not really meaningful in the sense of practical chemical reaction kinetics, because the reactions violate the component mass conservation principle, see, e.g. the reaction $2A_1 \rightarrow 3A_1$. However, the authors in [1] do not exclude this possibility (see, e.g. $A_i \rightarrow 2A_i$ in Eq. 11).

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Reference

1. G. Craciun, C. Pantea, J. Math. Chem. **44**, 244 (2008)