

On the Darboux integrability of a cubic CRNT model in \mathbb{R}^5

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Abstract

We study the Darboux integrability of a differential system with parameters coming from a chemical reaction model in \mathbb{R}^5 . We find all its Darboux polynomials and exponential factors and we prove that it is not Darboux integrable.

Keywords. Darboux polynomial; exponential factor; Darboux integrability; chemical reaction network

1 Introduction and statement of the main result

Consider an n -dimensional polynomial differential system of degree $d \in \mathbb{N}$

$$\dot{\mathbf{x}} = P(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n, \quad (1.1)$$

where $P(\mathbf{x}) = (P_1(\mathbf{x}), \dots, P_n(\mathbf{x}))$, $P_i \in \mathbb{C}[\mathbf{x}]$, and the dot denotes derivative with respect to the independent variable t .

A function $H(\mathbf{x})$ is a *first integral* of system (1.1) if it is continuous and defined in a full Lebesgue measure subset $\Omega \subseteq \mathbb{R}^n$, is not locally constant on any positive Lebesgue measure subset of Ω and moreover is constant along each orbit of system (1.1) in Ω . If H is \mathcal{C}^1 and we name \mathcal{X} the vector field associated to system (1.1), then we have

$$\mathcal{X}(H) = P_1 \frac{\partial H}{\partial x_1} + \dots + P_n \frac{\partial H}{\partial x_n} = 0.$$

System (1.1) is \mathcal{C}^k -completely integrable in Ω if it has $n - 1$ functionally independent \mathcal{C}^k first integrals in Ω . Recall that k functions $H_1(\mathbf{x}), \dots, H_k(\mathbf{x})$ are *functionally independent* in Ω if the matrix of gradients $(\nabla H_1, \dots, \nabla H_k)$ has rank k in a full Lebesgue measure subset of Ω .

For an n -dimensional system of differential equations the existence of some first integrals reduces the complexity of its dynamics and the existence of $n - 1$ functionally independent first

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Mathematics Subject Classification (2010): 34C05, 34A34, 34C14

integrals solves completely the problem (at least theoretically) of determining its phase portrait. In general for a given differential system it is a difficult problem to determine the existence or non-existence of first integrals.

During recent years the interest in the study of the integrability of differential equations has attracted much attention from the mathematical community. Darboux theory of integrability plays a central role in the integrability of the polynomial differential systems since it gives a sufficient condition for the integrability inside a wide family of functions. We highlight that it works for real or complex polynomial ordinary differential equations and that the study of complex algebraic solutions is necessary for obtaining all the real first integrals of a real polynomial differential equation.

A *Darboux polynomial* of (1.1) is a polynomial $f \in \mathbb{C}[\mathbf{x}]$ such that

$$\mathcal{X}(f) = P_1 \frac{\partial f}{\partial x_1} + \cdots + P_n \frac{\partial f}{\partial x_n} = kf,$$

where $\mathbf{x} = (x_1, \dots, x_n)$ and $k \in \mathbb{C}[\mathbf{x}]$, which is called the *cofactor* of f , has degree at most $d - 1$.

An *exponential factor* of (1.1) is a function $F = \exp(g/f)$, with $f, g \in \mathbb{C}[\mathbf{x}]$, such that

$$\mathcal{X}(F) = P_1 \frac{\partial F}{\partial x_1} + \cdots + P_n \frac{\partial F}{\partial x_n} = LF,$$

where $L \in \mathbb{C}[\mathbf{x}]$, which is called the *cofactor* of F , has degree at most $d - 1$. We note that in this case f is a Darboux polynomial of (1.1) and that $\mathcal{X}(g) = kg + Lf$, where k is the cofactor of f .

If H is a Darboux first integral then it has the form

$$H = f_1^{\lambda_1} \cdots f_p^{\lambda_p} F_1^{\mu_1} \cdots F_q^{\mu_q},$$

where f_1, \dots, f_p are Darboux polynomials, F_1, \dots, F_q are exponential factors and λ_i, μ_j are complex numbers, for $i = 1, \dots, p$ and $j = 1, \dots, q$.

The Darboux theory of integrability relates the number of Darboux polynomials and exponential factors with the existence of a Darboux first integral, see for example [10]. We recall that a Darboux first integral is a product of complex powers of Darboux polynomials and exponential factors.

The main aim in this paper is to study the Darboux integrability of a cubic differential system that belongs to \mathbb{R}^5 and has an important contribution in Chemical Reaction Network Theory (CRNT). A reaction network $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ is defined as a set of species \mathcal{S} , a set of complexes \mathcal{C} and a set of reactions \mathcal{R} between complexes; each complex is a combination of species. It is assumed that a reaction occurs according to mass-action kinetics, that is, at a rate proportional to the product of the species concentrations in the reactant or source complex. The set of reactions together with a rate vector give rise to a polynomial system of ordinary differential equations. We refer the reader to [7, 8, 9] for more information about CRNT. For a concrete system of chemical reactions the parameter and state spaces are typically high-dimensional and one uses numerical

methods to analyze the solutions. Due to high computational complexity this can be done only for a small set of values of system's parameters. Thus instead of studying quantitative aspects of the dynamics, recently there has been an increasing interest in studying *qualitative* properties of the CRN. For example in [1, 2, 3, 4, 5, 6] the authors considered the question of existence of single versus multiple steady states (also referred to as multistationary). The existence of first integrals of a polynomial differential system describing a CRN often provides essential qualitative information (the level sets are invariant under the flow) about the solution or can be used, to reduce the dimension of the total state space. Since the computation of nonlinear conservation laws (i.e., first integrals) is highly nontrivial, most of the known results related to the CRN dynamics provide only trivial linear first integrals. Hence, in this paper, our purpose is to show, by following an example (see system (1.2)), how to apply Darboux theory of integrability to obtain nontrivial and nonlinear algebraic and Darboux first integrals.

We deal with the following differential system appearing in [9]:

$$\begin{aligned}
\dot{x}_1 &= -c_1 x_1 x_2^2 + c_2 x_4 + c_4 x_5, \\
\dot{x}_2 &= -2c_1 x_1 x_2^2 + c_4 x_5, \\
\dot{x}_3 &= c_2 x_4 - c_3 x_3 x_4, \\
\dot{x}_4 &= c_1 x_1 x_2^2 - c_2 x_4 - c_3 x_3 x_4, \\
\dot{x}_5 &= c_3 x_3 x_4 - c_4 x_5,
\end{aligned} \tag{1.2}$$

where c_1, c_2, c_3, c_4 are positive constants. We shall study the Darboux integrability of this system by characterizing its Darboux polynomials and exponential factors.

Next we provide the main result of the paper. We prove that there only exist two first integrals (one polynomial and one Darboux), one irreducible Darboux polynomial of degree one and six exponential factors. Indeed, we prove that the system is not Darboux integrable.

Theorem 1.1. *The following results hold for system (1.2).*

- (a) *The unique irreducible polynomial first integral is $H_1 = x_1 + x_4 + x_5$. Any other polynomial first integral is a polynomial function of H_1 .*
- (b) *The unique irreducible Darboux polynomial is $F = c_2 - c_3 x_3$. It has cofactor $k = -c_3 x_4$.*
- (c) *It has six exponential factors: $F_1 = e^{x_3}$, $F_2 = e^{x_2 - 2x_1}$, $F_3 = e^{x_1 + x_4}$, $F_4 = e^{(x_2 - 2x_1)^2}$, $F_5 = e^{(2x_1 - x_2)(x_1 - x_3 + x_4)}$ and $F_6 = e^{(x_1 - x_3 + x_4)^2}$. If e^g/h is another exponential factor, then $h \in \mathbb{C}[H_1]$ and*

$$\begin{aligned}
g(x_1, x_2, x_3, x_4) &= a_1 x_3 + a_2 (x_2 - 2x_1) + a_3 (x_1 + x_4) + a_4 (x_2 - 2x_1)^2 \\
&\quad + a_5 (x_2 - 2x_1)(x_1 - x_3 + x_4) + a_6 (x_1 - x_3 + x_4)^2, \tag{1.3}
\end{aligned}$$

with $a_i \in \mathbb{C}$, $i = 1, \dots, 6$.

(d) *It has the (non-rational) Darboux first integral*

$$H_2 = F^{3c_2/c_3} e^{-(x_1+x_4)} e^{-(x_2-2x_1)} e^{x_3}.$$

(e) *It is not Darboux completely integrable.*

2 Proof of the main result

Statement (e) follows immediately from statements (a)-(d), since there is no way to construct two Darboux first integrals functionally independent of H_1, H_2 . In particular, it is clear that the system has not rational first integrals. Hence, we need to prove only statements (a), (b), (c) and (d).

We prove the statements of Theorem 1.1 separately.

2.1 Proof of statement (a)

Straightforward computations show that H_1 is a first integral of (1.2). The restriction of system (1.2) to $H_1 = h$ is the differential system

$$\begin{aligned}\dot{x}_1 &= -c_1 x_1 x_2^2 - c_4 x_1 + (c_2 - c_4) x_4 + c_4 h, \\ \dot{x}_2 &= -2c_1 x_1 x_2^2 - c_4 x_1 - c_4 x_4 + c_4 h, \\ \dot{x}_3 &= (c_2 - c_3 x_3) x_4, \\ \dot{x}_4 &= c_1 x_1 x_2^2 - c_2 x_4 - c_3 x_3 x_4.\end{aligned}\tag{2.1}$$

Let \mathcal{Y} be the corresponding vector field. Next lemma shows that (2.1) has no polynomial first integrals.

Lemma 2.1. *System (2.1) has no polynomial first integrals.*

Proof. Let $g(x_1, x_2, x_3, x_4)$ be a polynomial first integral of degree $m \in \mathbb{N}$ of system (2.1). We write $g = \sum_{i=1}^m g_i(x_1, x_2, x_3, x_4)$, where g_i is a homogeneous polynomial of degree i . The equation corresponding to the terms of degree $m+2$ of $\mathcal{Y}(g) = 0$ is

$$-c_1 x_1 x_2^2 \left(\frac{\partial g_m}{\partial x_1} + 2 \frac{\partial g_m}{\partial x_2} - \frac{\partial g_m}{\partial x_4} \right) = 0,$$

from which we obtain $g_m(x_1, x_2, x_3, x_4) = g_m(x_3, X_1, X_2)$, where we have introduced the variables $(X_1, X_2) = (x_2 - 2x_1, x_1 + x_4)$. Concerning the terms of degree $m+1$ we have the equation

$$-c_1 x_1 x_2^2 \left(\frac{\partial g_{m-1}}{\partial x_1} + 2 \frac{\partial g_{m-1}}{\partial x_2} - \frac{\partial g_{m-1}}{\partial x_4} \right) - c_3 x_3 x_4 \left(\frac{\partial g_m}{\partial x_3} + \frac{\partial g_m}{\partial x_4} \right) = 0,$$

from which we get

$$\begin{aligned}g_{m-1} &= \frac{c_3 x_3}{c_1(x_2 - 2x_1)} \left(\frac{\partial g_m}{\partial x_3}(x_3, X_1, X_2) + \frac{\partial g_m}{\partial X_2}(x_3, X_1, X_2) \right) \left(\frac{x_1 + x_4}{x_2 - 2x_1} \log \frac{x_2}{4x_1} \right. \\ &\quad \left. + \frac{x_2 + 2x_4}{2x_2} \right) + \bar{g}_{m-1}(x_3, x_2 - 2x_1, x_1 + x_4),\end{aligned}$$

where \bar{g}_{m-1} is a polynomial. Since the logarithm must be removed, we have

$$g_m = g_m(X_1, X_3),$$

where we have introduced $X_3 = X_2 - x_3$. Hence $g_{m-1} = g_{m-1}(x_3, X_1, X_2)$. Next we deal with the terms of degree m . We obtain

$$g_{m-2} = \frac{X_2}{c_1 X_1^2} \left((2c_2 - c_4) \frac{\partial g_m}{\partial X_1} + (c_2 + c_4) \frac{\partial g_m}{\partial X_2} + c_3 x_3 \left(\frac{\partial g_{m-1}}{\partial x_3} + \frac{\partial g_{m-1}}{\partial X_2} \right) \right) \log \frac{x_2}{4x_1} + G_{m-2} + \bar{g}_{m-2}(x_3, X_1, X_2),$$

where G_{m-2} is a rational (maybe polynomial) function and \bar{g}_{m-2} is a polynomial. We must remove the logarithm, hence we must solve an ODE. We obtain

$$g_{m-1}(x_3, X_1, X_2) = -\frac{(c_2 + c_4) \frac{\partial g_m}{\partial X_3} + (2c_2 - c_4) \frac{\partial g_m}{\partial X_1}}{c_3} \log x_3 + \bar{g}_{m-1}(X_1, X_3).$$

A new logarithm appears. To remove it we must take

$$g_m(X_1, X_3) = ((c_2 + c_4)X_1 + (c_4 - 2c_2)X_3)^m,$$

and therefore $g_{m-1}(x_3, X_1, X_2) = g_{m-1}(X_1, X_3)$. Now back to the expression of g_{m-2} we have

$$g_{m-2} = \frac{3c_2 c_4 m}{2c_1} \frac{((c_2 + c_4)X_1 + (c_4 - 2c_2)X_3)^{m-1}}{x_2} + \bar{g}_{m-2}(x_3, X_1, X_2).$$

Since g_{m-2} is to be a polynomial, $x_2 \nmid ((c_2 + c_4)X_1 + (c_4 - 2c_2)X_3)$ and $c_i > 0$ for all i , we have $m = 0$. Then g is a constant and the lemma follows. \square

Remark 2.2. The sequence of resolution in the proof of Lemma 2.1 will be used later on for other purposes.

After Lemma 2.1 we can prove statement (a) of Theorem 1.1. Let f be a polynomial first integral of (1.2) which is not a function of H_1 . Write $f = (H_1 - h)^j F$, where $j \in \mathbb{N} \cup \{0\}$ and $(H_1 - h) \nmid F$. Since $X(f) = 0$, we have $X(F) = 0$. Let $g = F|_{H_1=h} \neq 0$. Then $\mathcal{Y}(g) = 0$. By Lemma 2.1 we have $g \equiv 0$, which is a contradiction. Hence such f cannot exist and therefore statement (a) of Theorem 1.1 follows.

2.2 Proof of statement (b)

We start the study of the Darboux polynomials of system (1.2) simplifying the general expression of the cofactor of any Darboux polynomial.

Proposition 2.3. *Let f be a Darboux polynomial of degree $m \in \mathbb{N}$ of system (1.2) with cofactor k . Then $k = k_0 + k_1 x_1 + k_2 x_2 + k_3 x_3 + k_4 x_4 + k_5 x_5 + k_6 x_2^2 + k_7 x_1 x_2$, where $k_i \in \mathbb{C}$. Moreover, $-k_6/c_1, -k_7/(2c_1) \in \mathbb{N} \cup \{0\}$.*

Proof. We write the cofactor $k \in \mathbb{C}[x_1, x_2, x_3, x_4, x_5]$ as

$$\begin{aligned} k = & k_0 + k_1x_1 + k_2x_2 + k_3x_3 + k_4x_4 + k_5x_5 + k_6x_1^2 + k_7x_1x_2 + k_8x_1x_3 \\ & + k_9x_1x_4 + k_{10}x_1x_5 + k_{11}x_2^2 + k_{12}x_2x_3 + k_{13}x_2x_4 + k_{14}x_2x_5 \\ & + k_{15}x_3^2 + k_{16}x_3x_4 + k_{17}x_3x_5 + k_{18}x_4^2 + k_{19}x_4x_5 + k_{20}x_5^2. \end{aligned}$$

Taking the homogeneous part of degree $m + 1$ of the equation $\mathcal{X}(f) = kf$ and using the Euler theorem of homogeneous functions for f_m we get the equation

$$\begin{aligned} - & (k_6x_1^2 + k_7x_1x_2 + k_8x_1x_3 + k_9x_1x_4 + k_{10}x_1x_5 + (c_1m + k_{11})x_2^2 + k_{12}x_2x_3 + k_{13}x_2x_4 \\ & + k_{14}x_2x_5 + k_{15}x_3^2 + k_{16}x_3x_4 + k_{17}x_3x_5 + k_{18}x_4^2 + k_{19}x_4x_5 + k_{20}x_5^2)f_m \\ & + c_1x_2^2 \left((x_2 - 2x_1) \frac{\partial f_m}{\partial x_2} + x_3 \frac{\partial f_m}{\partial x_3} + (x_1 + x_4) \frac{\partial f_m}{\partial x_4} + x_5 \frac{\partial f_m}{\partial x_5} \right) = 0. \end{aligned}$$

The general solution of this equation is

$$\begin{aligned} f_m(x_1, x_2, x_3, x_4, x_5) = & e^{\frac{x_1 P_1}{2c_1 x_2 (2x_1 - x_2)^2}} x_2^{\frac{P_2}{4c_1 (2x_1 - x_2)^2}} (2x_1 - x_2)^{m + \frac{P_3}{4c_1}} \\ & \times C_m \left(x_1, \frac{x_3}{2x_1 - x_2}, \frac{x_1 + x_4}{2x_1 - x_2}, \frac{x_5}{2x_1 - x_2} \right), \end{aligned}$$

where

$$\begin{aligned} P_1 = & 4k_{20}x_5^2 + 4k_{19}x_4x_5 + 4k_{18}x_4^2 + 4k_{17}x_3x_5 + 4k_{16}x_3x_4 + 4k_{15}x_3^2 \\ & + 2(k_{19} - k_{10})x_2x_5 + 2(2k_{18} - k_9)x_2x_4 + 2(k_{16} - k_8)x_2x_3 \\ & + 4k_{10}x_1x_5 + 4k_9x_1x_4 + 4k_8x_1x_3 + 2(k_9 - 2k_6)x_1x_2 + 4k_6x_1^2 + (k_{18} - k_9 + k_6)x_2^2; \\ P_2 = & 4k_{20}x_5^2 + 4k_{19}x_4x_5 + 4k_{18}x_4^2 + 4k_{17}x_3x_5 + 4k_{16}x_3x_4 + 4k_{15}x_3^2 + 4k_{14}x_2x_5 \\ & + 4k_{13}x_2x_4 + 4k_{12}x_2x_3 + 4(k_9 - 2k_7 - k_6)x_1^2 + (-k_{18} + 2k_{13} + k_9 - 2k_7 - k_6)x_2^2 \\ & + 4(k_{19} - 2k_{14})x_1x_5 + 8(k_{18} - k_{13})x_1x_4 + 4(k_{16} - 2k_{12})x_1x_3 \\ & + 4(k_{18} - k_{13} - k_9 + 2k_7 + k_6)x_1x_2; \\ P_3 = & k_{18} - 2k_{13} + 4k_{11} - k_9 + 2k_7 + k_6; \end{aligned}$$

and C_m is an arbitrary function. In order to get a polynomial the exponent of the exponential must be a constant and the exponents of x_2 and $2x_1 - x_2$ must be non-negative integers. Therefore we must take $k_{11} = -c_1n_1$ and $k_7 = -2c_1n_2$, where $n_1, n_2 \in \mathbb{N} \cup \{0\}$, and $k_6 = k_8 = k_9 = k_{10} = 0$, $k_{12} = \dots = k_{20} = 0$. We get

$$f_m(x_1, x_2, x_3, x_4, x_5) = x_2^{n_2} (x_2 - 2x_1)^{m - n_1 - n_2} C_m \left(x_1, \frac{x_3}{x_2 - 2x_1}, \frac{x_1 + x_4}{x_2 - 2x_1}, \frac{x_5}{x_2 - 2x_1} \right).$$

Since this is to be a polynomial of degree m , we take

$$f_m(x_1, x_2, x_3, x_4, x_5) = x_1^{n_1} x_2^{n_2} (x_2 - 2x_1)^{m - n_1 - n_2 - n} P_n(x_3, x_1 + x_4, x_5),$$

where P_n is a homogeneous polynomial of degree $n \in \mathbb{N} \cup \{0\}$. Renaming the coefficients of k , the proposition follows. \square

Lemma 2.4. *The unique Darboux polynomial of degree one of system (1.2) is $c_2 - c_3x_3$. Its cofactor is $k = -c_3x_4$.*

Proof. It follows after easy computations. \square

Next lemma shows that there are no more Darboux polynomials, and thus it finishes the proof of statement (b) of Theorem 1.1.

Lemma 2.5. *System (1.2) has no irreducible Darboux polynomials of degree greater than one.*

Proof. Since $H_1 = x_1 + x_4 + x_5$ is a first integral and $c_2 - c_3x_3 = 0$ is a Darboux polynomial, both of (1.2), we can write system (1.2) restricted to $x_1 + x_4 + x_5 = h$ and $c_2 - c_3x_3 = 0$:

$$\begin{aligned}\dot{x}_1 &= -c_1x_1x_2^2 - c_4x_1 + (c_2 - c_4)x_4 + c_4h, \\ \dot{x}_2 &= -2c_1x_1x_2^2 - c_4x_1 - c_4x_4 + c_4h, \\ \dot{x}_4 &= c_1x_1x_2^2 - 2c_2x_4.\end{aligned}\tag{2.2}$$

Let f be an irreducible Darboux polynomial of system (1.2). Let g be the Darboux polynomial of (2.2) corresponding to f restricted to $x_1 + x_4 + x_5 = h$ and $c_2 - c_3x_3 = 0$. Let $m \in \mathbb{N}$ be the degree of g . Then

$$\begin{aligned}(-c_1x_1x_2^2 - c_4x_1 + (c_2 - c_4)x_4 + c_4h)\frac{\partial g}{\partial x_1} \\ + (-2c_1x_1x_2^2 - c_4x_1 - c_4x_4 + c_4h)\frac{\partial g}{\partial x_2} + (c_1x_1x_2^2 - 2c_2x_4)\frac{\partial g}{\partial x_4} \\ - (k_0 + k_1x_1 + k_2x_2 + k_4x_4 - c_1n_1x_2^2 - 2c_1n_2x_1x_2)g = 0.\end{aligned}\tag{2.3}$$

We note that the expression of the cofactor of g can be obtained from Proposition 2.3 after the considered restrictions.

We write $g = \sum_{i=0}^m g_i(x, y)$, with g_i a homogeneous polynomial of degree i . From (2.3), the equation of degree $m + 2$ becomes, after canceling a common factor c_1x_2 ,

$$-x_1x_2 \left(\frac{\partial g_m}{\partial x_1} + 2\frac{\partial g_m}{\partial x_2} - \frac{\partial g_m}{\partial x_4} \right) + (n_1x_2 + 2n_2x_1)g_m = 0.$$

Then $g_m = x_1^{n_1}x_2^{n_2}\bar{g}_m(x_2 - 2x_1, x_1 + x_4)$, with \bar{g}_m a homogeneous polynomial of degree $m - n_1 - n_2$.

The equation of degree $m + 1$ of (2.3) is

$$\begin{aligned}-c_1x_1x_2^2 \left(\frac{\partial g_{m-1}}{\partial x_1} + 2\frac{\partial g_{m-1}}{\partial x_2} - \frac{\partial g_{m-1}}{\partial x_4} \right) + c_1x_2(n_1x_2 + 2n_2x_1)g_{m-1} \\ - (k_1x_1 + k_2x_2 + k_4x_4)x_1^{n_1}x_2^{n_2}\bar{g}_m(x_2 - 2x_1, x_1 + x_4) = 0.\end{aligned}$$

from which we obtain

$$\begin{aligned}g_{m-1} = & -\frac{2k_1x_1 - k_1x_2 + k_4x_2 + 2k_4x_4}{2c_1(x_2 - 2x_1)}x_1^{n_1}x_2^{n_2-1}\bar{g}_m(x_2 - 2x_1, x_1 + x_4) \\ & -\frac{2k_2x_1 - k_4x_1 - k_2x_2 - k_4x_4}{c_1(x_2 - 2x_1)^2} \log \frac{x_2}{4x_1}x_1^{n_1}x_2^{n_2}\bar{g}_m(x_2 - 2x_1, x_1 + x_4) \\ & + x_1^{n_1}x_2^{n_2}\bar{g}_{m-1}(x_2 - 2x_1, x_1 + x_4),\end{aligned}$$

where \bar{g}_{m-1} is a homogeneous polynomial of degree $m - 1 - n_1 - n_2$. Since the logarithm must be removed, we have $k_2 = k_4 = 0$. Hence

$$g_{m-1} = \frac{k_1}{2c_1} x_1^{n_1} x_2^{n_2-1} \bar{g}_m(x_2 - 2x_1, x_1 + x_4) + x_1^{n_1} x_2^{n_2} \bar{g}_{m-1}(x_2 - 2x_1, x_1 + x_4).$$

The equation of degree m of (2.3) is

$$\begin{aligned} & -c_1 x_1 x_2^2 \left(\frac{\partial g_{m-2}}{\partial x_1} + 2 \frac{\partial g_{m-2}}{\partial x_2} - \frac{\partial g_{m-2}}{\partial x_4} \right) + c_1 x_2 (n_1 x_2 + 2n_2 x_1) g_{m-2} \\ & + ((c_2 - c_4)x_4 - c_4 x_1) \frac{\partial g_m}{\partial x_1} - c_4 (x_1 + x_4) \frac{\partial g_m}{\partial x_2} - 2c_2 x_4 \frac{\partial g_m}{\partial x_4} - k_0 g_m - k_1 x_1 g_{m-1} = 0. \end{aligned}$$

We obtain

$$g_{m-2} = \frac{x_1^{n_1} x_2^{n_2} E_{m-2}(\bar{g}_m)}{c_1 (x_2 - 2x_1)^3} \log \frac{x_2}{x_1} + \frac{x_1^{n_1-1} x_2^{n_2-2} P_{m-2}}{c_1^2 (x_2 - 2x_1)^2} + x_1^{n_1} x_2^{n_2} \bar{g}_{m-2}(x_2 - 2x_1, x_1 + x_4),$$

where \bar{g}_{m-2} is a homogeneous polynomial of degree $m - 2 - n_1 - n_2$, P_{m-2} is a homogeneous polynomial and $E_{m-2}(\bar{g}_m) = 0$ is an ODE with solution

$$\bar{g}_m = (x_2 - 2x_1)^{n_3} (x_1 + x_4)^{n_4} ((4c_2 + c_4)x_1 - (c_2 + c_4)x_2 + (2c_2 - c_4)x_4)^{m-n_1-n_2-n_3-n_4},$$

with $n_i \in \mathbb{N} \cup \{0\}$, where we have fixed $k_0 = -c_2 n_1 - (c_2 + c_4)n_4$ and $c_4 n_2 + 4(c_2 - c_4)n_1 + (2c_2 - c_4)n_3 = 0$ for \bar{g}_m to be a polynomial. The logarithm in the expression of g_{m-2} must be removed, hence we have this expression for \bar{g}_m . Then

$$\begin{aligned} g_{m-2} &= x_1^{n_1-1} x_2^{n_2-2} (x_2 - 2x_1)^{n_3-1} (x_1 + x_4)^{n_4-1} \times \\ & \quad ((4c_2 + c_4)x_1 - (c_2 + c_4)x_2 + (2c_2 - c_4)x_4)^{m-1-n_1-n_2-n_3-n_4} P_4 \\ & \quad + \frac{k_1}{2c_1} x_1^{n_1} x_2^{n_2-1} \bar{g}_{m-1} + x_1^{n_1} x_2^{n_2} \bar{g}_{m-2}, \end{aligned}$$

where P_4 is a homogeneous polynomial of degree 4.

The equation of degree $m - 1$ of (2.3) is

$$\begin{aligned} & -c_1 x_1 x_2^2 \left(\frac{\partial g_{m-3}}{\partial x_1} + 2 \frac{\partial g_{m-3}}{\partial x_2} - \frac{\partial g_{m-3}}{\partial x_4} \right) + c_1 x_2 (n_1 x_2 + 2n_2 x_1) g_{m-3} \\ & + ((c_2 - c_4)x_4 - c_4 x_1) \frac{\partial g_{m-1}}{\partial x_1} - c_4 (x_1 + x_4) \frac{\partial g_{m-1}}{\partial x_2} - 2c_2 x_4 \frac{\partial g_{m-1}}{\partial x_4} \\ & + (c_2 n_1 + (c_2 + c_4)n_4) g_{m-1} - k_1 x_1 g_{m-2} + c_4 h \left(\frac{\partial g_m}{\partial x_1} + \frac{\partial g_m}{\partial x_2} \right) = 0. \end{aligned}$$

We do not write the expression of g_{m-3} because it is too long. In this expression there is a logarithm that must be removed. Its coefficient provides an ODE with unknown \bar{g}_{m-1} whose solution is:

$$\begin{aligned} \bar{g}_{m-1} &= \frac{-1}{2c_1(2c_2 - c_4)(c_2 + c_4)} X_1^{n_3-1} X_2^{n_4-1} (-c_2(X_1 - 2X_2) - c_4(X_1 + X_2))^{m-2-\sum_{i=1}^4 n_i} \times \\ & \quad \left(-c_4(2c_1(2c_2 - c_4)h n_4 X_1 + (c_2 + c_4)k_1 X_2)(c_2(X_1 - 2X_2) + c_4(X_1 + X_2)) \right. \\ & \quad + 2c_1 c_2 h (2c_2 - c_4) \left[2(c_2 + c_4)(2n_1 + n_3) X_1 X_2 \log(X_1) \right. \\ & \quad \left. \left. - (8c_2(2n_1 + n_3) + c_4(3m - 11n_1 - 4n_3 - 3n_4)) X_1 X_2 \log((2c_2 - c_4)X_2) \right] \right) \\ & \quad + C_{m-1} X_1^{n_3} X_2^{n_4} (-c_2 X_1 - c_4 X_1 + 2c_2 X_2 - c_4 X_2)^{m-1-\sum_{i=1}^4 n_i}, \end{aligned}$$

where C_{m-1} is a constant and where we have written $X_1 = x_2 - 2x_1$ and $X_2 = x_1 + x_4$ for simplicity. To remove these new logarithms we have two possibilities: either $c_4 = 2c_2$, or

$$2n_1 + n_3 = 0 \quad \text{and} \quad 8c_2(2n_1 + n_3) + c_4(3m - 11n_1 - 4n_3 - 3n_4) = 0.$$

We deal with the first case later on. The latter case implies $n_4 = m + n_3/2$ and $n_1 = -n_3/2$. Since $0 \leq n_i \leq m$, we must take $n_1 = n_3 = 0$, and hence $n_4 = m$. Thus we have $n_2 = 0$.

After these new conditions we have $g_m = \bar{g}_m = X_2^m$ and

$$g_{m-1} = \frac{k_1}{2c_1} \frac{X_2^m}{x_2} + \bar{g}_{m-1}.$$

Thus $k_1 = 0$. Moreover

$$g_{m-2} = -\frac{c_2 m}{2c_1} \frac{X_2^{m-1}}{x_2} + \bar{g}_{m-2}.$$

Therefore we get $m = 0$.

The case $c_4 = 2c_2$ follows in a similar way as the previous one: solving the ODE's as before, we obtain the following polynomials:

$$\begin{aligned} g_m &= x_1^{n_1} x_2^{n_2} \bar{g}_m(X_1, X_2); \\ g_{m-1} &= \frac{k_1}{2c_1} x_1^{n_1} x_2^{n_2-1} \bar{g}_m + x_1^{n_1} x_2^{n_2} \bar{g}_{m-1}(X_1, X_2); \\ g_{m-2} &= x_1^{n_1-1} x_2^{2n_1-2} X_1^{n_3-1} X_2^{n_4-1} P_3 + \frac{k_1}{2c_1} x_1^{n_1} x_2^{2n_1-1} \bar{g}_{m-1} + x_1^{n_1} x_2^{2n_1} \bar{g}_{m-2}(X_1, X_2), \end{aligned}$$

where P_3 is a polynomial; and the conditions $k_2 = k_4 = 0$, $n_2 = 2n_1$, $k_0 = -c_2(n_1 + 3n_4)$ and $\bar{g}_m = X_1^{n_3} X_2^{n_4}$, with $\sum_{i=1}^4 n_i = m$.

When solving the equation corresponding to g_{m-3} , as before a logarithm must be removed, and we obtain

$$\begin{aligned} \bar{g}_{m-1} &= -\frac{X_1^{n_3-2} X_2^{n_4-1} (2c_1 n_4 h X_1^2 - k_1 X_2^2)}{3c_1} + C_{m-1} X_1^{n_3-1} X_2^{n_4} \\ &\quad - \frac{2}{3} (2n_1 + n_3) h X_1^{n_3-1} X_2^{n_4} \log X_2, \end{aligned}$$

where C_{m-1} is a constant. Since \bar{g}_{m-1} must be a polynomial and h does not need to be zero, we must take $2n_1 + n_3 = 0$. Hence $n_1 = n_3 = 0$, and therefore from above $n_2 = 0$ and hence $n_4 = m$. So we have $g_m = \bar{g}_m = X_2^m$ and

$$g_{m-1} = \frac{k_1}{2c_1} \frac{X_2^m}{x_2} + \bar{g}_{m-1}.$$

Thus $k_1 = 0$. Moreover

$$g_{m-2} = -\frac{c_2 m}{2c_1} \frac{X_2^{m-1}}{x_2} + \bar{g}_{m-2}.$$

Therefore we get $m = 0$.

Since $\deg g = 0$ in all cases, we have that $(c_2 - c_3 x_3)|f$. But f is irreducible, therefore $f = c_2 - c_3 x_3$. Then the lemma follows. \square

2.3 Proof of statement (c)

We consider system (1.2) restricted to $H_1 = h$, i.e. we consider system (2.1). The following result characterizes its exponential factors of the form $\exp(g)$, with $g \in \mathbb{C}[x_1, x_2, x_3, x_4]$.

Lemma 2.6. *Let $\exp(g)$, with $g \in \mathbb{C}[x_1, x_2, x_3, x_4]$, be an exponential factor of system (2.1). Then g is a linear combination of x_3 , $x_2 - 2x_1$, $x_1 + x_4$, $(x_2 - 2x_1)^2$, $(x_2 - 2x_1)(x_1 - x_3 + x_4)$ and $(x_1 - x_3 + x_4)^2$.*

Proof. Since $\exp(g)$ is an exponential factor of system (2.1), g satisfies

$$\begin{aligned} \mathcal{Y}(g) = k = & k_0 + k_1x_1 + k_2x_2 + k_3x_3 + k_4x_4 + k_5x_1^2 + k_6x_1x_2 + k_7x_1x_3 + k_8x_1x_4 \\ & + k_9x_2^2 + k_{10}x_2x_3 + k_{11}x_2x_4 + k_{12}x_3^2 + k_{13}x_3x_4 + k_{14}x_4^2. \end{aligned} \quad (2.4)$$

Assume that g is a polynomial of degree $m \in \mathbb{N}$, with $m \geq 3$. We write it as sum of its homogeneous parts $g = \sum_{i=1}^m g_i(x_1, x_2, x_3, x_4)$, where g_i is a homogeneous polynomial of degree i and $g_m \neq 0$. Since the right hand side terms of (2.4) has degree two, its left hand side must also have degree two. Since $m \geq 3$, the computation of g_m , g_{m-1} and g_{m-2} follow in the same way as the proof of Lemma 2.1. Therefore we get $m = 0$, which is a contradiction. Hence g is a polynomial of degree less than or equal to two in the variables x_1, x_2, x_3, x_4 . Indeed easy computations show that g is a linear combination of x_3 , $x_2 - 2x_1$, $x_1 + x_4$, $(x_2 - 2x_1)^2$, $(x_2 - 2x_1)(x_1 - x_3 + x_4)$ and $(x_1 - x_3 + x_4)^2$. \square

Remark 2.7. In particular, the functions appearing in statement (c) of Theorem 1.1 are exponential factors.

In view of Lemma 2.6, if $E = \exp(g)$ is an exponential factor of system (2.1), then g writes as (1.3) and the cofactor of E has the form

$$L = L_0 + c_4L_1H_1, \quad (2.5)$$

where

$$\begin{aligned} L_0 = & (a_2 - a_3)c_4x_1 + ((a_1 - 2a_2)c_2 + (a_2 - a_3)c_4)x_4 - (4a_4 - 3a_5 + 2a_6)c_4x_1^2 \\ & + (2a_4 - a_5)c_4x_1x_2 - (a_5 - 2a_6)c_4x_1x_3 + 2((4a_4 - a_6)c_2 - 2(a_4 - a_5 + a_6)c_4)x_1x_4 \\ & + ((2a_4 - a_5)c_4 - (4a_4 + a_5)c_2)x_2x_4 + (2(a_5 + a_6) - (a_1 + a_3)c_3 + (2a_6 - a_5)c_4)x_3x_4 \\ & + ((a_5 - 2a_6)c_4 - 2(a_5 + a_6)c_2)x_4^2 \end{aligned}$$

and

$$L_1 = -(a_2 - a_3) + (4a_4 - 3a_5 + 2a_6)x_1 - (2a_4 - a_5)x_2 + (a_5 - 2a_6)x_3 - (a_5 - 2a_6)x_4.$$

We shall use these expressions later on in the proof of Lemma 2.9.

We go back now to system (1.2). Since it has only one Darboux polynomial and one polynomial first integral, if it has an exponential factor, then it must be of the form $\exp(f/(F^nQ(H_1)))$, with $n \in \mathbb{N} \cup \{0\}$ and $Q \in \mathbb{C}[H_1]$. Next we prove that the expression of an exponential factor of this form cannot contain a power of F in the denominator of the exponent.

Lemma 2.8. *Suppose that system (1.2) has the exponential factor $E = \exp(f/(F^n Q(H_1)))$, with $f \in \mathbb{C}[x_1, x_2, x_3, x_4, x_5]$, $n \in \mathbb{N} \cup \{0\}$, $F \nmid f$ and Q a polynomial. Then $n = 0$.*

Proof. Suppose that $n > 0$. Let L be the cofactor of E . Since $\mathcal{X}(Q(H_1)) = 0$, we have

$$LE = \mathcal{X}(E) = E \frac{\mathcal{X}(f) \cdot F^n - f \cdot \mathcal{X}(F^n)}{F^{2n} Q(H_1)}.$$

Hence

$$\mathcal{X}(f)F^n + nc_3x_4fF^n = LF^{2n}Q(H_1),$$

see Lemma 2.4. Therefore

$$\mathcal{X}(f) + nc_3x_4f = LF^nQ(H_1). \quad (2.6)$$

Since $n > 0$, equation (2.6) on $H_1 = h$ and $F = 0$ becomes

$$\begin{aligned} & (-c_1x_1x_2^2 - c_4x_1 + (c_2 - c_4)x_4 + c_4h) \frac{\partial \bar{f}}{\partial x_1} + (-2c_1x_1x_2^2 - c_4x_1 - c_4x_4 + c_4h) \frac{\partial \bar{f}}{\partial x_2} \\ & + (c_1x_1x_2^2 - 2c_2x_4) \frac{\partial \bar{f}}{\partial x_4} = -nc_3x_4\bar{f}. \end{aligned}$$

where \bar{f} is the restriction of f to $H_1 = h$ and $F = 0$. This means that \bar{f} is a Darboux polynomial of system (2.2) with cofactor $-nc_3x_4 \neq 0$. In view of the proof of Lemma 2.5 this is a contradiction, which comes from the assumption $n \neq 0$. Therefore $n = 0$ and the lemma follows. \square

The following result completes the proof of statement (c).

Lemma 2.9. *Let $E = \exp(f/Q(H_1))$ be an exponential factor of system (1.2), with $Q \in \mathbb{C}[H_1]$ and $f \in \mathbb{C}[x_1, x_2, x_3, x_4, x_5]$. Then $f - gQ(H_1)$, with g as in (1.3), is a polynomial function of H_1 .*

Proof. Set $x_5 = H_1 - x_1 - x_4$. We write the cofactor k of $\exp(f/Q(H_1))$ in the variables x_1, x_2, x_3, x_4, H_1 as follows:

$$\begin{aligned} k &= k_0 + k_1x_1 + k_2x_2 + k_3x_3 + k_4x_4 + k_5x_1^2 + k_6x_1x_2 + k_7x_1x_3 + k_8x_1x_4 \\ &+ k_9x_2^2 + k_{10}x_2x_3 + k_{11}x_2x_4 + k_{12}x_3^2 + k_{13}x_3x_4 + k_{14}x_4^2 \\ &+ (k_{15} + k_{16}x_1 + k_{17}x_2 + k_{18}x_3 + k_{19}x_4)H_1 + k_{20}H_1^2. \end{aligned}$$

We also write Q and f as polynomials in H_1 :

$$Q(H_1) = \sum_{j=0}^n d_j H_1^j \quad \text{and} \quad f = \sum_{j=0}^n f_j(x_1, x_2, x_3, x_4) H_1^j,$$

where $d_j \in \mathbb{C}$ and $f_j \in \mathbb{C}[x_1, x_2, x_3, x_4]$. Since E is an exponential factor, f satisfies

$$\mathcal{X}(f) = kQ(H_1). \quad (2.7)$$

Evaluating (2.7) on $H_1 = 0$, we have that $\exp(f_0)$, with $f_0 = f|_{H_1=0}$, is an exponential factor of system (2.1) with $h = 0$ with the cofactor $d_0\bar{k} = d_0k|_{H_1=0}$. In view of Lemma 2.6, we have

$f_0 = f_0^0 + d_0g$, with g as in (1.3). Moreover, $\bar{k} = L_0$. Now computing the coefficient of H_1 in (2.7) we get

$$\begin{aligned} & c_4 \frac{\partial f_0}{\partial x_1} + c_4 \frac{\partial f_0}{\partial x_2} + (-c_1x_1x_2^2 - c_4x_1 + (c_2 - c_4)x_4) \frac{\partial f_1}{\partial x_1} + (-2c_1x_1x_2^2 - c_4x_1 - c_4x_4) \frac{\partial f_1}{\partial x_2} \\ & + (c_2 - c_3x_3)x_4 \frac{\partial f_1}{\partial x_3} + (c_1x_1x_2^2 - c_2x_4 - c_3x_3x_4) \frac{\partial f_1}{\partial x_4} \\ & = d_1L_0 + d_0(k_{15} + k_{16}x_1 + k_{17}x_2 + k_{18}x_3 + k_{19}x_4). \end{aligned}$$

Proceeding as in the proof of Lemma 2.6, we obtain $f_1 = f_1^0 + d_1g$ and $k_{15} + k_{16}x_1 + k_{17}x_2 + k_{18}x_3 + k_{19}x_4 = c_4L_1$. Now computing the coefficient of H_1^2 in (2.7) we get

$$\begin{aligned} & c_4 \frac{\partial f_1}{\partial x_1} + c_4 \frac{\partial f_1}{\partial x_2} + (-c_1x_1x_2^2 - c_4x_1 + (c_2 - c_4)x_4) \frac{\partial f_2}{\partial x_1} + (-2c_1x_1x_2^2 - c_4x_1 - c_4x_4) \frac{\partial f_2}{\partial x_2} \\ & + (c_2 - c_3x_3)x_4 \frac{\partial f_2}{\partial x_3} + (c_1x_1x_2^2 - c_2x_4 - c_3x_3x_4) \frac{\partial f_2}{\partial x_4} \\ & = d_2L_0 + d_1L_1 + d_0k_{20}, \end{aligned}$$

or equivalently

$$\begin{aligned} & (-c_1x_1x_2^2 - c_4x_1 + (c_2 - c_4)x_4) \frac{\partial f_2}{\partial x_1} + (-2c_1x_1x_2^2 - c_4x_1 - c_4x_4) \frac{\partial f_2}{\partial x_2} \\ & + (c_2 - c_3x_3)x_4 \frac{\partial f_2}{\partial x_3} + (c_1x_1x_2^2 - c_2x_4 - c_3x_3x_4) \frac{\partial f_2}{\partial x_4} = d_2L_0 + d_0k_{20}. \end{aligned}$$

Proceeding again as in the proof of Lemma 2.6 we get $f_2 = f_2^0 + d_2g$ and $k_{20} = 0$. Therefore $k = L$, see (2.5). Now proceeding inductively with $k = L$ we get that $f_j = f_j^0 + d_jg$, for $j \geq 2$. In short,

$$f = \sum_{j=0}^n d_j (f_j^0 + g) H_1^j = P(H_1) + gQ(H_1),$$

with $P(H_1) = \sum_{j=0}^n d_j f_j^0 H_1^j$ and g as in (1.3). Then the lemma follows. \square

After Lemma 2.9, if $\exp(f/Q(H_1))$ is an exponential factor, then

$$e^{f/Q(H_1)} = e^g e^{P(H_1)/Q(H_1)},$$

with P a polynomial in H_1 . Then statement (c) follows.

2.4 Proof of statement (d)

Let H be a Darboux first integral of system (1.2). Then it must be of the form $H = F^{\lambda_1} \exp(g)$ where g is given in (1.3). The cofactor of H must be zero. That is,

$$\begin{aligned} 0 &= -\lambda_1 c_3 x_4 + L \\ &= ((a_1 - 2a_2)c_2 - \lambda_1 c_3)x_4 + (a_3 - a_2)c_4 x_5 + 2(4a_4 - a_6)c_2 x_1 x_4 \\ &+ (4a_4 + 3a_5 + 2a_6)c_4 x_1 x_5 + (a_5 - 4a_4)c_2 x_2 x_4 - (2a_4 + a_5)c_4 x_2 x_5 \\ &+ (-2a_5 c_2 + 2a_6 c_2 - a_1 c_3 - a_3 c_3)x_3 x_4 - (a_5 + 2a_6)c_4 x_3 x_5 \\ &+ 2(a_5 - a_6)c_2 x_4^2 + (a_5 + 2a_6)c_4 x_4 x_5, \end{aligned} \quad (2.8)$$

where L is the cofactor of $\exp(g)$, see (2.5). Solving (2.8) we get $\lambda = 3a_1c_2/c_3$, $a_2 = a_3 = -a_1$ and $a_4 = a_5 = a_6 = 0$. Therefore statement (d) follows.

Acknowledgments. A. Ferragut is partially supported by the Spanish Government grant MTM2013-40998-P and C. Valls is supported by Portuguese National Funds through FCT - Fundação para a Ciência e a Tecnologia within projects PTDC/MAT/117106/2010 and PEst-OE/EEI/LA0009/2013 (CAMGSD).

References

- [1] M. BANAJI, *P matrix properties, injectivity, and stability in chemical reaction systems*, SIAM J. Appl. Math. **67** (2007), 1523–1547.
- [2] M. BANAJI AND G. CRACIUN, *Graph-theoretic approaches to injectivity and multiple equilibria in systems of interacting elements*, Commun. Math. Sci. **7** (2009), 867–900.
- [3] M. BANAJI AND G. CRACIUN, *Graph-theoretic approaches for injectivity and unique equilibria in general chemical reaction systems*, Adv. Appl. Math. **44** (2010), 168–184.
- [4] G. CRACIUN AND M. FEINBERG, *Multiple equilibria in complex chemical reaction networks I: The injectivity property*, SIAM J. Appl. Math. **65** (2005), 1526–1546.
- [5] G. CRACIUN AND M. FEINBERG, *Multiple equilibria in complex chemical reaction networks II: The species reaction graph*, SIAM J. Appl. Math. **66** (2006), 1321–1338.
- [6] G. CRACIUN AND M. FEINBERG, *Multiple equilibria in complex chemical reaction networks: Semiopen mass action systems*, SIAM J. Appl. Math. **70** (2010), 1859–1877.
- [7] E. FELIU, C. WIUF, *Simplifying biochemical models with intermediate species*, J. R. Soc. Interface **10** (2013), 20130484.
- [8] E. FELIU, C. WIUF, *Preclusion of switch behavior in networks with mass-action kinetics*, Appl. Math. Comput. **219** (2012), 1449–1467.
- [9] E. FELIU, C. WIUF, *Variable Elimination in Chemical Reaction Networks with Mass-Action Kinetics*, SIAM J. Appl. Math., **72(4)** (2012), 959–981.
- [10] J. LLIBRE, X. ZHANG, *On the Darboux Integrability of Polynomial Differential Systems*, Qual. Theory Dyn. Syst. **11** (2012), 129–144.