

Forward-Invariant Peeling in Chemical Dynamics: a Simple Case Study

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Abstract. Forward-invariant peeling aims to produce forward-invariant subset from a given set in phase space. The structure of chemical kinetic equations allows us to describe the general operations of the forward-invariant peeling. For example, we study a simple reaction network with three components A_1, A_2, A_3 and reactions $A_1 \rightarrow A_2 \rightarrow A_3 \rightarrow A_1, 2A_1 \rightleftharpoons 3A_2$ (without any stoichiometric conservation law). We assume that kinetics obey the classical mass action law and reaction rate constants are positive intervals $0 < k_{i \min} \leq k_i \leq k_{i \max} < \infty$. Kinetics of this system is described by a system of differential inclusions. We produce forward-invariant sets for these kinetic inclusions from the sets $\{c|c_i \geq 0, \sum c_i \geq \varepsilon\}$ by the forward-invariant peeling (for sufficiently small $\varepsilon > 0$). In particular, this construction proves persistence of this kinetic system (a positive solution cannot approach the origin even asymptotically, as $t \rightarrow \infty$).

Keywords and phrases: chemical kinetics, Lyapunov function, persistence

Mathematics Subject Classification: 37C10, 34D20, 93D05

1. Introduction

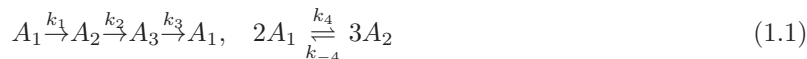
1.1. The problem

Differential inclusions for chemical kinetics with a given reaction mechanism, unknown rate constants but known thermodynamic data were introduced in 1979 [3] (for further references, generalizations and examples see [2, 4, 5, 7, 8, 10]; our works were mostly inspired by A.I.Volpert [9]). Solutions to these inclusions are forward-invariant sets of the kinetic equations.

In many important cases, the cones of the possible velocities in the concentration spaces are piecewise constant (for systems with a given reaction mechanism and the complex balance condition but unknown values of reaction rate constants, for example [7]). Two main approaches to evaluation of solutions to these kinetic inclusion have been proposed. If we start from an initial point and build the solutions stepwise by adding the cones of the possible velocities and intersection with the compartments where these cones are constant then the result is the minimal forward-invariant set which includes the initial point. The dual approach is the so-called *forward-invariant peeling*: we start from a domain in the concentration space and then delete some parts of this set (the ‘peel’ or the ‘rind’) to make it invariant [7].

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The goal of this note is to demonstrate how the procedure of forward-invariant peeling works on a simple but not yet trivial example. For this purpose, we take a system from a recent paper [8]



with the classical mass action law and interval constants $0 < \min k_i \leq k_i \leq \max k_i < \infty$. Consider the kinetic equations with such interval constants and classical mass action law. We will demonstrate how to use peeling for solution of the persistence problem for this system: is it possible that the solution of the differential inclusion with these interval constants starting from a positive vector will go to zero when $t \rightarrow \infty$? This question for that system was considered recently as an unsolved problem [8]. The solution was demonstrated in recent preprint [7]. The goal of this note is rather modest in the light of the general theory of toric inclusions announced very recently [1] but I believe that the publication of the straightforward analysis of an example of forward-invariant peeling still makes sense.

1.2. Mass action law

The *list of components* is a finite set of symbols A_1, \dots, A_n .

A *reaction mechanism* is a finite set of the *stoichiometric equations* of elementary reactions:



where $\rho = 1, \dots, m$ is the reaction number and the *stoichiometric coefficients* $\alpha_{\rho i}, \beta_{\rho i}$ are nonnegative numbers. Usually, these numbers are assumed to be integer but in some applications the construction should be more flexible and admit real nonnegative values. Let α_ρ, β_ρ be the vectors with coordinates $\alpha_{\rho i}, \beta_{\rho i}$ correspondingly.

A *stoichiometric vector* γ_ρ of the reaction in Equation (1.2) is a n -dimensional vector $\gamma_\rho = \beta_\rho - \alpha_\rho$ with coordinates

$$\gamma_{\rho i} = \beta_{\rho i} - \alpha_{\rho i} \quad (1.3)$$

that is, “gain minus loss” in the ρ th elementary reaction. We assume $\alpha_\rho \neq \beta_\rho$ to avoid trivial reactions with zero γ_ρ .

A non-negative intensive variable, the reaction rate r_ρ , corresponds to each elementary reaction.

The kinetic equations for a homogeneous system in the absence of external fluxes are

$$\frac{dN}{dt} = V \sum_\rho r_\rho \gamma_\rho. \quad (1.4)$$

If the volume is not constant then the equations for concentrations include \dot{V} and have different form (this is typical for combustion reactions, for example). In our case study we assume that the volume is constant and the equation for concentration can be used

$$\frac{dc}{dt} = \sum_\rho r_\rho \gamma_\rho. \quad (1.5)$$

Mass Action Law (MAL) gives a representation of the reaction rate as the functions of concentrations:

$$r_\rho = k_\rho \prod_{i=1}^n c_i^{\alpha_{\rho i}}, \quad (1.6)$$

where k_ρ are kinetic constants (they depend on the temperature but not on the concentrations).

For the intervals of kinetic constants, we work with differential inclusions

$$\frac{dc}{dt} \in \sum_\rho r_\rho \gamma_\rho; \quad \min k_\rho \leq k_\rho \leq \max k_\rho \quad (1.7)$$

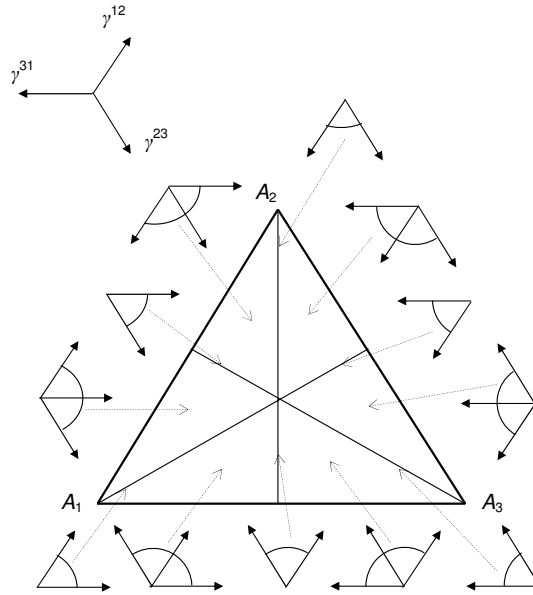


FIGURE 1. Kinetic inclusion for first order kinetics with three components and given equilibrium. The triangle of concentrations is split into compartments by the partial equilibria lines. The corresponding cones of possible vectors \dot{c} (the angles) for given equilibrium are piecewise constant (without any assumption of detailed balance).

2. A toy example

2.1. The system

Let us consider a reaction mechanism (1.1) [8].

The stoichiometric vectors of the reactions are

$$\gamma_1 = \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}; \quad \gamma_2 = \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}; \quad \gamma_3 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; \quad \gamma_4 = \gamma_{-4} = \begin{pmatrix} -2 \\ 3 \\ 0 \end{pmatrix}; \quad (2.1)$$

The reaction rates are: $r_1 = k_1 c_1$, $r_2 = k_2 c_2$, $r_3 = k_3 c_3$, $r_4 = k_4 c_1^2$, $r_{-4} = k_{-4} c_2^3$

The chemical kinetic inclusions for the given interval of constants are

$$\frac{dc}{dt} \in k_1 c_1 \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} + k_2 c_2 \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix} + k_3 c_3 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} + (k_4 c_1^2 - k_{-4} c_2^3) \begin{pmatrix} -2 \\ 3 \\ 0 \end{pmatrix}, \quad (2.2)$$

where $k_i \in [\min k_i, \max k_i]$.

This system has no linear conservation law (like mass balance). In chemical kinetics such systems might appear as subsystems of larger systems. For example, we can assume that the nonlinear reaction $2A_1 \rightleftharpoons 3A_2$ includes one more reagent, B : $2A_1 + B \rightleftharpoons 3A_2$ and the concentration of B is kept constant.

The systems with total mass balance cannot approach zero from a positive initial state, this means, it is *persistent*. Without such a conservation law persistence depends on the reaction mechanism. Nevertheless, we will demonstrate that solution of inclusion 2.2 cannot tend to zero from positive initial conditions.

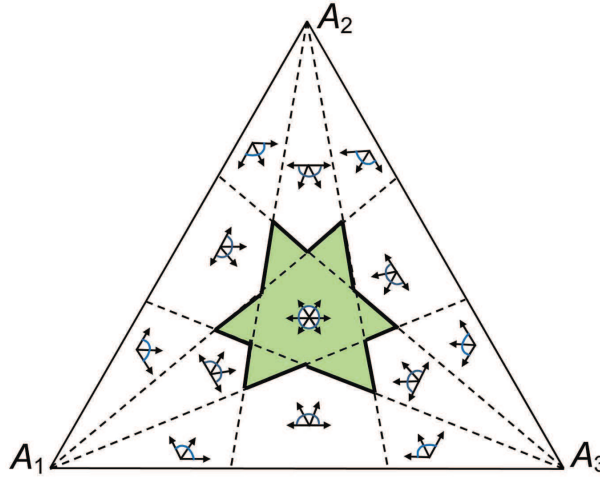


FIGURE 2. Partial equilibria of the reversible cycle with interval restrictions on the equilibrium constants. The lines of partial equilibria $A_i \rightleftharpoons A_j$, which correspond to the end of the intervals of equilibrium constants, split the triangle into several compartments. The borders of these compartments are combined from the intervals of the dashed lines. These dashed lines correspond to the minima and maxima of the equilibrium constants κ_j/κ_{-j} . In each compartment, the cone (the angle) of possible directions of \dot{c} is given. This is a proper cone (an angle that is less than π) outside the equilibria strips, a halfplane in an equilibrium strip of a single reaction, and a whole plane in the intersection of two such strips. The area of the possible equilibria (the angle of possible directions of \dot{c} is the whole plane) is outlined by bold line and colored in green.

2.2. Transformation to fully reversible system

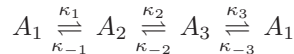
Let us use the local equivalence of reversible and general Markov chains with the same equilibrium [6] (this is a particular case of local equivalence of systems with detailed and complex balance [7]) and represent the system (2.2) as a particular case of differential inclusion for a reversible reaction network $A_1 \rightleftharpoons A_2 \rightleftharpoons A_3 \rightleftharpoons A_1$, $2A_1 \rightleftharpoons 3A_2$ (with possible extension of the interval of constants).

For every first order kinetics with given equilibrium the velocity vector \dot{c} at each state c may be expressed as a velocity vector for a first order system with detailed balance and the same equilibrium (the choice of this system with detailed balance depends on the state c). The cone of the possible velocity vectors is piecewise constant (Fig. 1).

The equilibrium concentrations c_i^* in the irreversible cycle satisfy the following identities:

$$k_1 c_1^* = k_2 c_2^* = k_3 c_3^*, \quad \frac{c_i^*}{c_j^*} = \frac{k_j}{k_i}$$

Instead of the irreversible cycle of linear reactions we will take the reversible cycle



with the interval restrictions on the *equilibrium constants* (the ratios of the reaction rate constants κ_j/κ_{-j})

$$\frac{\min k_2}{\max k_1} \leq \frac{\kappa_1}{\kappa_{-1}} \leq \frac{\max k_2}{\min k_1}, \quad \frac{\min k_3}{\max k_2} \leq \frac{\kappa_2}{\kappa_{-2}} \leq \frac{\max k_3}{\min k_2}, \quad \frac{\min k_1}{\max k_3} \leq \frac{\kappa_3}{\kappa_{-3}} \leq \frac{\max k_1}{\min k_3} \quad (2.3)$$

The detailed balance condition should also hold for the constants $\kappa_{\pm j}$:

$$\kappa_1 \kappa_2 \kappa_3 = \kappa_{-1} \kappa_{-2} \kappa_{-3}$$

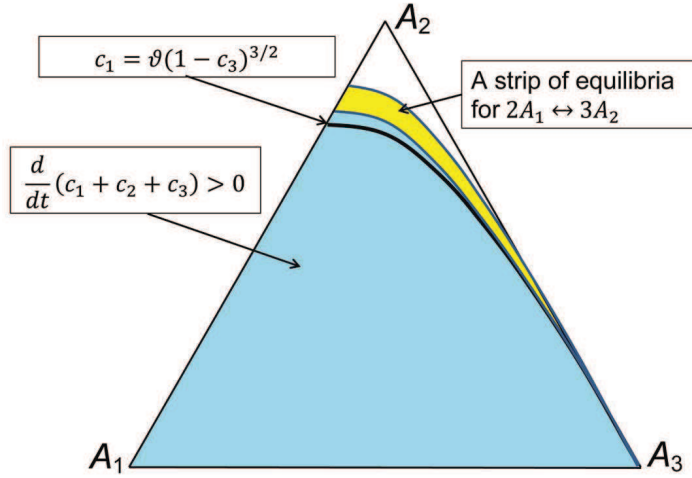


FIGURE 3. The equilibrium strip of the reaction $2A_1 \rightleftharpoons 3A_2$ (yellow) and the area where $\sum_i \dot{c}_i > 0$ (blue) rescaled from the triangle with $\sum c_i = \varepsilon$ to the unit triangle

In the graphic illustrations below we use the symmetric intervals for κ_i/κ_{-i} in the form

$$\frac{1}{\omega} \leq \frac{\kappa_1}{\kappa_{-1}} \leq \omega$$

for some $\omega > 1$. Every interval could be included into such a symmetric one. Therefore, if we demonstrate persistence for the systems with symmetric intervals then it the persistence for all positive intervals is also proven.

The equilibria for this cycle satisfy the conditions

$$\kappa_1 c_1^* = \kappa_{-1} c_2^*, \quad \kappa_2 c_2^* = \kappa_{-2} c_3^*, \quad \kappa_3 c_3^* = \kappa_{-3} c_1^*$$

These conditions provide the same range of equilibrium concentrations for the reversible and irreversible cycles. Therefore, the possible value of \dot{c} for the irreversible cycle in the given interval of reaction rate constants always belongs to the cone of possible values of \dot{c} of the reversible cycle under given restrictions.

For the reversible cycle the reaction rates are

$$r_1 = \kappa_1 c_1 - \kappa_{-1} c_2, \quad r_2 = \kappa_2 c_2 - \kappa_{-2} c_3, \quad r_3 = \kappa_3 c_3 - \kappa_{-3} c_1$$

The differential inclusion for the linear cycle is represented in Fig. 2. There are three types of areas: (i) area where the equilibria may be located and the direction of \dot{c} may coincide with any vector of the linear subspace $\sum_i \dot{c}_i = 0$, (ii) areas where direction of one reaction is indefinite but the signs of two other reactions rates are fixed, and (iii) areas where signs of all reaction rates are fixed. The cones (angles) of possible vectors \dot{c} are drawn in Fig. 2.

2.3. Separation of equilibria for different subsystems near origin

For the linear system the scheme presented in Fig. 2 does not depend on the positive value of the balance $\sum_i c_i = \varepsilon$. We can just rescale $c_i \leftarrow c_i/\varepsilon$ and return to the unit triangle with the unit sum of c_i . The situation is different for the nonlinear reaction $2A_1 \rightleftharpoons 3A_2$. Consider the “equilibrium strip” where the reaction rate $r_4 = k_4 c_1^2 - k_{-4} c_2^3$ may be zero for the admissible reaction rate constants:

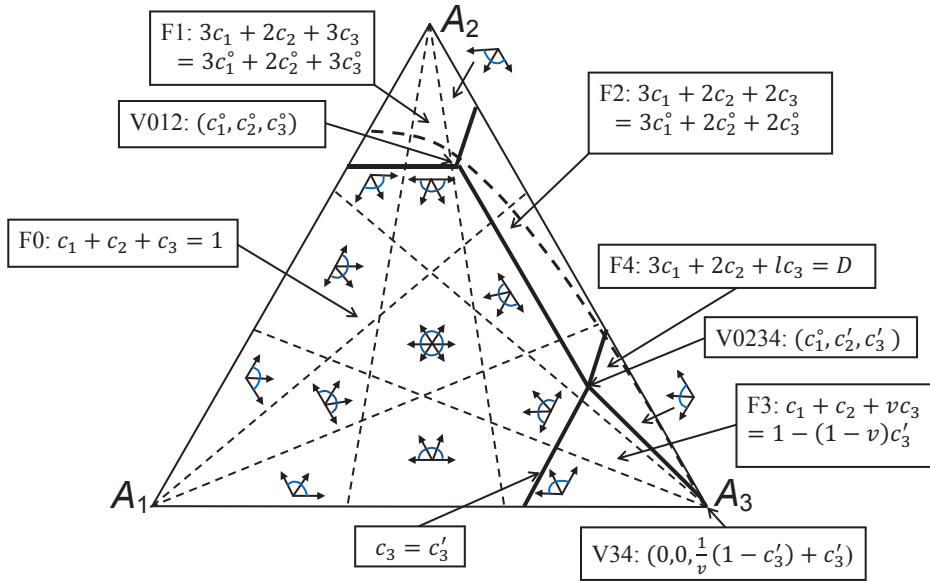


FIGURE 4. Faces of the peeled invariant set in the central projection onto unit triangle. The borders between faces are highlighted by bold.

$$\frac{\min k_{-4}}{\max k_4} \leq \frac{c_1^2}{c_2^3} \leq \frac{\max k_{-4}}{\min k_4}$$

Let us take this strip on the plane $\sum_i c_i = \varepsilon$ and return it to the unit triangle by rescaling ($c_i \leftarrow c_i/\varepsilon$). For small ε this strip approaches the $[A_2, A_3]$ edge of the triangle. It is situated between the line

$$c_1 = \sqrt{\varepsilon} \sqrt{\frac{\max k_{-4}}{\min k_4}} (1 - c_3)^{3/2}$$

and the segment $[A_2, A_3]$. Further we use the notation ϑ for the coefficient in this formula:

$$\vartheta = \sqrt{\varepsilon} \sqrt{\frac{\max k_{-4}}{\min k_4}}$$

The line

$$c_1 = \vartheta(1 - c_3)^{3/2} \quad (2.4)$$

separates the equilibrium strip of the reaction $2A_1 \rightleftharpoons 3A_2$ (where $r_4 = 0$ for some admissible combinations of the reaction rate constants) from the area where $r_4 > 0$ (i.e. $k_4(\varepsilon c_1)^2 - k_{-4}(\varepsilon c_2)^3 > 0$ for all admissible k_4, k_{-4} . (We use the rescaling from the triangle with $\sum c_i = \varepsilon$ to the unit triangle without further comments.)

This line is tangent to the segment at the vertex A_3 (Fig. 3). On the other side of the line the time derivative of $\sum_i c_i$ is positive:

$$\sum_i \dot{c}_i = r_4 > 0$$

2.4. Faces of peeled set and separation from origin

Let us describe first the structure of the peeled set. Select for peeling the set $U = \{c \mid \sum_i c_i \geq \varepsilon, c_i \geq 0\}$. The structure of peeling scaled to $c_1 + c_2 + c_3 = 1$ is presented in Fig. 4. It appears that the piecewise linear peeling is sufficient. There are five faces different from the coordinate planes. The face F0 is a polygon on the plane $\sum c_i = 1$. The face F1 is situated at the A_2 corner. It is produced by the peeling parallel to $\text{Span}\{\gamma_3, \gamma_4\}$. The plane of F1 is given by the equation $3c_1 + 2c_2 + 3c_3 = \text{const}$. The face F2 is presented by a parallelogram at the middle of the edge $[A_2, A_3]$ (Fig. 4). It covers the intersection of the equilibrium strips of the reactions $2A_1 \rightleftharpoons 3A_2$ and the reaction $A_2 \rightleftharpoons A_3$. F2 is produced by the peeling parallel to $\text{Span}\{\gamma_2, \gamma_4\}$. The plane is given by the equation $3c_1 + 2c_2 + 2c_3 = \text{const}$. Its intersection with the plane $c_1 + c_2 + c_3 = 1$ is a straight line $c_1 = c_1^\circ, c_2 + c_3 = 1 - c_1^\circ$ for a sufficiently small $c_1^\circ > 0$.

The final fragment of peeling is situated near the vertex A_3 (Fig. 4). It consists of two triangles. The first (F3) is a fragment of a plane $c_1 + c_2 + vc_3 = \text{const}$ ($0 < v < 1$). Parameter v is defined from the condition of positive invariance below.

The second triangle (F4) situated near the vertex A_3 is parallel to γ_4 and the common edge with F3. The general plane parallel to γ_4 is given by the equation $3c_1 + 2c_2 + lc_3 = D$. We will define the parameters l and D from the vertices of the face F3,

Let us define the parameters of this peeling. At the A_2 corner the peeling is parallel to $\text{Span}\{\gamma_3, \gamma_4\}$. The plane can be given by the equation $3c_1 + 2c_2 + 3c_3 = \text{const}$. The edge between this face and the face $\sum c_i = 1$ belongs to the straight line $c_2 = c_2^\circ, c_1 + c_3 = 1 - c_2^\circ$. The level c_2° should be selected above all the equilibria of the linear reactions (Fig. 2) but below the intersection of the curve (2.4) with the right border of the equilibrium strip of the reaction $A_1 \rightleftharpoons A_3$ given by the equation $c_3 = c_1 \max\left\{\frac{\kappa-3}{\kappa_3}\right\}$. For the intersection we have

$$c_3 = \vartheta \max\left\{\frac{\kappa-3}{\kappa_3}\right\} (1 - c_3)^{3/2}$$

Therefore, at this point

$$c_3 < \vartheta \max\left\{\frac{\kappa-3}{\kappa_3}\right\}$$

and $c_1 < \vartheta$ on the line (2.4). Therefore, we can select

$$c_2^\circ = 1 - \vartheta \left(\max\left\{\frac{\kappa-3}{\kappa_3}\right\} + 1 \right)$$

This c_2° is smaller than the value of c_2 at the intersection and for sufficiently small ϑ , the line $c_2 = c_2^\circ$ is close to the vertex A_2 and does not intersect the area of possible equilibria of linear reactions.

Consider intersection of the straight line $c_2 = c_2^\circ, c_1 + c_3 = 1 - c_2^\circ$ with the curve (2.4) and evaluate the value of c_1 at this intersection from above: $c_1 = \vartheta(c_2^\circ + c_1)^{3/2}$, $c_1 < \vartheta$, hence, $c_1 < c_1^\circ = \vartheta(c_2^\circ + \vartheta)^{3/2}$.

Thus, the vertex V012 at the intersection of three faces, F0, F1, and F2 is selected as $(c_1^\circ, c_2^\circ, c_3^\circ)$, where

$$\begin{aligned} c_1^\circ &= \vartheta \left(1 - \vartheta \max\left\{\frac{\kappa-3}{\kappa_3}\right\} \right)^{3/2} \\ c_2^\circ &= 1 - \vartheta \left(\max\left\{\frac{\kappa-3}{\kappa_3}\right\} + 1 \right) \\ c_3^\circ &= 1 - c_1^\circ - c_2^\circ = \vartheta \left(1 + \max\left\{\frac{\kappa-3}{\kappa_3}\right\} - \left(1 - \vartheta \max\left\{\frac{\kappa-3}{\kappa_3}\right\} \right)^{3/2} \right) \end{aligned}$$

To check that this point is outside the equilibrium strip of the reaction $A_1 \rightleftharpoons A_3$, we calculate

$$\frac{c_3^\circ}{c_1^\circ} = \frac{1 + \max\left\{\frac{\kappa-3}{\kappa_3}\right\}}{\left(1 - \vartheta \max\left\{\frac{\kappa-3}{\kappa_3}\right\} \right)^{3/2}} - 1 > \max\left\{\frac{\kappa-3}{\kappa_3}\right\}$$

The next group of parameters we have to identify are the coordinates of the vertex V0234 (c'_1, c'_2, c'_3) at the intersection of four faces F0, F2, F3, and F4. We will define it as the intersection of F0, F2, and F3 and then use its coordinates for definition of parameters of F4. One coordinate, c'_1 is, obviously, $c'_1 = c_1^\circ$ because the intersection of F2 and F0 is parallel to γ_2 , i.e. it is parallel to the edge $[A_2, A_3]$ of the unit triangle and c_1 is constant on this edge. Another coordinate, c'_3 can be easily determined from the condition that the line $c_3 = c'_3$ in the unit triangle should not intersect the strips of equilibria for the reactions $A_2 \rightleftharpoons A_3$ and $A_1 \rightleftharpoons A_3$. Immediately, these conditions give the inequalities that should hold for all admissible reaction rate constants:

$$c'_3 > \frac{\kappa_{-3}}{\kappa_3 + \kappa_{-3}}, \quad c'_3 > \frac{\kappa_2}{\kappa_2 + \kappa_{-2}}$$

Finally,

$$c'_3 > \max \left\{ \frac{1}{\min \left\{ \frac{\kappa_3}{\kappa_{-3}} \right\} + 1}, \frac{1}{1 + \min \left\{ \frac{\kappa_{-2}}{\kappa_2} \right\}} \right\}$$

We can take c'_3 between this maximum and 1, for example we propose

$$c'_3 = \frac{1}{2} + \frac{1}{2} \max \left\{ \frac{1}{\min \left\{ \frac{\kappa_3}{\kappa_{-3}} \right\} + 1}, \frac{1}{1 + \min \left\{ \frac{\kappa_{-2}}{\kappa_2} \right\}} \right\}$$

For sufficiently small ϑ , the inequality $c'_3 + c_1^\circ < 1$ holds, and we can take $c'_2 = 1 - c'_3 - c_1^\circ > 0$.

If we know c'_3 and v then we know the equation of the plane F4:

$$c_1 + c_2 + vc_3 = 1 - (1 - v)c'_3$$

We also find immediately the coordinates of the vertex V34, the intersection of F3 (and F4) with the coordinate axis A_3 . This vertex is $(0, 0, \frac{1}{v}(1 - c'_3) + c'_3)$.

Let us define the parameters l and D for the face F4. This face should include the vertices V0234 (c_1°, c'_2, c'_3) and V34 $(0, 0, \frac{1}{v}(1 - c'_3) + c'_3)$. Therefore,

$$l = v \left(2 + \frac{c_1^\circ}{c_1^\circ + c'_2} \right), \quad D = 3c_1^\circ + 2c'_2 + lc'_3$$

To demonstrate the positive invariance of the peeled set we have to evaluate the sign of the inner product of \dot{c} onto the inner normals to the faces on the faces.

The time derivatives of the concentrations are

$$\dot{c}_1 = -r_1 + r_3 - 2r_4, \quad \dot{c}_2 = r_1 - r_2 + 3r_4, \quad \dot{c}_3 = r_2 - r_3$$

The signs of some reaction rates are unambiguously defined on the faces:

- On F0 $r_4 > 0$;
- On F1 $r_1 < 0$, and $r_2 > 0$;
- On F2 $r_1 < 0$, and $r_3 > 0$;
- On F3 $r_2 < 0$, $r_3 > 0$, and $r_4 > 0$;
- On F4 $r_1 < 0$, $r_2 < 0$, and $r_3 > 0$.

The inner products of \dot{c} onto the inner normals to the faces are:

- On F0 $\frac{d}{dt}(c_1 + c_2 + c_3) = r_4 > 0$;
- On F1 $\frac{d}{dt}(3c_1 + 2c_2 + 3c_3) = -r_1 + r_2 > 0$;
- On F2 $\frac{d}{dt}(3c_1 + 2c_2 + 2c_3) = -r_1 + r_3 > 0$;

- On F3 $\frac{d}{dt}(c_1 + c_2 + vc_3) = (1 - v)(-r_2 + r_3) + r_4 > 0$ ($0 < v < 1$);
- On F4 $\frac{d}{dt}(3c_1 + 2c_2 + lc_3) = -r_1 - (2 - l)r_2 + (3 - l)r_3 < 0$ if $0 < l < 2$.

Thus, the peeled set is positively invariant if $0 < l < 2$. This means

$$0 < v < \frac{1}{1 + \frac{c_1^0}{2(c_1^0 + c_2^0)}}$$

It is sufficient to take $0 < v < \frac{2}{3}$ because of obvious inequality.

We have demonstrated that for any given range of positive kinetic constants any solution of the kinetic inclusion for the system (1.1) cannot approach the origin when $t \rightarrow \infty$. We have constructed a piecewise-linear surface that isolated the ε -vicinity of the origin from the outside. If $\varepsilon > 0$ is sufficiently small then this surface cannot be intersected by the solutions of the kinetic inclusion in the motion from the outside to the origin.

3. Discussion

The forward-invariant peeling is a universal procedure for producing forward-invariant sets for kinetic equations and inclusions. The peeling procedure used in this toy-example for isolation from zero differs from the general greedy peeling [7]. (It is a simplified version of the greedy peeling.) We have guessed the structure of the corner near A_3 and build two plain faces, F3 and F4, instead of a sequence of the curvilinear “cylindric” faces. This piecewise peeling is not minimal but is simpler for drawing.

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