ISSN 0012-9593

quatrième série - tome 43 *fascicule 1* *janvier-février 2010*

ANNALES SCIENTIFIQUES de L'ÉCOLE NORMALE SUPÉRIEURE

Thierry GOUDON & Alexis VASSEUR

Regularity analysis for systems of reaction-diffusion equations

SOCIÉTÉ MATHÉMATIQUE DE FRANCE

Ann. Scient. Éc. Norm. Sup.
4^e série, t. 43, 2010, p. 117 à 142

REGULARITY ANALYSIS FOR SYSTEMS OF REACTION-DIFFUSION EQUATIONS

BY THIERRY GOUDON AND ALEXIS VASSEUR

ABSTRACT. – This paper is devoted to the study of the regularity of solutions to some systems of reaction–diffusion equations. In particular, we show the global boundedness and regularity of the solutions in one and two dimensions. In addition, we discuss the Hausdorff dimension of the set of singularities in higher dimensions. Our approach is inspired by De Giorgi's method for elliptic regularity with rough coefficients. The proof uses the specific structure of the system to be considered and is not a mere adaptation of scalar techniques; in particular the natural entropy of the system plays a crucial role in the analysis.

RÉSUMÉ. – Ce travail est consacré à l'étude de la régularité des solutions de certains systèmes d'équations de réaction-diffusion. En particulier, nous montrons que les solutions peuvent être bornées et régulières en dimensions un et deux alors qu'en dimensions supérieures nous discutons la dimension de Hausdorff de l'ensemble des points singuliers. L'approche proposée ici s'inspire de la méthode de De Giorgi pour étudier la régularité de problèmes elliptiques avec des coefficients discontinus. La preuve exploite la stucture spécifique des systèmes considérés et n'est pas une simple adaptation de techniques scalaires. L'entropie associée naturellement au système joue un rôle crucial dans cette analyse.

1. Introduction

This paper is devoted to the analysis of the following system of reaction-diffusion equations

$$\begin{cases} \partial_t a_i - \nabla \cdot (D_i \nabla a_i) = Q_i(a), \qquad i \in \{1, \dots, p\}, \\ Q_i(a) = (\mu_i - \nu_i) \left(k_{\mathrm{f}} \prod_{j=1}^{p} a_j^{\nu_j} - k_{\mathrm{b}} \prod_{j=1}^{p} a_j^{\mu_j} \right), \\ a_{i\,|t=0} = a_i^0. \end{cases} \tag{1.1}$$

This work has been done while the first author was visiting ICES and the University of Texas at Austin. Thanks are addressed for their warm hospitality and support. We also thank J.-F. Coulombel who read preliminary versions and has suggested many improvements. The second author was partially supported by the NSF grant DMS-0607053.

The equation holds for $t \geq 0$ and the space variable x lies in Ω where

- either $\Omega = \mathbb{R}^N$,
- or $\Omega \subset \mathbb{R}^N$ is a bounded domain with smooth boundary and the system is completed by imposing the Neumann boundary condition

$$D_i \nabla a_i \cdot \nu(x)_{|\partial\Omega} = 0,$$

where $\nu(x)$ stands for the outer normal vector at $x \in \partial\Omega$.

Throughout the paper, the symbol ∇ denotes the gradient operator with respect to the space variable x only. The matrices $D_i(x)$ are required to satisfy

$$\begin{aligned} &D_i \in \big(L^\infty(\Omega)\big)^{N\times N}, \\ &D_i(x)\xi\cdot\xi \geq \alpha|\xi|^2, \qquad \alpha > 0 \qquad \text{for any } \xi \in \mathbb{R}^N,\ x \in \Omega. \end{aligned} \tag{1.2}$$

Let us comment this assumption:

- the analysis below is interesting when there are different diffusion matrices: assuming $D_i = D$, a common value, makes the problem easier;
- there is no regularity assumption on the coefficients;
- the standard uniform coercivity condition is assumed. The case of degenerate coefficients leads to specific difficulties which are beyond the scope of this paper.

Such a system is intended to describe e.g. the evolution of a chemical solution: the unknown a_i stands for the density of the species labelled by $i \in \{1,\dots,p\}$ within the solution. The right hand side of (1.1) follows from the mass action principle applied to the reversible reaction

$$\sum_{i=1}^p \nu_i A_i \leftrightarrow \sum_{i=1}^p \mu_i A_i,$$

where the μ_i and ν_i's—the so-called stoichiometric coefficients—are integers. The (positive) coefficients k_f and k_b are the rates corresponding to the forward and backward reactions, respectively. According to the physical interpretation, the unknowns are implicitly non-negative quantities: $a_i \geq 0$. In fact, this property holds thanks to the structure of the system. Indeed, (1.1) can be written

$$\partial_t a_i - \nabla\cdot(D_i\nabla a_i) + L_i(a)a_i = G_i(a) \tag{1.3}$$

where the nonlinear functions G_i and L_i have the property: if the components a_k of a are non-negative then $G_i(a) \geq 0$ and $L_i(a) \geq 0$. Hence preservation of non-negativity, when starting from a non-negative initial data, can be considered among the a priori estimates of the problem (see appendix for more details). The main ingredients of our analysis rely on the following properties:

- The mass is conserved. The stoichiometric coefficients satisfy

$$\text{There exists } (m_1,\dots,m_p) \in \mathbb{N}^p,\ m_i \neq 0, \text{ such that } \sum_{i=1}^p m_i\mu_i = \sum_{i=1}^p m_i\nu_i. \tag{1.4}$$

It implies the mass conservation

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=1}^p \int_\Omega m_i\, a_i\, \mathrm{d}x = 0.$$

– The entropy is dissipated. We set $K = k_{\rm b}/k_{\rm f}$, then

$$\sum_{i=1}^{p} Q_i(a)\ln(a_i/K^{1/(p(\mu_i-\nu_i))}) = -k_{\rm f}\Big(\prod_{i=1}^{p} a_i^{\mu_i} - K\prod_{i=1}^{p} a_i^{\nu_i}\Big)\ln\Big(\frac{\prod_{i=1}^{p} a_i^{\mu_i}}{K\prod_{i=1}^{p} a_i^{\nu_i}}\Big) \le 0. \tag{1.5}$$

In order to simplify the notations, and without loss of generality, we restrict ourselves to the case

$$m_i = 1, \qquad k_{\rm f} = 1 = k_{\rm b}.$$

A crucial role will be played by the quantity

$$\overline{\mu} = \sum_{i=1}^{p} \mu_i = \sum_{i=1}^{p} \nu_i,$$

where the coefficients μ_i and ν_i are still integers.

In our study of such systems restrictions on the space dimension N and the parameter $\overline{\mu}$ appear. One of the most interesting situations we are able to deal with is the following example corresponding to 4 species subject to the reactions

$$A_1 + A_3 \leftrightarrow A_2 + A_4.$$

It leads to

$$Q_i(a) = (-1)^{i+1}(a_2a_4 - a_1a_3). \tag{1.6}$$

We refer for a thorough introduction to the modeling issues and mathematical properties of such reaction diffusion systems to [11, 13, 14, 19, 20, 21, 23, 28, 31]. Information can also be found in the survey [6] with connection to coagulation-fragmentation models and in [24] for applications in biology. Let us also mention that (1.1) can be derived through hydrodynamic scaling from kinetic models, see [2].

In this contribution we are interested in the derivation of new L^∞ estimates and we investigate the regularity of the solutions of (1.1). Quite surprisingly, the question of global boundedness becomes trivial when the diffusion coefficients vanish. Indeed, consider $D_i = 0$, and a bounded initial value. The property (1.4) implies that for each x fixed, the total mass $\sum_{i=1}^{p} m_i a_i(t,x)$ is time independent. Then, the non-negativity of the a_i's implies that each a_i is uniformly bounded. Conversely, certain reaction diffusion systems might exhibit blow-up phenomena, see e.g. [22, 26], as it is also well known when considering nonlinear heat equations [15, 35]. Therefore global well-posedness and discussion of smoothing effects—that is gain of regularity of the solution compared to the initial data—is an issue.

Standard techniques can indeed be applied to show the existence of a smooth solution of (1.1) locally in time, with, say, initial data in $L^1 \cap L^\infty(\Omega)$. We sketch in the appendix the basic argument that proves the local existence of a smooth non negative solution. The challenging question consists in extending the result on arbitrarily large time intervals. Roughly speaking, this is due to a lack of estimates since the only natural bounds are provided by the mass conservation (1.4) and the entropy dissipation (1.5). In particular, the mass conservation only provides an estimate of the solution in L^1 which is not enough for the right hand side $Q_i(a)$ to make sense as a distribution! However, by using the sophisticated techniques introduced in [25, 26], it has been shown recently in [10] that the solutions of (1.1) in the quadratic case (1.6) are a priori bounded in $L^2((0,T)\times\Omega)$ so that the nonlinear reaction term makes sense at least in L^1. This non-trivial estimate can be obtained by exploiting

the entropy dissipation and the non-degeneracy of the diffusion coefficients. In [10], using also the arguments introduced in [25], it allows us to establish the global existence of weak solutions of (1.1), (1.6). Dealing with higher order nonlinearities or degenerate coefficients the difficulty might lead us to introduce a suitable notion of renormalized solutions, see [10] again. We also mention the recent work [27] where the quadratic system is analyzed with diffusion acting only in one direction. The dissipation property (1.5) is also the basis for studying the asymptotic trend to equilibrium [8, 9] in the spirit of the entropy/entropy dissipation techniques which are presented e.g. in [34] (we refer also to [1] for further investigation of the large time behavior of nonlinear evolution systems using the entropy dissipation).

Our approach is inspired by De Giorgi's methods for studying the regularity of solution of diffusion equations without requiring the regularity of the coefficients, see [7]. The crucial step consists in establishing a L^∞ estimate on the solution. Regularity of the solution follows in a classical way (see appendix). This approach has been used in [33] to obtain an alternative proof to the regularity results for the Navier-Stokes equation [4, 17] and it also shares some features with the strategy introduced in [29, 30]. It has also been applied to study convection-diffusion equations [18] and regularity for the quasi-geostrophic equation [5]. Here, it is worth pointing out that the proof utilizes strongly the structure of the whole system and the argument is not a mere refinement of a scalar approach. As we shall see however, restrictions appear between the space dimension N and the degree of nonlinearity of the reaction term measured by means of $\overline{\mu}$. For this reason, the L^∞ estimates can be proved in two dimension for the quadratic operator (1.6) or in one dimension considering cubic terms.

THEOREM 1.1. – *We consider the quadratic operator* (1.6) *(or assume* $\overline{\mu} = 2$*). Let* $N = 2$ *and suppose that the diffusion coefficients fulfill* (1.2)*. Let* $a_i^0 \geq 0$ *satisfy*

$$\sum_{i=1}^{4} \int_\Omega a_i^0 \big(1 + |x| + |\ln(a_i^0)|\big)\, \mathrm{d}x = M_0 < \infty. \tag{1.7}$$

Then, (1.1) *admits a global solution such that for any* $0 < T \leq T^\star < \infty$*,* a_i *belongs to* $L^\infty((T, T^\star) \times \Omega)$*.*

THEOREM 1.2. – *Let* $N = 1$ *with* $\overline{\mu} \leq 3$ *and suppose that the diffusion coefficients fulfill* (1.2)*. Let* $a_i^0 \geq 0$ *satisfy* (1.7)*. Then,* (1.1) *admits a global solution such that for any* $0 < T \leq T^\star < \infty$*,* a_i *belongs to* $L^\infty((T, T^\star) \times \Omega)$*.*

We point out that these statements do not require any regularity property on the diffusion coefficients D_i which are only supposed to be bounded. As a byproduct, by using the new bound, a direct bootstrap argument shows the global regularity of the solution (see appendix).

COROLLARY 1.1. – *Let the assumptions of Theorem 1.1 or 1.2 be fulfilled. Suppose moreover that the* D_i*'s belong to* $C^k(\Omega)$ *with bounded derivatives up to order* k*. Then, for any* $0 < T \leq T^\star < \infty$*, the solution belongs to* $L^\infty(T, T^\star; C^k(\Omega))$*. Accordingly for* C^∞ *coefficients with bounded derivatives, the solution is* C^∞ *on* $(T, T^\star) \times \Omega$*.*