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Global existence of renormalized solutions to entropy-dissipating reaction-diffusion systems

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Reaction-diffusion equations with mass-action kinetics occur in the mathematical modeling of many phenomena, e.g. in the modeling of chemical reactions or in drift-diffusion models for semiconductors. Consider a single reversible chemical reaction of the form

$$\alpha_1\mathcal{A}_1 + \ldots + \alpha_S\mathcal{A}_S \rightleftharpoons \beta_1\mathcal{A}_1 + \ldots + \beta_S\mathcal{A}_S$$

(with $\alpha_i, \beta_i \in \mathbb{N}_0$), where the $\mathcal{A}_i$ denote the different chemical species (i.e. the different types of molecules; e.g. $\mathcal{A}_1$ could be H_2O or O_2). Introduce the notation u_i for the concentration of the chemical species $\mathcal{A}_i$. The simplest corresponding reaction-diffusion equation with mass-action kinetics is then given by

$$\frac{d}{dt}u_i = a_i\Delta u_i + \underbrace{(\beta_i - \alpha_i)\left(c_F\prod_{k=1}^{S}u_k^{\alpha_k} - c_B\prod_{k=1}^{S}u_k^{\beta_k}\right)}_{=:R_i(u)} \quad \forall i \in \{1,\ldots,S\}, \tag{1}$$

where the $a_i > 0$ denote the species-dependent diffusion coefficients and where $c_F, c_B > 0$ denote reaction constants. For this equation, the entropy estimate

$$\frac{d}{dt}\int_\Omega \sum_{i=1}^{S}(\mu_i - 1 + \log u_i)u_i \; dx \leq -c\int_\Omega \sum_{i=1}^{S}|\nabla\sqrt{u_i}|^2 \; dx \tag{2}$$

(which is a consequence of the particular structure of the reaction terms $R_i(u)$ and which is valid for classical solutions e.g. in case of homogeneous Neumann boundary conditions and for appropriately chosen $\mu_i \in \mathbb{R}$, $c > 0$) prevents global blowup of solutions. Note that formally, the reaction-diffusion equation (1) may even be written as a gradient flow of the entropy [7].

Despite this absence of global blowup, even for the simple reaction-diffusion equation (1) global existence of any kind of solution in general has been an open problem, even for smooth initial data and bounded smooth domains. The key issue in establishing global existence of solutions is to give a meaning to the reaction terms $R_i(u)$: besides the entropy estimate, already on a formal level only an $L^2(\Omega\times[0,T])$ estimate is available for solutions [9]; however, in general higher powers of the solution occur in the reaction terms $R_i(u)$. Thus, *a priori* it is not known whether the reaction terms in (1) even define a distribution. For this reason, previous existence results have been limited to reactions of low degree, i.e. (very) small values of $\sum\alpha_k$ or $\sum\beta_k$, or almost coinciding diffusion coefficients, see e.g. [1, 4, 6, 8] and the references therein.

In the recent paper [5], we propose a notion of renormalized solutions for reaction-diffusion equations of the form

$$\frac{d}{dt}u_i = \nabla\cdot(A_i\nabla u_i) - \nabla\cdot(u_i\vec{b}_i) + R_i(u) \quad \forall i \in \{1,\ldots,S\}$$

and establish global existence of solutions. For the reaction rates $R_i(\cdot)$, besides local Lipschitz continuity and the natural condition $R_i(v) \geq 0$ in case $v_i = 0$ (a chemical species that is not present may not be consumed by reactions) our only assumption is that the entropy condition

$$\sum_{i=1}^{S} R_i(v)(\log v_i + \mu_i) \leq 0 \quad \forall v \in (\mathbb{R}_0^+)^S$$

holds for appropriate $\mu_i \in \mathbb{R}$. We would like to emphasize that this entropy condition is satisfied for all reversible reactions with mass-action kinetics; furthermore, it holds for all systems of reversible reactions with mass-action kinetics that are subject to the so-called condition of detailed balance; see e.g. [10].

In general, the concept of *renormalized solutions* for a partial differential equation (introduced by DiPerna and Lions [2, 3]) imposes an evolution equation for nonlinear functions $\xi(u)$ of the actual solution u, whenever ξ belongs to some suitable class of functions; more precisely, $\xi(u)$ is required to satisfy the equation deduced from the original PDE by a formal application of the chain rule. In case of the simplified equation (1), our definition of renormalized solutions consists of requiring that the equation

$$\begin{aligned} \int_\Omega \xi(u)\psi \, dx \bigg|_0^T = &- \int_0^T \int_\Omega \sum_{i,j=1}^{S} \psi a_i \partial_i \partial_j \xi(u) \nabla u_i \cdot \nabla u_j \, dx \, dt \\ &- \int_0^T \int_\Omega \sum_{i=1}^{S} a_i \partial_i \xi(u) \nabla u_i \cdot \nabla \psi \, dx \, dt \\ &+ \int_0^T \int_\Omega \sum_{i=1}^{S} \partial_i \xi(u) R_i(u) \psi \, dx \, dt \end{aligned} \tag{3}$$

must be satisfied for any $\xi \in C^\infty((\mathbb{R}_0^+)^S)$ with compactly supported derivatives, any test function $\psi \in W^{1,\infty}(\Omega)$, and any $T > 0$. Furthermore, we impose the regularity constraints $u_i \in L^\infty([0,T]; L^1(\Omega; \mathbb{R}_0^+))$ and $\sqrt{u_i} \in L^2([0,T]; H^1(\Omega))$.

In the construction of such renormalized solutions, two major difficulties occur: first, for the family of solutions u^ε to the regularized problems

$$\frac{d}{dt} u_i^\varepsilon = a_i \Delta u_i^\varepsilon + \frac{R_i(u^\varepsilon)}{1 + \varepsilon |R(u^\varepsilon)|} \quad \forall i \in \{1, \ldots, S\}, \tag{4}$$

compactness in $L^1(\Omega \times [0,T])$ is not immediate: a direct application of the Aubin-Lions Lemma is not possible due to the potential failure of the uniform boundedness of $\frac{d}{dt} u^\varepsilon$ in $L^1([0,T]; (H^m(\Omega))')$ for all m. Introducing a family φ_i^E of multi-variable truncations of the map $v \mapsto v_i$ – the truncation occurring whenever $\sum_{k=1}^S v_k$ exceeds E –, this problem can be overcome by applying the Aubin-Lions Lemma to the family $\varphi_i^E(u^\varepsilon)$ instead.

The key difficulty in the construction of renormalized solutions, however, is the lack of compactness in $L^2(\Omega \times [0,T])$ of the spatial derivatives ∇u^ε of the approximating sequence. Only *weak* convergence of $\nabla \sqrt{u_i^\varepsilon}$ in $L^2(\Omega \times [0,T])$ is implied by the known mathematical energy estimates (which basically consist just of the entropy estimate (2)). The functions u^ε can be shown to satisfy a renormalized formulation of the regularized equation (4) which is completely analogous to (3). However, in the limit $\varepsilon \to 0$ convergence of the first term on the right-hand side of the ε-regularized version of (3) cannot be established directly for our approximating sequence u^ε, as this term contains a product of spatial derivatives.

Instead, we resort to an alternative strategy: we pass to the limit $\varepsilon \to 0$ in the equation satisfied by $\varphi_i^E(u^\varepsilon)$; in this limit, only the oscillations of the sequence

$\nabla\sqrt{u_j^\varepsilon}$ on the set $\{E \leq \sum_{k=1}^S u_k^\varepsilon \leq 2E\}$ may cause a convergence defect in our equation, as only in this range $\varphi_i^E(\cdot)$ is non-affine. From the resulting equation for $\varphi_i^E(u)$ which is only satisfied up to this convergence defect, an equation for $\xi(\varphi^E(u))$ which also only holds up to this convergence defect may be derived by a generalized chain rule. Finally passing to the limit $E \to \infty$, an exact equation for $\xi(u)$ is derived by showing that the convergence defect vanishes in the limit $E \to \infty$. The latter issue is the most delicate part of the proof. It is accomplished by a Fatou-type estimate of the form

$$\sum_{\hat{E}=0}^{\infty} \lim_{\varepsilon\to 0} \int_0^T \int_\Omega \chi_{\{\hat{E}\leq\sum_{k=1}^S u_k^\varepsilon<\hat{E}+1\}} |\nabla\sqrt{u_i^\varepsilon}|^2 \, dx \, dt \leq \liminf_{\varepsilon\to 0} \int_0^T \int_\Omega |\nabla\sqrt{u_i^\varepsilon}|^2 \, dx \, dt$$

(the expression on the right-hand side being finite due to the entropy estimate) which entails the desired decay of oscillations as $E \to \infty$

$$\lim_{E\to\infty} \lim_{\varepsilon\to 0} \int_0^T \int_\Omega \chi_{\{E\leq\sum_{k=1}^S u_k^\varepsilon\leq 2E\}} |\nabla\sqrt{u_i^\varepsilon}|^2 \, dx \, dt = 0.$$

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