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Partial Differential Equations

Strong solutions to a class of air quality models

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Abstract

We are concerned with strong L_2 solutions to a class of degenerate elliptic reaction diffusion systems associated with air quality models. ***To cite this article: W.E. Fitzgibbon et al., C. R. Acad. Sci. Paris, Ser. I 339 (2004).***

Résumé

Solutions fortes pour une classe de modèles de qualité de l'air. On étudie l'existence de solutions fortes dans L_2 pour une classe de systèmes de réaction diffusion elliptiques dégénérés associés à des modèles de qualité de l'air. ***Pour citer cet article : W.E. Fitzgibbon et al., C. R. Acad. Sci. Paris, Ser. I 339 (2004).***

Version française abrégée

On s'intéresse à l'existence de solutions fortes pour le système de réaction diffusion dégénéré suivant

$$\partial\varphi_i/\partial t = d\,\partial^2\varphi_i/\partial z^2 + \nabla\cdot\omega\varphi_i + f_i(\varphi_1,\dots,\varphi_N) + g_i, \quad 1 \leqslant i \leqslant N,$$

posé dans le domaine $Q = \Omega\times[0,1]\times[0,T]$; ici Ω est un ouvert du plan de variables (x,y), $[0,1]$ représente la variable z verticale et $[0,T]$ l'intervalle de temps de l'étude. Le champ de vecteurs $\vec{\omega} = (\omega_1,\omega_2,\omega_3)$ est à divergence nulle dans $\Omega\times[0,1]$. Ce système est issu d'un modèle de qualité de l'air, cf. [5,9].

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On lui associe des conditions de flux sur les bords supérieur et inférieur de Q :

$$\partial\varphi_i/\partial z + \upsilon_i\varphi = e_i \quad \text{pour } z = 0 \quad \text{et} \quad \partial\varphi_i/\partial z = 0 \quad \text{pour } z = 1,$$

des conditions initiales en $t = 0$,

$$\varphi_i(x, y, z, 0) = \varphi_{i_o}(x, y, z)$$

ainsi que des conditions aux limites sur la partie Σ_- de la frontière latérale de Q où le champ de vecteur $\vec{\omega}$ est sortant.

On peut alors considérer ce système comme un système parabolique dégénéré ou mieux comme un système elliptique dégénéré. Sous l'hypothèse que le terme de réaction est conservatif et quasipositif on peut alors établir des estimations a priori dans L_∞ pour des solutions fortes dans L_2. L'existence résulte alors de techniques de perturbations pour des opérateurs maximaux monotones.

1. Introduction

The photochemical production and atmospheric dispersion of ozone and other pollutants is traditionally modeled by advection reaction diffusion systems. In many cases, cf. [5,9], one ignores the horizontal components of diffusion and assumes that diffusion transpires only vertically. This produces a degenerate reaction diffusion system of the form:

$$\partial\varphi_i/\partial t = d\,\partial^2\varphi_i/\partial z^2 + \nabla\cdot\omega\varphi_i + f_i(\varphi_1,\ldots,\varphi_N) + g_i$$

where $d > 0$ and $i = 1,\ldots,N$. The state variables, φ_i, represent concentration densities of the chemical species involved in the photochemical reaction. The relevant chemistry of the reaction process appears in the nonlinear functions, $f_i(\varphi_1,\ldots,\varphi_N)$, with the terms, g_i, representing elevated point sources. In practice these systems can be extraordinarily large with N possibly in the hundreds. The advection terms, $\vec{\omega} = (\omega_1, \omega_2, \omega_3)$, describe transport from the velocity vector field of atmospheric current or wind. Typically one is interested in distribution of chemical concentrations over a specified geographic area. We therefore take as a modeling region a spatial cylinder of fixed height over a fixed two dimensional region, Ω. The bottom of the cylinder lies on the land surface of the earth and the top is the boundary of the troposphere. For our purposes we shall normalize the height to be one. Chemical species involved in the photochemical process are emitted upward from both anthropogenic and biogenic sources. Here set the upward flux equal minus a deposition flux,

$$\partial\varphi_i/\partial z + \upsilon_i\varphi = e_i \quad \text{for } z = 0. \tag{1}$$

We stipulate that e_i is a smooth, nonnegative function of space and time and $\upsilon_i > 0$ is a positive constant, cf. [5]. On the top of the cylinder we prescribe a simple no flux boundary condition,

$$\partial\varphi_i/\partial z = 0, \quad \text{for } z = 1. \tag{2}$$

The boundary conditions for the cylinder use measured concentrations together with meteorological data for the wind to describe the chemical flux into the cylinder. The exact description of the boundary conditions is quite technical [1,3,6–8]; see below. Finally we need to provide initial conditions. We require the initial data,

$$\varphi_i(x, y, z, 0) = \varphi_{i_o}(x, y, z) \tag{3}$$

for $i = 1$ to N is a smooth, nonnegative function of space. As previously mentioned the reaction vector field is complex and can be quite large possibly having hundreds of components. Typically, the reaction vector field satisfies a system of conservation laws and does not point out of the positive cone of $\Re^N$. For present purpose we shall assume that:

(i) $\sum_{i=1}^{N} f_i(\varphi) \leqslant 0 \quad \text{for } \varphi \in (\Re^N)^+,$

(ii) $f_i(\varphi) \geqslant 0 \quad \text{for } \varphi \in (\Re^N)^+, \text{ with } \varphi_i = 0.$

It has become common to call vector fields that satisfy (i) and (ii) conservative, quasipositive vector fields.

We also make the standard assumption of incompressibility (in this case three dimensional), i.e., we have $\partial\omega_1/\partial x + \partial\omega_2/\partial y + \partial\omega_3/\partial z = 0$. Taken together these assumptions produce a system of the form,

$$\partial\varphi_i/\partial t = d\,\partial^2\varphi_i/\partial z^2 + \omega_1\partial\varphi_i/\partial x + \omega_2\partial\varphi_i/\partial y + \omega_3\partial\varphi_i/\partial z + f_i(\varphi) + g_i. \tag{4}$$

Standard practice would be to be to view (4)-(3)-(2)-(1) as a degenerate parabolic (or ultra parabolic) evolution system with degeneracies in the horizontal spatial components and to obtain well-posedness via application of a time dependent variation of parameters or Duhamel formula. However, we shall find convenient to view it as a degenerate elliptic system with degeneracies in the space and time variables on the four dimensional vector field. In this context we can find a natural way of using the advective flux define boundary provide boundary conditions on those portions of the our domain. We have a four dimensional vector field of the form $(\omega_1, \omega_2, \omega_3, -1)$ and we make note of the fact that our initial condition will be prescribed as via the fact that the four-component vector field points into the four dimensional region on the face prescribed by $t = 0$. We shall obtain a priori estimates by virtue of a weak maximum principle and our existence results will follow.

2. Details of the problem

We shall use existing theory of degenerate elliptic operators and scalar equations. For a complete development of this theory the reader is referred to [1,3,6,7] [8]. If our systems had no vertical diffusion they would be reactive transport equations and the fundamental linear transport theory of [1] would be applicable. We introduce the space time cylinder, $Q = \Omega \times [0,1] \times [0,T]$, for some $T > 0$. We hope that we do not do not belabor the obvious by pointing out that the advection field for the parabolic operator is $\omega = (\omega_1(x,y,z,t), \omega_2(x,y,z,t), \omega_3(x,y,z,t))$ and that the advection vector for the degenerate elliptic operator is the four-dimensional vector field $\widetilde{\omega} = (\omega_1(x,y,t), \omega_2(x,y,t), \omega_3(x,y,z,t), -1)$. We make a smoothness assumption, $(\omega_1, \omega_2, \omega_3) \in C^1(\overline{Q})$. We introduce the first order differential operator with the equation

$$\Lambda\phi = \partial/\partial x(\omega_1\phi) + \partial/\partial y(\omega_2\phi) + \partial/\partial z(\omega_3\phi) - \partial\phi/\partial t = \omega_1\partial\phi/\partial x + \omega_2\partial\phi/\partial y + \omega_3\partial\phi/\partial z - \partial\phi/\partial t,$$

and the second order differential operator

$$£_*\phi = d\,\partial^2\phi/\partial z^2 \tag{5}$$

with constant $d > 0$. We set

$$£\phi = £_*\phi + \Lambda\phi. \tag{6}$$

We let $\eta = (\eta_1, \eta_2, \eta_3, \eta_4)$ denote the unit outward normal on the boundary of our space time cylinder Q. We let

$$Q_e = \{(x,y,1,t) \in \partial Q\} \cup \{(x,y,0,t) \in \partial Q\} = Q_{e_U} \cup Q_{e_B} \tag{7}$$

and introduce the Fichera function $l = -\omega_1\eta_1 - \omega_2\eta_2 - \omega_3\eta_3 + \eta_4$. We denote by ∂Q_-, ∂Q_0 and ∂Q_+ the subsets of $\partial Q - \partial Q_e$ where $l < 0$, $l = 0$ and $l > 0$ respectively. We impose the technical regularity assumption on the boundaries of ∂Q_e, ∂Q_-, ∂Q_0 and ∂Q_+ given by A_2 in [6], this is it is either smooth or small enough. We set:

$$L_l^2(\partial Q_-) = \left\{\phi : \partial Q_- \to \Re \,\Big|\, \int_{\partial Q_-} |l|\phi^2\,\mathrm{d}\sigma < \infty\right\},$$

$$L_l^2(\partial Q_+) = \left\{\phi : \partial Q_+ \to \Re \,\Big|\, \int\limits_{\partial Q_-} l\phi^2 \,\mathrm{d}\sigma < \infty\right\}.$$

Our boundary conditions assume the form,

$$\partial\phi/\partial z = 0, \quad \text{on } (x, y, 1, t) \in \partial Q \tag{8}$$

and

$$\partial\phi/\partial z + \upsilon\phi = e, \quad \text{on } (x, y, 0, t) \in \partial Q \tag{9}$$

and

$$\phi(x, y, z, 0) = \phi_0(x, y, z), \quad \text{for } (x, y, z) \in \Omega \times (0, 1) \tag{10}$$

and

$$\phi(x, y, z, t) = \theta(x, y, z, t) \quad \text{for } (x, y, z, t) \in \partial Q_- - \big(\Omega \times \{0\}\big). \tag{11}$$

We require that $\varphi_{0_i} \in C^1(\Omega)$ with $\varphi_{0_i}(x, y, z) \geqslant 0$ for $(x, y, z) \in \Omega$ and $\theta_i \in L_2(\overline{\partial Q_-} - (\Omega \times \{0\}))$ with $\theta_i(x, y, z, t) \geqslant 0$ for $(x, y, z, t) \in \partial Q_- - (\Omega \times \{0\})$. Finally we stipulate that the constants $\upsilon_i > 0$ and that $e_i \in C^1(\overline{\Omega} \times [0, T])$ with $e_i(x, y, t) \geqslant 0$ on $\Omega \times [0, T]$.

In this setting our system has the form,

$$-\pounds(\varphi_i) = -d\, \partial^2\varphi_i/\partial z^2 - \omega_1\partial\varphi_i/\partial x - \omega_2\partial\varphi_i/\partial y - \omega_3\partial\varphi_i/\partial z + \partial\varphi_i/\partial t = f_i(\varphi) + g_i. \tag{12}$$

By a strong L_2 solution to the degenerate elliptic boundary value problem we mean $\varphi = \{\varphi_1, \ldots, \varphi_N\}$ so that:

$$\varphi_i \in L_\infty(Q), \quad \partial^2\varphi_i/\partial z^2 \in L_2(Q),$$
$$\omega_1\partial\varphi_i/\partial x + \omega_2\partial\varphi_i/\partial y + \omega_3\partial\varphi_i/\partial z - \partial\varphi_i/\partial t \in L_2(Q) \quad \text{with } \varphi_i\,|_{\partial Q\_} \in L_2(\partial Q\_)$$

so that each φ_i satisfies the partial differential equation (12) and boundary conditions (8)–(11) in the a.e. sense (with respect to the appropriate measures). If $\varphi = \{\varphi_1, \ldots, \varphi_N\}$ is a strong solution we can a obtain an a priori L_∞ estimate for strong solutions. Our estimate is derived from a maximum principle for degenerate elliptic systems, cf. [6]. It is based on an estimate for $\Phi = \sum_{i=1}^N \varphi_i$ and it makes strong use of the quasipositivity and the balancing property of the reaction vector field. However, given this it is independent of a particular choice of reaction vector field, $f = \{f_i\}_{i=1}^N$. We have:

Theorem 2.1. *If the foregoing hypotheses are satisfied and $\varphi = \{\varphi_1, \ldots, \varphi_N\}$ is a strong L_2 solution to* (4), (8)–(11) *on Q with nonnegative components, then there exists an $M = M(Q)$ so that*

$$\max\big\{\|\varphi_i\|_{\infty,Q},\ 1 \leqslant i \leqslant N\big\} \leqslant M.$$

We can also guarantee the existence of strong L_2 solutions. The proof uses the a priori estimates of the previous theorem and an abstract surjectivity result for perturbations of maximal monotone operators, cf. [2].

Theorem 2.2. *If $f = \{f_i\}_{i=1}^N : \Re^N \to \Re^N$ is a balanced quasipositive vector field satisfying* (i) *and* (ii) *then there exists a strong L_2 solution to* (4) *with boundary conditions* (8)–(11) *on ∂Q.*

More details are found in [4].

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