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Singular shock solutions in nonlinear chromatography

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HIGHLIGHTS

- Investigation of a system of hyperbolic PDEs applied in nonlinear chromatography.
- Presentation of initial and feed conditions resulting in singular solutions.
- Derivation of properties of the singular shocks by two different approaches.
- Consistent results with both approaches.

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ABSTRACT

We consider a hyperbolic system of partial differential equations which is of interest in the context of nonlinear chromatography. Under certain initial and feed conditions, specified in the first part of this contribution, solutions to this system are unbounded. Characteristic properties of the singular shocks, i.e. propagation velocity and strength, are derived by two different approaches, based on Colombeau generalized functions and on box approximations of the unbounded solution, respectively. The derived expressions are found to be consistent for both approaches.

1. Introduction

Let us consider the two dimensional system of first order PDEs, which are of the conservation laws type:

$$\left(u_i + \frac{a_i u_i}{1 - u_1 + u_2}\right)_\tau + (u_i)_x = 0 \qquad (i = 1, 2)\,, \tag{1}$$

where only the pairs (u_1, u_2) that fulfill the conditions $u_1 \geq 0$, $u_2 \geq 0$ and $d = 1 - u_1 + u_2 > 0$ are allowed, and the inequality $a_2 > a_1 > 0$ holds true [1]. For convenience, we also define

$$v_i = \frac{a_i u_i}{1 - u_1 + u_2} = \frac{a_i u_i}{d} \qquad (i = 1, 2). \tag{2}$$

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For this system, the following Riemann problem will be studied:

$$\begin{aligned} &\text{at} \quad \tau = 0,\ 0 \le x \le 1: \quad u_i = u_i^B\ , \quad \text{(state B)}, \\ &\text{at} \quad x = 0,\ 0 < \tau < +\infty: \quad u_i = u_i^A\ , \quad \text{(state A)}. \end{aligned} \tag{3}$$

The equations above describe a system of great interest in nonlinear chromatography when u_i and v_i are interpreted as dimensionless fluid phase and adsorbed phase concentrations of the chemical species of index i, whereas a_i is the retention factor of species i; τ is a dimensionless time and x is the normalized space coordinate along the chromatographic column [2]. This is the so called equilibrium theory model of chromatography, and Eq. (2) is the so called adsorption isotherm, written for the case of competitive (species 2)-cooperative (species 1) adsorption.

Note that several researchers [3–5] have recently studied Eqs. (1), but in the special case where $a_1 = a_2 = 1$, which leads admittedly to a rather different and possibly simpler mathematical solution. The condition $a_1 = a_2 = 1$ is non-generic from a physical point of view, as it represents a combination of values of physical parameters, which is impossible in practice. Moreover, if $a_1 = a_2$, independently of their specific value, the two species have the same retention factor, i.e. they cannot be separated by chromatography, thus making its use pointless.

The interest for system (1) stems from three facts. First, under well specified conditions the Riemann problem (3) admits a singular solution of the delta-shock type that is in line with numerical solutions of a regularization of Eqs. (1), including a dispersion term [1]. Secondly, exact expressions for the delta shock's rate of propagation and for the rate of change of the delta shock's strength have been obtained [1]. Finally, there is an ongoing effort to find experimental evidence of the delta-shock, which has so far only been derived mathematically. In a first study, an experimental system was identified, which apparently fulfilled all prerequisites (adsorption behavior) to exhibit a delta-shock. At conditions which theoretically should result in a delta-shock, this system exhibited a very similar behavior, which was at the time interpreted as the experimental evidence of the delta-shock [6]. However, during a more in depth analysis, inconsistencies between theory and experimental behavior became evident; and it was finally shown that the adsorption behavior of the experimental system differed in fact from the adsorption isotherm defined in Eq. (2) [7,8].

In a previous paper, Eqs. (1) were proven to exhibit singular solutions, exact criteria on the Riemann problem were derived for the occurrence of the singular solution, a smooth approximation, constituting a solution to Eq. (1) in the sense of weak convergence, was introduced first and then used to derive closed expressions for the rate of propagation of the delta-shock and for the rate of growth of its strength [1]. The latter was achieved by following an approach similar to what Keyfitz and Kranzer used in section 2.2 of their 1995 seminal paper [9]. The expressions derived in [1] have been confirmed very recently by Tsikkou [10], who used the Geometric Singular Perturbation Theory to show existence of a singular solution to Eqs. (1).

In this work, again in the same spirit of the previous paper [1], we present two alternative ways of reaching the same results. The first approach is based on Colombeau generalized functions, whose representatives can be considered as the smooth approximations used in [1]. Although the presented approach is basically analogue to the one presented in [1], in this contribution we make rigorous use of the Colombeau algebra, and thus use that approach in more general terms. The second approach, which is novel in the context of the considered system of PDEs, is based on box approximations (as in section 2.3 of [9]). The manuscript is structured as follows: First the key features of Eqs. (1) are summarized in Section 2, then the approaches based on Colombeau generalized functions (Section 3), and on box approximations (Section 4), are presented and discussed. Section 5 finally brings the two approaches together to obtain exact results about the delta-shock solutions.