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The variational formulation of a non-equilibrium traffic flow model: theory and implications

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Abstract

The analysis and numerical solution of non-equilibrium traffic flow models in current literature are almost exclusively carried out in the hyperbolic conservation law framework, which requires a good understanding of the delicate and non-trivial Riemann problem for conservation laws. In this paper, we present a novel formulation of certain non-equilibrium traffic flow models based on their isomorphic relation with optimal control problems. This formulation extends the minimum principle observed by the LWR model. We demonstrate that with the new formulation, generic initial-boundary conditions can be conveniently handled and a simplified numerical solution scheme for non-equilibrium models can be devised. Besides deriving the variational formulation, we provide a comprehensive discussion on its mathematical properties and physical implications.

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1. Introduction

Despite the extensive applications of the Lighthill-Whitham-Richards (LWR) model for solving various real-world transportation problems, its capability of modeling some practically important phenomena, e.g. capacity drop and stop-and-go waves, is known to be limited. Various extensions of the LWR model have been developed to address this issue, among which the non-equilibrium traffic flow models constitute a major category. Most non-equilibrium traffic flow models consist of two equations, which can usually be written in the following form,

$$\begin{cases} \partial_t \rho + \partial_x(\rho v) = 0 \\ F(\rho, v, \partial_x v, \partial_t v, \partial_x \rho, \partial_t \rho) = 0 \end{cases} \tag{1}$$

Here ρ, v, and $\partial_t \cdot$, $\partial_x \cdot$ denote traffic density, traffic speed, the partial derivative with respect to time t and space x, respectively. The first equation of (1) simply expresses the fact that total number of vehicles

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is conserved. The second equation of (1) prescribes a dynamical relation between traffic speed and density, which reflects certain behavioral postulations or empirical measurements.

Despite its ability in explaining complicated macroscopic traffic phenomena and its intimate relation with car-following behaviors, the non-equilibrium modeling paradigm has raised numerable puzzles and debates, on issues such as wrong-way travel and violation of anisotropic property (Daganzo, 1995; Zhang, 2009; Helbing & Johansson, 2009; Helbing, 2009). Substantial efforts have been devoted to resolving these puzzles from behavioral and mathematical perspectives (e.g., Zhang, 2002; Aw & Rascle, 2000). It is recognized that some mathematical artifacts, e.g. faster-than-traffic waves, can be rectified in the classical hyperbolic conservation law (i.e. kinematic wave, KW) framework (Dafermos, 2005).

In this paper, we aim to provide an alternative angle to understand the traits of system (1), in particular its dynamics in the vicinity of complicated boundaries. Our approach is based on the variational formulation (VF) of KW models, which originates from their connection with Hamilton-Jacobi equations. In the equilibrium case, such a connection is realized and it is known that the variational formulation can provide several important enhancements over the traditional KW treatments in the traffic flow modeling context, including a compact analytical solution form, relative easiness to handle discrete objects in traffic streams, etc. (Daganzo, 2005a,b). We will show constructively that for a certain case of system (1), its VF exists and hence these appealing features carry over to the non-equilibrium model. With the VF perspective, we acquire deeper understanding of the mathematical properties, physical implications and numerical solutions of System (1), such that the basis of non-equilibrium modeling is further reinforced.

The remainder of this paper is organized as follows. In Section 2, we discuss the qualitative properties and physical implications of non-equilibrium traffic flow models in conservative form. In Section 3, through exploiting their special mathematical structure, we develop a variational formulation of non-equilibrium traffic models that adopt conservative forms. In Section 4, a numerical scheme based on the variational characterization of these non-equilibrium models is given. In Section 5, we summarize the findings and briefly remark on some ongoing problems related to the variational formulation of traffic flow models.

2. Non-equilibrium model as a 2 × 2 conservative system

As we mentioned earlier, System (1) consists of a conservation equation and an equation of motion. Since the second equation encapsulates the behavioral aspects of vehicular traffic flow, it is anticipated that solution properties of (1) are mainly dictated by it. Many early traffic models, usually derived from car-following heuristics, amounts to letting the total derivative of traffic speeds $\partial_t v + v\partial_x v$ be a function of various stimuli, including $\rho, \partial_x\rho, v - v_e(\rho)$ ($v_e(\cdot)$ is a nominal equilibrium speed-density relation). One example is the model of Payne (1971), which defines (T is so-called relaxation time)

$$\partial_t v + v\partial_x v = -\frac{v - v_e(\rho)}{T} + \frac{v_e'(\rho)}{2T\rho}\frac{\partial\rho}{\partial x} \tag{2}$$

For a review of models alike and their shortcomings, the reader is referred to Daganzo (1995) and Zhang (1998). We note that one major reason accounting for the fallacy associated with such models, e.g. wrong-way travel, is due to lack of mathematical consciousness in tackling discontinuities (shocks) in solutions.

2.1. Conservative form

Better insights into non-equilibrium models, regarding well-posedness, admissible wave patterns and valid numerical discretizations, are obtained when they are treated in the hyperbolic conservation law framework (Dafermos, 2005). Thus not surprisingly, most recent non-equilibrium models, e.g. Aw & Rascle (2000) and Zhang (2002), employ hyperbolic conservation law methodologies intensively.

A system of conservation law refers to the following set of equations

$$\begin{cases} \partial_t u_1 + \partial_x f(u_1, u_2) = 0 \\ \partial_t u_2 + \partial_x g(u_1, u_2) = 0 \end{cases} \tag{3}$$

where u_1, u_2 are state variables and (f, g) is called a flux pair. This set of equations is an evident extension of the LWR model, which considers a coupled pair of state variables $U \equiv (u_1, u_2)$ instead of a single scalar state variable ρ. As in the LWR model, essentially all information on dynamics of this system is encoded in the flux pair. Actually, it is straightforward to write (3) in a compact vectorial form

$$\partial_t U + A(U)\partial_x U = 0 \tag{4}$$

where A is a matrix depending on (f, g). When A has real eigenvalues, the system (4) is called a hyperbolic system and (3) is called a hyperbolic system of conservation laws. Quantitative and qualitative characters of such systems, most prominently admissible wave patterns, are then inferrable from traits of A, which amounts to applying entropy and shock conditions appropriately. The reader is referred to Dafermos (2005) for a systematic explanation of hyperbolic conservation laws.

Interestingly, in traffic flow modeling context, though conservation of vehicle number is the only univocal principle, macroscopic models developed based on various car-following heuristics usually turn out to have form (3), with or without a relaxation term on the right-hand side. Here are several examples.

- *Payne-Whitham model*. As noted in Jin & Zhang (2003), it adopts the following equation of motion when q, instead of v, is used as state variable

  $$\partial_t q + \partial_x (q^2/\rho + c_0^2 \rho) = \frac{\rho v_e(\rho) - q}{T} \tag{5}$$

  where c_0 is a constant interpreted as 'sound speed', in analogy of the same concept in gas dynamics.

- *Model of Aw & Rascle (2000)*. The equation of motion proposed therein reads

  $$\partial_t (v + p(\rho)) + v\partial_x (v + p(\rho)) = 0 \tag{6}$$

  where $p(\cdot)$ is an increasing function named pressure, which is nothing else than a stimulus whose rate of change determines the acceleration of a car. The conservative form of (6) can be obtained as

  $$\partial_t (\rho(v + p(\rho))) + \partial_x (\rho v(v + p(\rho))) = 0 \tag{7}$$

- *Model of Lebacque* et al. *(2007)*. It is a generalization of the model of Aw & Rascle (2000), which has the following equation of motion

  $$\partial_t (\rho I) + \partial_x (\rho v I) = -\rho f(I) \tag{8}$$

  where I is interpreted as an invariant quantity pertaining to vehicle-driver characters, e.g. preferred speed-spacing relation. The relaxation term is suggested to be $f(I) = I/T$.

It is perceivable that not all non-equilibrium models can be written in form (3), though they adopt form (4), because this requires $a_{21}\partial_x \rho + a_{22}\partial_x s$ (a_{ij} denotes element of A) be a total derivative. One example is the model of Zhang (2002), which has equation of motion

$$\partial_t v + v\partial_x v = -c(\rho) v_x \tag{9}$$

where $c(\rho)$ is a function of ρ, similar to c_0 in Example 1. This equation has an obvious quasilinear form

$$\partial_t v + (v + c(\rho))\partial_x v = 0 \tag{10}$$

but does not admit any obvious conservative form.

2.2. Further analysis

Due to the formal resemblance of (3) to the LWR model, it is anticipated that models of this form may adopt a similar variational formulation. However, before deriving relevant results, it would be essential to look into the physical content and limitations of non-equilibrium models in the form of (3).

We first discuss when (3) is appropriate to model traffic flow. Minimal requirements include the following: a) Total traffic volume is conserved; b) The fastest wave is less than or equal to traffic speed.

The requirement a) means one of the variables in (3) is traffic density. Since we know that its corresponding flux is ρv, we let $u_1 = \rho$ and $f(u_1, u_2) = \rho v(\rho, u_2)$. Then (3) can be written in quasilinear from, with

$$A = \begin{pmatrix} v + \rho v_\rho & \rho v_s \\ g_\rho & g_s \end{pmatrix} \tag{11}$$

where we use subscripts to denote partial derivatives (e.g. v_ρ stands for $\partial_\rho v(\rho, s)$). The requirement b) implies matrix A must be diagonalizable and has all its eigenvalues upper bounded by v. This in turn leads to a first characterization of flux $g(\rho, s)$.

Proposition 2.1. *Flux function g satisfies* $(v_s, -v_\rho)\nabla g \geq v v_\rho$*, if (3) is anisotropic, where* $\nabla\cdot$ *denotes gradient with respect to* ρ *and s. Moreover, the equality is attained when one characteristic speed of (3) is v.*

Proof We consider $y(\lambda) \equiv det(A - \lambda I)$. It represents a parabola with respect to λ, whose roots are characteristic speeds of (3). Anisotropy of (3) means the largest root of $y(\lambda)$ is upper bounded by v, which holds only if $y(v) \geq 0$. This leads to the inequality to prove after simple algebra. Moreover, existence of a characteristic with speed v means $y(v) = 0$, i.e. the equality is attained.

As an exercise, the reader may verify that when $s = \rho(v - v_e(\rho))$, its flux $g(\rho, s) = s^2/\rho + v_e(\rho)s$ satisfies the inequality and the equality is also attained. A very interesting implication of Proposition 2.1 is that though we do not specify what is the second conservative variable, gradient of its flux g naturally satisfies constraints related to traffic speed. We can characterize flux g better when extra physical constraints are imposed. For instance, when $s = \rho I$ as postulated in Lebacque *et al.* (2007), we can derive its property from an invariant assumption.

Proposition 2.2. *Flux function g satisfies* $(\rho_x, s_x)\nabla g = s v_x + v s_x$*, if quantity* $s = \rho I(\rho, v)$ *and I is constant along vehicle trajectories.*

Proof The assumption says that when $dx/dt = v$, there is $d(s/\rho)/dt = 0$. This expression can be simplified to $sv_x + s_t + vs_x = 0$. We obtain the formula to prove by combining this expression with the conservation equation $s_t + g(\rho, s)_x = s_t + g_\rho \rho_x + g_s s_x = 0$.

A corollary regarding $\|\nabla g\|$ easily follows from Proposition 2.1 and 2.2. By applying the Cauchy-Schwartz inequality ($\|a\|\|b\| \geq |a \cdot b|$, where a, b are vectors, $a \cdot b$ is their inner product and $\| \cdot \|$ is second norm), we obtain the following estimate of $\|\nabla g\|$

$$\|\nabla g\| \geq \max\{\frac{v v_\rho}{\|\nabla v\|}, \frac{s v_x + v s_x}{\|(\rho_x, s_x)\|}\} \tag{12}$$

In above we derive two conditions, based on respectively anisotropic principle and an invariant property, that flux g necessarily satisfies if models of form (3) are appropriate to describe traffic flow. These conditions can screen out models that are physically unreal and provide *a priori* estimates for solutions of a given model. Yet, we want to stress that the validity of a specific model is subject to experimental assessment. Cautions should be taken when determining the conservative forms of (3), i.e. conservative variables and their fluxes. Manipulation of conservation equations can result in artificial solutions, due to discontinuities resulted from shocks. This complication is well-known in the case of Burger's equation (LeVeque, 1992). Investigation of this issue is left to future studies.

2.3. Physics: inhomogeneity and relaxation

From now on, we restrict our attention to the model of Lebacque *et al.* (2007). When relaxation term is not included, interestingly, this model resembles an inhomogeneous LWR model (see Li & Zhang (in press) for an overview). Actually, it has two waves, of speed $\lambda_1 = \partial_\rho Q = \partial_\rho(\rho v)$ and $\lambda_2 = v$ respectively. This roughly means local information propagates along two directions in traffic (refer to Fig.1). One wave is attached to vehicles, the other wave propagates forwards (in light traffic) or backwards (in heavy traffic), similar to the kinematic waves in the classical LWR model. Speed of the latter wave could fluctuate if I is inhomogeneous across drivers.

In simple cases, we can predict traffic evolutions at least qualitatively based on this theory. For example, in Fig.2, We assume initial data on ρ, I prescribe there are three platoons, labeled respectively as U, M, D, which locate from upstream to downstream. Also, we assume platoon U moves at its initial speed. The first wave determines that platoon M and D slow down to U′ and D′ respectively. The second wave determines that vehicles in each platoon retain their preference (on deviation from some nominal 'equilibrium' relation), which means their states remain on the fundamental diagrams that they initially situated on, while moving in the direction of solid arrow lines. Accordingly, a loop detector installed downstream would observe state transitions illustrated by the dotted arrow line.

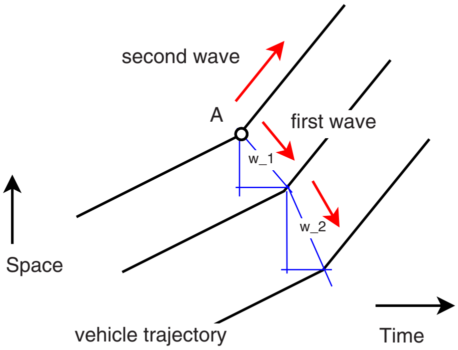

Fig. 1. Traffic and wave relation in Lebacque's model

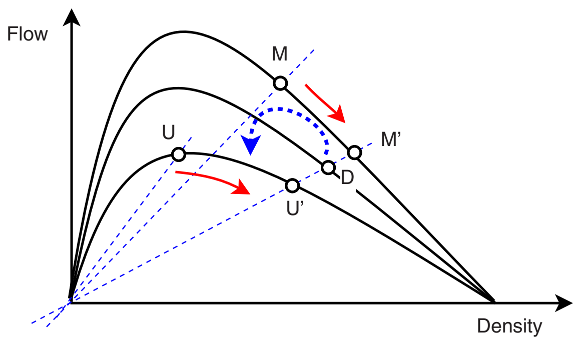

Fig. 2. An example of state transition

One may question the validity regarding invariance of I along vehicle trajectories, because this assumption is essentially an equilibrium assumption for each vehicle. While a comprehensive empirical validation of this assumption is beyond the scope of this paper, evidences in literature show that it constitutes a good approximation to the reality. For instance, Duret *et al.* (2008) looked into NGSIM I-80 trajectory data and their result (Fig.2b therein) indicated that in usual congested situations, speed-spacing data of individual vehicles exhibit a well-defined bivariate relation. Li & Zhang (2011) explored single loop detector data on freeway I-80 near Sacramento, California and found that speed-constant fluctuations are common. Such fluctuations, though alien to other theories (e.g. homogenous LWR), have a very natural explanation based on the example just given (see Fig.2).

Meanwhile, this theory provides a mechanism for individual vehicles to have transitions surrounding the equilibrium curve when relaxation term is included. In this case, it resembles many early non-equilibrium traffic flow models (e.g. model of Payne-Whitham) and suggests transient car-following behaviors. We can see this clearly by writing its equation of motion ((14) with $I = v - v_e(\rho)$ and relaxation $f(I) = -I/\tau$) as

$$\frac{d}{dt}v = -\frac{v - v_e(\rho)}{\tau} - \rho v_e'(\rho) v_x \tag{13}$$

The first term in the right-hand side of (13) represents relaxation, the second term is exactly the acceleration of traffic predicted by the LWR model if $v = v_e(\rho)$. This equation resembles the one proposed in Zhang (1998) in structure. Rigorous analysis of effects of relaxation can be carried out in a similar way as that presented in Zhang (2000), which amounts to looking into behaviors of Riemann invariants. We give a result characterizing the decaying influence of the relaxation term on solutions. The equation of motion in Lebacque *et al.* (2007) is equivalent (at least formally) to

$$\partial_t I + v \partial_x I = -f(I) \tag{14}$$

We take $f(I) = -\frac{I}{\tau}$, where τ is relaxation time. This means along vehicle trajectory (i.e. second wave), we have

$$\frac{d}{dt}\ln(I) = -\frac{1}{\tau} \tag{15}$$

Therefore,

$$I = I_0 \exp(-\frac{1}{\tau}t) \tag{16}$$

where I_0 is initial value of I. This means variations in initial data of I are dampened out exponentially fast if relaxation term is added. In large time, the original model reduces to an homogeneous LWR model.

2.4. *Convexity of flux pair* (f, g)

Before proceeding to the variational formulation of System (3), out of well-posedness considerations, we impose restrictions on the concavity of flux pair (f, g). In general, it is desirable that f and g are not convex-concave in ρ and s, i.e. their second derivatives with respect to ρ and s have fixed signs. This requirement is mild. Take flux pair for model of Lebacque *et al.* (2007) for example,

$$\begin{cases} f(\rho, s) = \rho v_e(\rho) + s \\ g(\rho, s) = v_e(\rho)s + \frac{s^2}{\rho} \end{cases} \tag{17}$$

it is satisfied when assuming $v_e(\rho)$ is continuous, strictly monotone and piecewise linear. In fact, it is then straightforward to verify that $\partial^2_\rho f < 0$, $\partial^2_s f = 0$, $\partial^2_\rho g \geq 0$ and $\partial^2_s g > 0$. This property roughly implies that over the feasible set of (ρ, s), which is compact, the maximizer of f and minimizer of g are unique. One may refer to Fig.3 for an intuition on the shape of (f, g), which is obtained by assuming $v_e(\rho) = -65/200(\rho - 200)$. Similarly, the reader could verify that the flux of Payne-Whitham model (refer to (5)) are both convex.

3. Variational formulation

From now on, we use $P, Q, \ldots$ to denote points $(t_P, x_P), (t_Q, x_Q), \ldots$ on time-space plane, and N_P stands for the cumulative traffic count at point P, i.e. $N_P = N(t_P, x_P)$. Moreover, x_{PQ} denotes a path from P to Q, $x_{\cdot Q}$ denotes a path to Q, and $x_{P\cdot}$ denotes a path from P. Notation such as $x_{PQ}(t)$ denotes the point on path x_{PQ} at time t. Path here means a Lipschitz continuous curve directed with time. When necessary, superscript will be added, e.g. $x^1_{PQ}, \ldots, x^n_{PQ}$, to differentiate paths with identical end points. Letters $\mathcal{B}, \mathcal{C}, \ldots$ are reserved for boundaries (continuous curves where data are available or constraints are imposed) on the time-space plane.

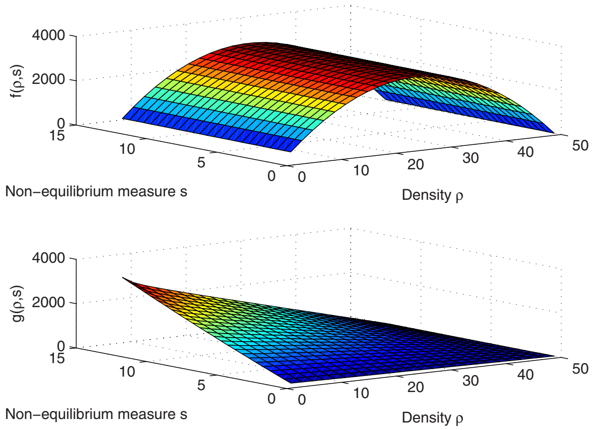

Fig. 3. One example of flux pair (f,g).

3.1. An overview of the scalar case

In traffic flow literature, the variational formulation of traffic flow models was first proposed in Newell (1993a,b), coined as a minimum principle therein. The motivation of this work is to simplify the computation of first-order kinematic wave model (i.e. the LWR model), through updating cumulative traffic count $N(t,x)$ instead of traffic density $\rho(t,x)$. In case a triangular fundamental diagram is adopted, the calculation can actually be done explicitly, by noting that

$$\frac{dN}{dt} = \begin{cases} 0 & \text{if wave speed equals } v_f \\ w\rho_j & \text{if wave speed equals } -w \end{cases} \tag{18}$$

along the two kinematic waves, independent of the initial-boundary data. Here v_f, $-w$ $(w>0)$ and ρ_j denote free flow speed, wave speed in congestion and jam density, respectively. The minimum principle is used to single out a unique N from multiple values that are possibly obtained. It says that actual value of N at some (t,x) is the minimum of all candidates values from different characteristics. In case where the fundamental diagram is triangular, calculation amounts to comparing at most two values at each point.

This line of reasoning was further exploited in the variational formulation in Daganzo (2005a,b). This work tackles the LWR model equipped with a general concave fundamental diagram. Connection of the LWR model with the Hamilton-Jacobi theory was realized therein and it was shown that the minimum principle can be generalized to include non-wave paths, when a proper cost functional is defined. Roughly, in the homogeneous case, the variational formulation of a LWR model states that the cumulative traffic count N at some point Q is the minimum of a real set,

$$N_Q = \inf\{N_P + \int_{x_{PQ}} \sup_{\rho}\{f(\rho) - \rho\dot{x}_{PQ}\} : P \in \mathcal{B}, x_{PQ} \text{ is a path}\} \tag{19}$$

where $f(\cdot)$ is the fundamental diagram. Function $\sup_\rho\{f(\rho)-\rho\dot{x}_{PQ}\}$ of $\dot{x}_{PQ}$ is Legendre transform of $f(\cdot)$. It is the maximum passing flow for observer with instantaneous speed $\dot{x}_{PQ}$ at density ρ. We write this term as $R(\dot{x}_{PQ})$ for simplicity.

We note that in the above discussion (19) has an optimal control interpretation, which stems from the equivalence of conservation law equations (C1) and Hamilton-Jacobi equation endowed with a scalar Hamiltonian (H1), that has been used for numerical analysis purposes (see Caselles, 1992; Jin & Xin, 1998 and references therein). This equivalence establishes the one-to-one correspondence between the entropy solutions to (C1) and viscosity solutions to (H1), under certain regularity conditions on initial-boundary data and the concavity condition of the Hamiltonian. In the perspective of optimal control, the problem of determining the N-value at (t,x) is cast as a terminal cost problem (i.e. Bolza problem, see Naidu, 2003), which finds the optimal path $\eta^* \in \Omega(t,x)$ such that the total cost, i.e. $N(t_\eta, \eta(t_\eta)) + \int_\eta \sup_\rho \{f(\rho) - \rho\dot{\eta}\}$ is minimized.

The attractiveness of expression (19) (also called the Lax-Hopf formula in PDE and optimal control literature) lies in its variational structure, which allows optimization techniques (e.g. dynamic programming) be used to solve conservation law problems. The variational formulation is advantageous over the conventional kinematic wave formulation, in terms of modeling flexibility and easiness of computation under complex initial/boundary conditions, e.g. when traffic signals and moving bottlenecks are involved..

3.2. The auxiliary optimal control problem

Before proceeding to the extension of the variational formulation of non-equilibrium traffic flow models, it is worth looking into the physics underpinning such a formulation. Significance of (19) lies in that it reveals an isomorphic relation between a conservation law problem and an optimal control problem.

Suppose on a time-space region Ω with proper initial-boundary conditions, a LWR model is well-posed and solved by $\rho(t,x)$, with $(t,x) \in \Omega$, which maps to a proper N-surface over Ω. Then formula (19) implies that for any point Q, calculating N_Q amounts to solving the following optimal control problem

$$\begin{array}{rl} \text{minimize} & C(x_{PQ}) = N_P + \int_{t_P}^{t_Q} R(\dot{x}_{PQ})dt \\ \text{s.t.} & \frac{d}{dt}C = q(t, x_{PQ}(t)) - \dot{x}_{PQ}(t)\rho(t,x(t)) \\ & q = f(\rho) \\ & P \in \mathcal{B}; Q \text{ is as given} \end{array} \tag{20}$$

and letting N_Q be the minimal value of $C(x_{PQ})$. In (20), the first equation in the constraints represents the instantaneous changing rate of cost C along a trajectory PQ, which corresponds to observation of N in a moving coordinate of speed $\dot{x}_{PQ}(t)$; the second equation corresponds to the equilibrium assumption (i.e. fundamental diagram) in the LWR model; and the last row gives boundary conditions. This problem is the familiar Bolza problem in the optimal control context (Naidu, 2003). Solution of this problem is nothing else than the kinematic wave emitting from Q (Daganzo, 2005a).

3.3. Extension to non-equilibrium systems

Ever since its discovery, the variational formulation of the LWR model has found numerous practical applications, e.g. in modeling moving bottlenecks, developing simplified numerical solution schemes, devising data assimilation algorithms for probe vehicle measurements, etc. Major examples include Daganzo & Laval (2005), Daganzo (2005b), Daganzo & Menendez (2005), Claudel & Bayen (2010a,b, 2011), and Mazaré *et al.* (2011). It is thus natural to ask whether other type of traffic flow models possess formulations alike, so that similar advantages could be attained.

To answer this question, we can consider a moving observer. Suppose this observer observes certain conservative quantity y and records its cumulative amount Y. Then we can calculate the cumulative increment of Y along a path x_{PQ} from P to Q,

$$Y_Q = Y_P + \int_{t_P}^{t_Q} r_y(t, x_{PQ}(t), \dot{x}_{PQ}(t))dt \tag{21}$$

where $r_y(t,x,v)$ is the passing rate of y at (t,x) relative to an observer of speed v. In the case of the homogeneous LWR model, we have the following observations: 1) $R(v)$ is an upper bound of $r(t,x,v)$, for all valid paths; and 2) $R(\dot{x}) = r(t,x,\dot{x})$ determines a valid path. Actually, these two conditions are sufficient to ensure that Y_Q assumes a variational form:

$$Y_Q = \inf\{Y_P + \int_{t_P}^{t_Q} R(\dot{x}_{PQ})dt\} \tag{22}$$

Proof of this claim is straightforward upon noting that condition 1) and 2) respectively implies right-hand side of (22) is an upper bound of left-hand side and that it is tight.

3.4. Systems with no relaxation

Now we extend the above argument to System (3). For simplicity, we first tackle the case $h = 0$, i.e. system without relaxation. We first define cost functions (23), assuming f is concave in ρ for each s, and g is convex in s for each ρ. Physically, similar to the scalar case (Daganzo, 2006), $R_\rho(\rho, v)$ characterizes the upper bound of passing flow relative to an observer of speed v when the other conservative quantity is s. Due to the symmetric relation of s and ρ, s can be understood as a density-like quantity, measuring the intensity of 'off-equilibrium'. Function R_s gives the lower bound of corresponding flux at any density.

Definition We define the cost pair (R_ρ, R_s) as the Legendre-Fenchel type transform of the flux pair (f, g)

$$\begin{cases} R_\rho(s,v) = \sup_\rho\{f(\rho,s) - \rho v\} \\ R_s(\rho,v) = \inf_s\{g(\rho,s) - sv\} \end{cases} \tag{23}$$

Lemma 3.1. *Suppose $h(x,y)$ is strictly concave with respect to x for any given y, then* $\sup_s\{h(s,y) - s\partial_x h(x,y)\} = h(x,y) - x\partial_x h(x,y)$.

Proof Let $g(s) = h(s,y) - su$. It is straightforward to verify that $g(s)$ is concave, therefore attains its supremum when $g'(s) = 0$, i.e. $\partial_s h(s,y) = u$. This lemma is proved by letting $u = \partial_x h(x,y)$ and noting that $\partial_s h(s,y) = \partial_x h(x,y)$ if and only if $s = x$, due to the strict concavity of h.

Now we have the main result of this paper, which gives the form of variational solutions and a sufficient condition for their existence.

Definition Suppose $y(x,t)$ is a scalar field on the time-space plane, we define its corresponding cumulative count N_y as follows

$$N_l(x,t) = \int_x^\infty l(s,t)ds$$

Theorem 3.2. *Consider System (3) with zero relaxation and proper initial-boundary data on $\mathcal{B} \subset \mathbb{R}^+ \times \mathbb{R}$. Then N_ρ and N_s adopt the following variational representations*

$$\begin{cases} N_\rho(t,x) = \inf\{N_\rho(t_{\eta_\rho}, \eta_\rho(t_{\eta_\rho})) + \int_{t_{\eta_\rho}}^t R_\rho(s(\tau,\eta_\rho(\tau)), \dot\eta_\rho)d\tau : \eta_\rho \textit{ is a path from } \mathcal{B} \textit{ to } (t,x)\} \\ N_s(t,x) = \sup\{N_s(t_{\eta_s}, \eta_s(t_{\eta_s})) + \int_{t_{\eta_s}}^t R_s(\rho(\tau,\eta_s(\tau)), \dot\eta_s)d\tau : \eta_s \textit{ is a path from } \mathcal{B} \textit{ to } (t,x)\} \end{cases} \tag{24}$$

if the following ordinary differential equations (ODEs) admit Lipschitz continuous solutions

$$\begin{cases} \dot\eta_\rho(\tau) = \partial_\rho f(\rho(\tau,\eta_\rho(\tau)), s(\tau,\eta_\rho(\tau))) \\ \eta_\rho(t) = x \end{cases} \tag{25}$$

$$\begin{cases} \dot\eta_s(\tau) = \partial_s g(\rho(\tau,\eta_s(\tau)), s(\tau,\eta_s(\tau))) \\ \eta_s(t) = x \end{cases} \tag{26}$$

where $\rho(t,x)$ and $s(t,x)$ are proper solutions to system (3) with the given initial-boundary data. We call the solutions to these ODEs optimal paths pertaining to scalar field ρ and s respectively.

Proof First, consider two arbitrary paths connecting the boundary $\mathcal{B}$ and point (t,x), denoted as η_ρ and η_s. They start from time t_{η_ρ} and t_{η_s} respectively. We calculate changes of N_ρ and N_s along these paths, and observe that there are always

$$N_\rho(t,x) - N_\rho(t_{\eta_\rho}, \eta_\rho(t_{\eta_\rho})) \le \int_{t_{\eta_\rho}}^t R_\rho(s(\tau,\eta_\rho(\tau)), \dot\eta_\rho)d\tau \tag{27}$$

and

$$N_s(t,x) - N_s(t_{\eta_s}, \eta_s(t_{\eta_s})) \geq \int_{t_{\eta_s}}^{t} R_s(\rho(\tau, \eta_s(\tau)), \dot{\eta}_s) d\tau \tag{28}$$

This is because the left-hand sides of (27) and (28) represent the path integral of instantaneous passing rate along η_ρ and η_s, while the right-hand sides of these inequalities represent their upper and lower bounds, according to the definitions of R_ρ and R_s. Since η_ρ and η_s are arbitrary, (27) and (28) imply that

$$N_\rho(t,x) \leq \inf\{N_\rho(t_{\eta_\rho}, \eta_\rho(t_{\eta_\rho})) + \int_{t_{\eta_\rho}}^{t} R_\rho(s(\tau, \eta_\rho(\tau)), \dot{\eta}_\rho) d\tau\} \tag{29}$$

and

$$N_s(t,x) \geq \sup\{N_s(t_{\eta_s}, \eta_s(t_{\eta_s})) + \int_{t_{\eta_s}}^{t} R_s(\rho(\tau, \eta_s(\tau)), \dot{\eta}_s) d\tau\} \tag{30}$$

To obtain the variational formulation, it remains to show that the inequalities (29) and (30) are indeed binding. This is true because of the assumption we made, i.e. that the two ODEs admit Lipschitz continuous solutions. To see this, we take (29) for example, and denote the solution to (25) as η_ρ^*. It is then easy to see $\eta_\rho^* \in \Omega(t,x)$ and at each time instant $s \in [t_{\eta^*}, t]$, there is

$$f(\rho, s) - \rho\dot{\eta}_\rho^* = f(\rho, s) - \rho\partial_\rho f(\rho, s) = \sup_y\{f(y,s) - y\partial_\rho f(\rho, s)\} \tag{31}$$

where the first equality is due to the construction of η_ρ^*, and second equality is implied by Lemma 3.1. The fact that the left-hand side equals the right-hand side in (31) means the observed passing flow equals the relative capacity almost everywhere, when the moving observer has trajectory η_ρ^* on the time-space plane. This thus shows constructively the inequality (29) must be binding, which is simply an alternative way of expressing the desired variational formulation of N_ρ. The same procedure can be applied to (26) and (30) to obtain the variational formulation of N_s. This completes our proof.

Remark 1: Several intrinsically related approaches exist in the literature to develop the variational formulation of scalar conservation law, e.g. based on Green's theorem (Lax, 1973; Dafermos, 2005), exploiting the special role of characteristic curves (Newell, 1993a; Daganzo, 2005a), and using the viability theory (Aubin *et al.* , 2008). Our proof revolves estimating and closing the gap between $N_\rho(t,x)$ and $N_s(t,x)$, which are unknown, and infimum/supremum of their upper/lower bounds, which are obtainable for every possible path of an imaginary observer. Refer to the illustration of Fig.4, in general, the paths over which the upper/lower bounds are binding are different, which could be interpreted as a pair of coupled controls. This is in a similar spirit to the interpretation of variational formulation raised in Daganzo (2006), though that paper focused on the first-order model and did not discuss the issue of binding.

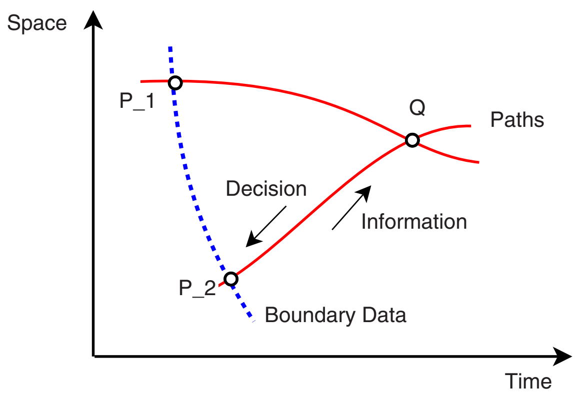

Fig. 4. Concept of a variational solution.

Remark 2: It can be seen that in our proof, the existence of a variational formulation for a system of PDEs (partial differential equations) is linked with the existence of proper solutions to the corresponding ODEs, which are in principle easier to deal with. In particular, an ODE like (25) or (26) admits a unique solution when its right-hand side is bounded and sufficiently smooth. When shocks only exist on a set of zero measure (this is always the case for a scalar conservation law, i.e. the LWR model, see Dafermos (2005)), the corresponding ODEs are locally well-posed. Therefore, intuitively, requirement looks mild for the existence of proposed variational formulation. Nonetheless, rigorously proving that the ODEs in Theorem 3.2 always have solution requires substantial analysis of the complications caused by shocks in ρ and s. It amounts to proving the well-posedness of

$$\begin{cases} \dot{x} = h(\rho(t,x), s(t,x)) \\ x(0) = \bar{x} \end{cases} \tag{32}$$

for some smooth function h. A similar problem (in (33), $\rho(x,t)$ solves a scalar conservation law),

$$\begin{cases} \dot{x} = h(\rho(t,x)) \\ x(0) = \bar{x} \end{cases} \tag{33}$$

has been tackled in Bressan & Shen (1998), and the reader is referred there for a discussion of discontinuous ODE problems.

Remark 3: In the optimal control context, the two controls induce an external cost to each other, due to the coupled form of cost pair (R_ρ, R_s). This gives an interpretation of the trajectories η^*_ρ and η^*_s as solutions to an externality problem. The reader is referred to Loreti & Vergara Caffarelli (2000, 2004) for in-depth discussions along this line of reasoning.

Remark 4: The variable $s = \rho I$ is interpreted as 'a density of an off-equilibrium measure', with the unit of traffic volume when $I = v - v_e(\rho)$. Unlike ρ, s does not has a fixed sign, so N_s is in general not monotone with respect to time or space. This is different from N_ρ, specification of which needs extra cares.

3.5. Systems with relaxation

Earlier in this paper we estimated the influence of relaxation on traffic state, which was shown to decay exponentially fast (see (16)). In this case, the model ultimately degenerates to a LWR model ($s = 0$). We thus can infer the true value of N_ρ (with relaxation) from a LWR model with speed-density relation $v = v_e(\rho)$. Let us consider a leading vehicle, which represents a given boundary condition, and a following vehicle. Suppose the leading vehicle has trajectory $x_L(t)$, $t \geq 0$, their initial gap is ρ_0^{-1} and initial speed of the following vehicle is v_F. Then initially, the quantity I attached to the following vehicle is $I_0 = \rho_0(v_F - v_e(\rho_0))$. We can evaluate the deviation of trajectories of the following vehicle in two models, denoted as $x_F(t)$ (original model) and $\tilde{x}_F(t)$ (the LWR approximation) respectively. It is

$$|x_F(t) - \tilde{x}_F(t)| = |\int_0^t (\dot{x}_F(s) - \dot{\tilde{x}}_F(s))ds| \tag{34}$$

From (16), we have

$$\rho(t)(\dot{x}_F - v_e(\rho(t))) = I_0 \exp(-t/T) \tag{35}$$

while in the LWR model,

$$\dot{\tilde{x}}_F - v_e(\rho(t)) = 0 \tag{36}$$

We assume $|\rho(t) - \rho_0| \leq a$ from some constant a strictly less than ρ_0, which means the gap has a bounded variation over time. Then we can combine these relations and obtain

$$|x_F(t) - \tilde{x}_F(t)| \leq \frac{I_0}{a} \int_0^t \exp(-s/T)ds = \frac{I_0}{a} \frac{1 - \exp(-t/T)}{T} \leq \frac{I_0}{aT} \tag{37}$$

Note that the right-hand side of (37) is independent of t and N_ρ is constant along trajectories $x_F(t)$ and $\tilde{x}_F(t)$, we can see that the two N-surfaces formed under the two different models has bounded deviation to each other. Therefore, when relaxation exists, the problem reduces to solving a LWR model in large time.

4. Simplified numerical scheme

One main application of the variational formulation is on developing numerical solution schemes or estimators that incorporate moving elements in traffic flow models, e.g. moving bottlenecks and probe vehicles. Compared to the cell-based algorithms (Daganzo, 1994; Lebacque, 1996), the numerical scheme based on variational formulation does not require cell partitions, thus is much more flexible with the type of input data or imposed constraints. Moreover, the variational formulation itself naturally ensures the uniqueness of solution. Therefore, entropy conditions are not explicitly stated. This is favorable because as such the preliminary work of solving Riemann problem can be skipped.

4.1. The scheme

We present a numerical scheme below to illustrate how the variational formulation (24) is used for the computational purposes. The idea resembles the one in Daganzo (2005b): A dense mesh is laid on the time-space plane, whose connected arcs approximate the paths and N_ρ and N_s values on its nodes are updated. The discrete time and location are labeled by positive integers i and j, respectively. Concerned nodes are divided into two categories: boundary set $\mathcal{B}$ and interior set O of a prescribed computational region. The update strategy is described as below,

1. Set current time $i_0 = 0$;
2. For all (i, j) such that $i = i_0$, we calculate the approximate value of ρ and s,

$$\rho(i,j) = \sum_{|j'-j|=1} |N_\rho(i,j') - N_\rho(i,j)|/|\{j'\}|\Delta x$$

$$s(i,j) = \sum_{|j'-j|=1} |N_s(i,j') - N_s(i,j)|/|\{j'\}|\Delta x$$

3. Update N-values of ρ and s according to the variational formulas derived above

$$N_\rho(i+1,j) = \min_{j'\in A}\{N_\rho(i,j') + \Delta t R_\rho(s(i,j'),(j'-j)\Delta x/\Delta t)\}$$

$$N_s(i+1,j) = \max_{j'\in A}\{N_s(i,j') + \Delta t R_s(\rho(i,j'),(j'-j)\Delta x/\Delta t)\}$$

   where $A = \{j : (i, j) \in \mathcal{B}\}$;
4. If N-values of all nodes in O are obtained, stop; otherwise, set $i_0 = i+1$, $\mathcal{B} = \mathcal{B} \cup \{(i, j) : i = i_0\}$, and go to step 2.

This algorithm looks simple and should be self-explanatory. We only mention that in step 2, the ρ and s values are calculated, which are used in step 3 for updating N_ρ and N_s. Note that although the mesh used in this algorithm has a grid like structure, it is not essential. In addition, moving objects can be conveniently handled in this numerical scheme, because of the variational character of the proposed numerical scheme. The technical details are similar to that of the first-order model (Daganzo, 2005b; Leclercq *et al.* , 2007) and omitted here.

4.2. Error bounds

The proposed scheme essentially approximates optimal paths (see Theorem 3.2 and Fig.4) with piecewise linear curves, whose slopes are $m\Delta x/\Delta t$, with m belonging to a proper integer set. Therefore, we can in principle evaluate the error of this scheme by tracking the change of state variables along an optimal path $x(t)$, and its approximation $\tilde{x}(t)$. We point out the following necessary condition for the numerical solution to be exact.

Proposition 4.1. *The proposed numerical scheme is exact only if $\partial_\rho f$ and $\partial_s g$ are piecewise constant, and they take values in the set $\{m\Delta x/\Delta t\}$.*

Proof If the given scheme generates exact solutions, we know that the optimal paths are piecewise linear. Since the optimal paths solve (25) and (26), we know the right-hand side of these equations, i.e. $\partial_\rho f$ and $\partial_s g$, must also be piecewise constant, taking their values in the set $\{m\Delta x/\Delta t\}$.

Remark: In the VF of the LWR model, we know exact numerical solution is possible only if corresponding fundamental diagram is piecewise linear. The above proposition is a generalization of this fact.

5. Conclusions

In this paper, we revisit the variational theory of traffic flow modeling and derive the variational formulation for a generic class of non-equilibrium traffic flow models. We achieve this goal through characterizing the binding conditions relevant to moving observations. This approach reflects the intrinsic connection of conservation law problems with optimal control problems.

Our finding enables the LWR model and a class of non-equilibrium traffic models to be tackled in a unified mathematical framework. In particular, this novel formulation of non-equilibrium models make the incorporation of peculiar boundary conditions and moving objects straightforward, which is favorable for numerous applications, e.g. simulations involving slow moving vehicles, probe data fusion, etc.

There are several directions to go based on the current work. We believe that the full potential of the variational formulation has not been explored. Its physical implications, mathematical and numerical properties, and applications to various real-world problems are worth further investigations. In particular, our ongoing work is focusing on the implementation and analysis of the proposed numerical solution scheme and testing it in various scenarios of practical significance.

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References

Aubin, J.P., Bayen, A.M., & Saint-Pierre, P. 2008. Dirichlet problems for some Hamilton-Jacobi equations with inequality constraints. *SIAM Journal on Control and Optimization*, **47**(5), 2348–2380.

Aw, A., & Rascle, M. 2000. Resurrection of "second order" models of traffic flow. *SIAM journal on applied mathematics*, 916–938.

Bressan, A., & Shen, W. 1998. Uniqueness for discontinuous ODE and conservation laws. *Nonlinear analysis*, **34**(5), 637–652.

Caselles, V. 1992. Scalar conservation laws and Hamilton-Jacobi equations in one-space variable. *Nonlinear analysis: Theory, Methods & Applications*, **18**(5), 461–465.

Claudel, C.G., & Bayen, A.M. 2010a. Lax–Hopf Based Incorporation of Internal Boundary Conditions Into Hamilton–Jacobi Equation. Part I: Theory. *IEEE Transactions on Automatic Control*, **55**(5), 1142–1157.

Claudel, C.G., & Bayen, A.M. 2010b. Lax–Hopf based incorporation of internal boundary conditions into Hamilton-Jacobi equation. Part II: Computational methods. *IEEE Transactions on Automatic Control*, **55**(5), 1158–1174.

Claudel, Christian G, & Bayen, Alexandre M. 2011. Convex formulations of data assimilation problems for a class of Hamilton-Jacobi equations. *SIAM Journal on Control and Optimization*, **49**(2), 383–402.

Dafermos, C.M. 2005. *Hyperbolic conservation laws in continuum physics*. Springer Verlag.

Daganzo, Carlos F, & Menendez, Monica. 2005. A variational formulation of kinematic waves: Bottleneck properties and examples. *In: Transportation and Traffic Theory. Flow, Dynamics and Human Interaction. 16th International Symposium on Transportation and Traffic Theory*.

Daganzo, C.F. 1994. The cell transmission model: A dynamic representation of highway traffic consistent with the hydrodynamic theory. *Transportation Research Part B: Methodological*, **28**(4), 269–287.

Daganzo, C.F. 1995. Requiem for second-order fluid approximations of traffic flow. *Transportation Research Part B*, **29**(4), 277–286.

Daganzo, C.F. 2005a. A variational formulation of kinematic waves: basic theory and complex boundary conditions. *Transportation Research Part B*, **39**(2), 187–196.

Daganzo, C.F. 2005b. A variational formulation of kinematic waves: Solution methods. *Transportation Research Part B*, **39**(10), 934–950.

Daganzo, C.F. 2006. On the variational theory of traffic flow: well-posedness, duality and applications. *Networks and Heterogeneous Media*, **1**(4), 601–619.

Daganzo, C.F., & Laval, J.A. 2005. Moving bottlenecks: A numerical method that converges in flows. *Transportation Research Part B: Methodological*, **39**(9), 855–863.

Duret, Aurélien, Buisson, Christine, & Chiabaut, Nicolas. 2008. Estimating Individual Speed-Spacing Relationship and Assessing Ability of Newell's Car-Following Model to Reproduce Trajectories. *Transportation Research Record: Journal of the Transportation Research Board*, **2088**(-1), 188–197.

Helbing, D. 2009. Reply to comment on "On the controversy around Daganzo's requiem for and Aw-Rascle's resurrection of second-order traffic flow models" by HM Zhang. *The European Physical Journal B*, **69**(4), 569–570.

Helbing, D., & Johansson, AF. 2009. On the controversy around Daganzos requiem for and Aw-Rascles resurrection of second-order traffic flow models. *The European Physical Journal B-Condensed Matter and Complex Systems*, **69**(4), 549–562.

Jin, S., & Xin, Z. 1998. Numerical passage from systems of conservation laws to Hamilton-Jacobi equations, and relaxation schemes. *SIAM Journal on Numerical Analysis*, 2385–2404.

Jin, WL, & Zhang, HM. 2003. The formation and structure of vehicle clusters in the Payne–Whitham traffic flow model. *Transportation Research Part B*, **37**(3), 207–223.

Lax, P.D. 1973. *Hyperbolic systems of conservation laws and the mathematical theory of shock waves*. Society for Industrial Mathematics.

Lebacque, J.P. 1996. The Godunov scheme and what it means for first order traffic flow models. *Pages 647–677 of: Internaional symposium on transportation and traffic theory*.

Lebacque, J.P., Mammar, S., & Salem, H.H. 2007. Generic second order traffic flow modelling. *In: Transportation and Traffic Theory 2007. Papers Selected for Presentation at ISTTT17*.

Leclercq, L., Laval, J.A., & Chevallier, E. 2007. The Lagrangian coordinates and what it means for first order traffic flow models. *In: Transportation and Traffic Theory 2007. Papers Selected for Presentation at ISTTT17*.

LeVeque, R.J. 1992. *Numerical methods for conservation laws*. Birkhäuser.

Li, J., & Zhang, H.M. 2011. The fundamental diagram of traffic flow: A new identification scheme and further evidences from empirical data. *Transportation Research Record: Journal of Transporation Research Board*, 50–59.

Li, J., & Zhang, H.M. in press. Modeling space-time inhomogeneity with kinematic wave theory. *Transportation Research Part B*.

Loreti, P., & Vergara Caffarelli, G. 2000. Variational solutions of coupled Hamilton-Jacobi equations. *Applied Mathematics & Optimization*, **41**(1), 9–24.

Loreti, P., & Vergara Caffarelli, G. 2004. Externality and Hamilton-Jacobi equations. *NoDEA: Nonlinear Differential Equations and Applications*, **11**(2), 123–136.

Mazaré, Pierre-Emmanuel, Dehwah, Ahmad H, Claudel, Christian G, & Bayen, Alexandre M. 2011. Analytical and grid-free solutions to the Lighthill–Whitham–Richards traffic flow model. *Transportation Research Part B: Methodological*, **45**(10), 1727–1748.

Naidu, D.S. 2003. *Optimal control systems*. CRC.

Newell, G.F. 1993a. A simplified theory of kinematic waves in highway traffic, part I: general theory. *Transportation Research Part B: Methodological*, **27**(4), 281–287.

Newell, G.F. 1993b. A simplified theory of kinematic waves in highway traffic, Part II: Queueing at freeway bottlenecks. *Transportation Research Part B: Methodological*, **27**(4), 289–303.

Payne, H.J. 1971. Models of freeway traffic and control. *Mathematical models of public systems*, **1**(1), 51–61.

Zhang, H.M. 1998. A theory of nonequilibrium traffic flow. *Transportation Research Part B*, **32**(7), 485–498.

Zhang, HM. 2000. Structural properties of solutions arising from a nonequilibrium traffic flow theory. *Transportation Research Part B*, **34**(7), 583–603.

Zhang, H.M. 2002. A non-equilibrium traffic model devoid of gas-like behavior. *Transportation Research Part B: Methodological*, **36**(3), 275–290.

Zhang, HM. 2009. Comment on "On the controversy around Daganzo's requiem for and Aw-Rascle's resurrection of second-order traffic flow models" by D. Helbing and AF Johansson. *The European Physical Journal B-Condensed Matter and Complex Systems*, **69**(4), 563–568.