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STABILITY OF INTERACTING TRAVELING WAVES IN REACTION-CONVECTION-DIFFUSION SYSTEMS

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Abstract. The stability of isolated combustion traveling waves has been exhaustively studied in the literature of reaction-diffusion systems. The analysis has been done mainly by neglecting other waves that are usually present in the solution and that can influence the stability of the combustion wave. In this paper, a numerical example on the influence of such interaction on wave stability are presented.

The paper is illustrated through a simple model for the injection of air into a porous medium that contains a solid fuel. The model considered here reproduces a variety of observed phenomena and yet is simple enough to allow rigorous investigation. We refer on earlier work containing proofs of existence of traveling waves corresponding to combustion waves by phase plane analysis were presented; wave sequences that can occur as solutions of Riemann problems were identified.

1. Introduction.

Combustion traveling waves arise in many applications such as oil recovery [14], burners [4], smoldering combustion [23] and others [12]. One of the most important aspects in the study of such waves is combustion extinction. This problem can be addressed mathematically through stability analysis.

Large efforts were applied in this direction over the last few decades. For example in [5, 18] the stability of gas-less combustion waves was studied using the spectral method applied to simple models of two reaction-diffusion equations.

In [15] a model involving in situ combustion of oil with pyrolysis and vaporization was analyzed. In [2] a filtration combustion model was studied, where the reaction rate was modeled as delta function and the stability analysis was performed using spectral analysis.

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Some other works also addressing stability analytically are [20, 21, 24, 25]. Other works address this issue numerically [7, 6], [24].

A common feature of all these works is that they perform stability analysis of a single combustion wave without considering its interaction with other waves present in typical solutions. In the current paper we intend to show some numerical examples in which such an interaction leads to instability of the combustion wave.

This paper is part of long term research project the purpose of which is to identify waves that arise in one-dimensional models of combustion in porous media, and to understand how the waves fit together in solutions of Riemann problems; see [8, 10, 15, 16, 17, 19, 22], and references therein. Such flows give rise to reaction-convection-diffusion equations in which the three aspects are of roughly equal importance.

The paper presents a careful numerical analysis of waves arising in a model for the injection of air into a porous medium that contains a solid fuel with a pressure independent oxidation rate. The model was proposed in [1] and further studied in [10, 11], where it was simplified by ignoring the dependence of gas density on temperature. This simplification facilitates the study of traveling waves and the identification of the wave sequences that can occur as solutions of Riemann problems.

The model derived in [11], which is reviewed in Section 2, consists of three equations that express energy, oxygen, and fuel balance laws. We use a shifted reaction rate Arrhenius law for which combustion begins at a threshold temperature. We analyze the simple case in which the thermal capacity of the medium is negligible compared to that of the air. A consequence is that oxygen and heat are both transported at the velocity of the moving gas. The negligible thermal capacity assumption is not correct for oil recovery, but is approximately valid for polyurethane foam smoldering such as that used in furniture.

In [11] four types of combustion waves were found that approach their end states exponentially: two that propagate faster than oxygen and temperature, and two that propagate more slowly. Fast combustion waves represent "premixed combustion": an oxidation reaction, once it starts, races, in the form of a burning front, into a region where both solid fuel and oxygen are present. Behind the front either oxygen or fuel is exhausted. The slow combustion waves found have been called "reaction-trailing smolder waves" [23] and "coflow (or forward) filtration combustion waves" [3] in the context of more realistic models of air injection into a porous medium. The moving gas brings oxygen into a region where solid fuel is present. The oxygen is consumed in the reaction. Since the gas velocity is larger than that of the flame front, a region of high temperature and no oxygen is swept ahead of the front. Properties of both fast and slow combustion waves are reviewed in Section 3. The types of possible contact discontinuities that can occur in generic waves sequences were also studied in [11] and are reviewed in Section 3.3.

In Section 4 some numerical examples studying the combustion wave instability resulting from interaction between traveling reaction wave and diffusive contact wave are presented. Finally, in Section 5 some conclusions are discussed.

2. **Model.**

The system we consider is

$$\partial_t \theta + a\partial_x \theta = \partial_{xx}\theta + \rho Y \Phi, \tag{1}$$

$$\partial_t \rho = -\rho Y \Phi, \tag{2}$$

$$\partial_t Y + a\partial_x Y = -\rho Y \Phi, \tag{3}$$

$$\Phi = \begin{cases} \exp(-1/\theta), & \theta > 0 \\ 0, & \theta \le 0. \end{cases} \tag{4}$$

There are three dimensionless dependent scaled variables: temperature θ, solid fuel concentration ρ, and oxygen concentration Y. The oxygen is a component of gas that is moving with Darcy velocity $a > 0$. Both oxygen and heat are assumed to be transported with this velocity. An exothermic chemical reaction involving oxygen and solid fuel can occur only when the temperature is above a threshold temperature, which we have normalized to be $\theta = 0$. Because of this convention, the scaled temperature is allowed to be negative. The reaction rate is given as Arrhenius law in (4) by $\Phi(\theta)$. Equation (1) represents transport and diffusion of temperature, as well as generation of thermal energy by the chemical reaction. Equation (2) represents consumption of the solid fuel, which of course does not diffuse and is not transported by gas. Equation (3) represents transport of oxygen and consumption of oxygen in the chemical reaction. Diffusion of oxygen is ignored as in [1]. A derivation of the model, and discussion of its range of validity, can be found in Appendix A of [11].

We are of course interested in solutions with $\rho \geq 0$ and $Y \geq 0$ everywhere. It turns out that all waves have nonnegative speeds. The injection problem is therefore equivalent to considering (1)–(2) on $-\infty < x < \infty$, $t \geq 0$, with constant boundary conditions

$$(\theta, \rho, Y)(-\infty) = (\theta^L, \rho^L, Y^L), \qquad (\theta, \rho, Y)(\infty) = (\theta^R, \rho^R, Y^R). \tag{5}$$

As usual, we assume that the reaction does not occur at the boundaries, i.e., the reaction terms in (1)–(3) vanish at the boundary. There are three reasons for the reaction terms to vanish:

1. Temperature control (TC) – the reaction ceases due to low temperature $\theta \leq 0$;
2. Fuel control (FC) – the reaction ceases due to lack of fuel $\rho = 0$;
3. Oxygen control (OC) – the reaction ceases due to lack of oxygen $Y = 0$.

Of course, two or all of these conditions can occur simultaneously. In this paper we focus on the case when the left boundary condition corresponds to (OC) and the right boundary condition corresponds to (TC).

3. **Previous results.**

In this section we review nomenclature and some results obtained in [11]. We denote by $(\theta^-, \rho^-, Y^-) \xrightarrow{c} (\theta^+, \rho^+, Y^+)$ a wave of velocity c that connects (θ^-, ρ^-, Y^-) at the left to (θ^+, ρ^+, Y^+) at the right. At the end states of the wave, the reaction terms in (1)–(3) vanish.

States at which the reaction terms vanish were classified as TC, FC, OC, $TC \cap FC$, $TC \cap OC$, $FC \cap OC$, or $TC \cap FC \cap OC$. The type of the state indicates exactly which conditions hold at that state; for example, a $TC \cap FC$ state has $\theta \leq 0$, $\rho = 0$, and $Y > 0$. A wave with velocity c from a state of type $FC \cap OC$ to one of type TC, for example, would be indicated $FC \cap OC \xrightarrow{c} TC$. In [11] it was assumed that the boundary conditions can be FC, OC or TC with no intersections. However, they cannot be ignored as possible intermediate states.

By a "combustion wave" we shall mean a continuous nontrivial traveling wave with velocity $c > 0$, $c \neq a$. Following [11], we are concerned especially with combustion waves that approach both end states exponentially. This limitation allows us to ignore certain waves that exist only when $\theta^+ = 0$, but approach the right state more slowly than exponentially. The consequence is that we can treat right states with $\theta^+ = 0$ exactly like right states with $\theta^+ < 0$. The limitation also allows us to ignore traveling waves with $\theta^- = 0$, since it turns out that they necessarily approach the left state more slowly than exponentially. For other approaches see [1, 3, 10, 13, 23, 26].

In [11] it was established that there are exactly four types of combustion waves that approach both end states exponentially, two fast (wave velocity $c_f > a$) and two slow (positive wave velocity $c_s < a$): $FC \xrightarrow{c_f} TC$, $OC \xrightarrow{c_f} TC$, $FC \xrightarrow{c_s} OC$, $TC \xrightarrow{c_s} OC$.

3.1. **Fast combustion wave.**

In a fast combustion wave, the burning front moves toward the low-temperature region containing both solid fuel and oxygen; this is often called "premixed combustion." The heat produced remains behind the combustion front because the moving gas that could transport it has a lower velocity. These fronts were studied in [11], where the following result was proven:

Theorem 3.1 (Fast Combustion Waves)**.** *Fix $a > 0$. Let (θ^+, ρ^+, Y^+) be a state of type TC, i.e., $\theta^+ \le 0$, $\rho^+ > 0$, $Y^+ > 0$. Assume in addition that $\theta^+ + Y^+ > 0$. Then there exists a state (θ^-, ρ^-, Y^-) and a velocity $c_f > a$ such that there is a combustion wave $(\theta^-, \rho^-, Y^-) \xrightarrow{c_f} (\theta^+, \rho^+, Y^+)$ that approaches its right state exponentially. It has $\theta^- > 0$, and ρ^- or Y^- or both equal to 0. More precisely, for fixed (θ^+, ρ^+), there is a unique Y^+_* with $\theta^+ + Y^+_* > 0$ such that*

1. *if $-\theta^+ < Y^+ < Y^+_*$, then there exists a combustion wave of type $OC \xrightarrow{c_f} TC$;*
2. *if $Y^+ = Y^+_*$, then there exists a combustion wave of type $FC \cap OC \xrightarrow{c_f} TC$;*
3. *if $Y^+ > Y^+_*$, then there exists a combustion wave of type $FC \xrightarrow{c_f} TC$.*

In all cases, $\theta^+ + Y^+ = \theta^- + Y^-$ and

$$c_f = \frac{aY^+ - aY^-}{Y^+ - Y^- + \rho^- - \rho^+}. \tag{6}$$

In the first and third cases the wave also approaches its left state exponentially; in the second case it does not. There are no combustion waves with $c > a$ and $\theta^+ + Y^+ \le 0$.

Remark 1. In fact, given (θ^-, ρ^-, Y^-), the values of Y^* define a three dimensional manifold in parameter space $\{(\theta^-, \rho^-, Y^-, a)\}$. This manifold was studied numerically in [9].

Theorem 3.1 says that if the right state has too little oxygen (i.e., if $\theta^+ + Y^+ \le 0$), then the reaction cannot occur; if it has a moderate amount of oxygen, then there exists a combustion wave in which all the oxygen is used up in the reaction; and if it has a large amount of oxygen, then there exists a combustion wave in which all the fuel is used up in the reaction.

We conjecture that the combustion waves described in Theorem 3.1 are unique and depend smoothly on the right state. Explicitly, given $a > 0$, $\theta^+ \le 0$, $\rho^+ > 0$, and $Y^+ > -\theta^+$, there is a unique $c > a$, given by a smooth function of (θ^+, ρ^+, Y^+), such that there is a combustion wave with velocity c and left state (θ^+, ρ^+, Y^+). In Section 9 of [11] numerical evidence for the uniqueness was presented.

When the right state of a combustion wave is temperature-controlled, the oxygen concentration there, Y^+, is typically $\mathcal{O}(1)$. Thus the assumption $\theta^+ + Y^+ > 0$ holds whenever the temperature θ^+ at the right state is not too far below ignition temperature 0. This assumption is reasonable; in engineering it is often assumed that the two are equal.

3.2. **Slow combustion wave.** In a slow combustion wave, gas bringing oxygen flows into a region in which solid fuel is present but oxygen is not. Combustion occurs behind the incoming gas; it cannot occur in front since ahead of the gas there is no oxygen. Thus the speed c of the combustion front cannot be greater than a. In fact $c < a$, so heat produced by combustion, which also moves with speed a, is swept head of the combustion front. Hence the high-temperature region is ahead of the front. The oxygen is entirely consumed in the reaction. These fronts have been called "reaction-trailing smolder waves" [23] and "coflow (or forward) filtration combustion waves" [3]. They were studied in [11], where the following result was established.

Theorem 3.2 (Slow Combustion Waves)**.** *1. Consider $FC \xrightarrow{c_s} OC$ and $FC \cap TC \xrightarrow{c_s} OC$ waves. Fix $a > 0$. Let $(\theta^-, 0, Y^-)$ have $\theta^- \ge 0$ and $Y^- > 0$. Then for each $\rho^+ > 0$, there are unique numbers $\theta^+ > 0$ and c_s, $0 < c_s < a$, such that there exists a combustion wave of velocity c_s from $(\theta^-, 0, Y^-)$ to $(\theta^+, \rho^+, 0)$. In fact,*

$$\theta^+ = \theta^- + Y^-, \quad c_s = \frac{Y^-}{\rho^+ + Y^-} a. \tag{7}$$

These waves approach their right state exponentially, and approach their left state exponentially if and only if $\theta^- > 0$, i.e., if and only if the left state is of type FC.

2. *$TC \xrightarrow{c_s} OC$ waves. Fix $a > 0$. Let $\theta^- < 0$, Y^- with $\theta^- + Y^- > 0$, and $\rho^+ > 0$ be given. Then there are numbers $\rho^- > 0$, $\theta^+ > 0$, and c_s, $0 < c_s < a$, such that there exists a combustion wave of velocity c_s from (θ^-, ρ^-, Y^-) to $(\theta^+, \rho^+, 0)$. Moreover $\theta^+ = \theta^- + Y^-$, and the quantities c_s and ρ^- are related by the formula*

$$c_s = \frac{aY^-}{Y^- - \rho^- + \rho^+}.$$

These waves approach both end states exponentially.
3. *There are no other combustion waves with velocity satisfying $0 < c < a$. In particular, there are no slow combustion waves with $\theta^- + Y^- \leq 0$.*

Theorem 3.2 (1) says that for each left state of type FC, and for the left state $(0, 0, Y^-)$ with $Y^- > 0$, there is a one-parameter family of right states of type OC to which the left state can be connected by a slow combustion wave.

Theorem 3.2 (2) says that for a slow combustion wave of speed c_s from a left state (θ^-, ρ^-, Y^-) of type TC to a right state $(\theta^+, \rho^+, 0)$ of type OC to exist, the triple (θ^-, Y^-, ρ^+) may be chosen arbitrarily, and then a corresponding triple (ρ^-, θ^+, c_s) can be found. In [11] we present numerical evidence that the triple (ρ^-, θ^+, c_s) is unique.

3.3. **Contact discontinuities.** In the absence of reaction and diffusion terms, the characteristic velocities of (1)–(3) are 0 for the solid fuel and a for temperature and oxygen. Contact discontinuity[1] waves therefore have velocity 0 or a. The solid fuel concentration can change across a contact discontinuity of velocity 0, while temperature or oxygen concentration or both can change across a contact discontinuity of velocity a. Contact discontinuities must separate intervals in which the reaction does not occur (since (θ, ρ, Y) is constant).

The waves in a wave train must occur in order of increasing velocity from left to right. It is easy to see that there is at most one slow combustion wave and one fast combustion wave. We may also assume that there is at most one wave of velocity 0 and one of velocity a. The reason is that a sequence of two contact discontinuities with the same velocity can be combined into one discontinuity.

The *dimension number* of a contact discontinuity is the dimension of the set of right states that can be reached from a fixed left state by a contact discontinuity of the given type. For example, for a contact discontinuity of speed 0, the ρ-component of the right state can vary (dimension 1) unless it is 0 (dimension 0). For a contact discontinuity of speed a, both the the θ- and Y-components of the right state can vary (dimension 2), unless the Y-component of the right state is 0 (dimension 1). The following result was proven in [11]:

Theorem 3.3. *With assumptions (L), (R), and (O), the contact discontinuities that occur in generic wave sequences are*

$$\begin{gathered} TC \xrightarrow{0} TC\ (1); \quad TC \xrightarrow{0} TC \cap FC\ (0); \quad OC \xrightarrow{0} OC\ (1); \\ OC \xrightarrow{0} FC \cap OC\ (0); \quad TC \xrightarrow{a} TC\ (2); \quad TC \xrightarrow{a} OC\ (1); \\ FC \xrightarrow{a} FC\ (2); \quad OC \xrightarrow{a} OC\ (1); \quad OC \xrightarrow{a} TC\ (2); \\ TC \cap FC \xrightarrow{a} FC\ (2); \quad FC \cap OC \xrightarrow{a} FC\ (2), \end{gathered} \tag{8}$$

where the corresponding dimension number is given inside the parentheses.

[1] Because some of these waves widen with time, they are not classical contact discontinuities. However, they are analogous to them. For more details see [11]. A better name for the wave with constant velocity a in variable θ would be diffusive contact. For simplicity, we abuse the notation and use the term "contact wave" to describe it.

3.4. **Wave Sequences.** In [11] 18 possible wave sequences were classified and numerically illustrated. In [9] this classification was refined and expanded to 26 wave sequences. As our interest in the present paper is showing an example of instability resulting from the interaction between traveling and contact waves, we will concentrate only in the sequences corresponding to the cases

$$OC \xrightarrow{0} OC \xrightarrow{a} TC; \tag{9}$$

$$OC \xrightarrow{0} OC \xrightarrow{c_f} TC; \tag{10}$$

$$OC \xrightarrow{0} OC \xrightarrow{a} OC \xrightarrow{c_f} TC. \tag{11}$$

4. **Numerical examples.** In this section we present a numerical example showing the interactions between traveling and contact waves. We simulate the system (1)-(4) using a Crank-Nicolson difference scheme. The simulation used the parameter $a = 0.1$, space step $\Delta x = 1.0$, time step $\Delta t = 5$ and a total grid number 1900. This example corresponds to the boundary conditions OC on the left and TC on the right. The possible wave sequences for this Riemann problem are given by (9)-(11).

The first simulation starts with the contact and traveling wave profiles placed far from each other, as plotted on the left side of Fig. 1. The contact and traveling waves do not interact and separate from each other. The stable combustion front can be observed on the right side of Fig. 1. It is clear that the distance between the waves grows linearly.

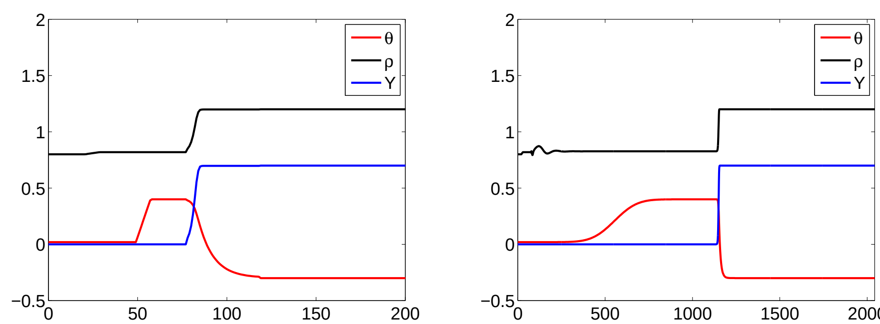

Figure 1. Initial condition is plotted on the left and the simulation result at time 5000 on the right. Both figures correspond to the sequence given in (11). Horizontal axis – variable x.

The second and first simulations differ only in the distance between the contact and traveling wave initial profiles, which are placed close to each other in the second simulation as plotted on the left side of Fig. 2. After some oscillations, the combustion wave vanishes, see the right side of Fig. 2. For the simulations described above the combustion wave satisfies the relation (6) in the following sense: given the right state of the fast combustion wave, the left state and speed obtained numerically coincide with those given by Eq. (6).

5. **Conclusions and discussion.** Let us try to understand the bifurcation occurring between Fig. 1 and Fig. 2. The combustion occurs in a small region around the intersection of oxygen and fuel profiles. The heat generated in this thin region is dissipated to the colder regions ahead and behind. However, dissipation to the region behind is smaller in Fig. 1 than in Fig. 2 because the width of the high temperature region is larger in Fig. 1. Thus enough heat is preserved in the reaction region plotted in Fig. 1 so that the combustion is maintained.

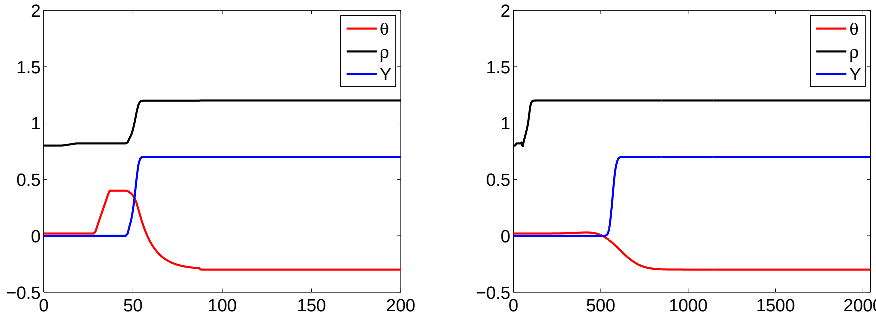

FIGURE 2. An initial condition corresponging to the sequence given in (11) is plotted on the left and the simulation result at time 5000 on the right; it corresponds to sequence given in (9). Horizontal axis – variable x.

In summary, we have presented a numerical example exhibiting the influence of the interaction between traveling and contact waves on the stability of the pair of waves. Such interaction, in fact, can change significantly the behavior of the solution, leading to instability absent from isolated waves. Describing this wave interaction from a mathematical point of view represents a challenge for the future.

Appendix A. Stability of isolated waves. As mentioned in the introduction, the stability of the combustion wave alone has been the subject of many studies. Here we verify that the combustion wave is stable by direct numerical simulation using the boundary conditions corresponding to those given by Eq. (6), as plotted on the left side of Fig. 3. One can observe a stable combustion wave the right side of Fig. 3.

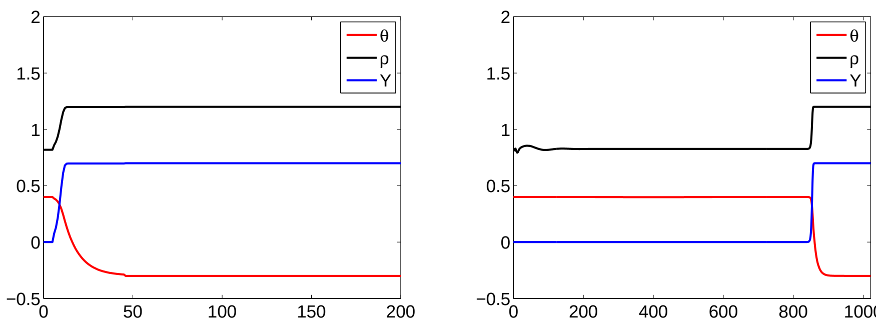

FIGURE 3. Initial condition is plotted on the left and simulation result at time 4000 on the right. Horizontal axis – variable x.

We stress the fact that initial and boundary conditions different from those used in Remark 1 can generate combustion waves of different nature. As an example, on the left and right sides of Fig. 4 we plot the initial condition and the corresponding simulation result at time 9000, a solution that oscillates periodically for as long as one cares to perform the simulations. Notice that the initial and boundary conditions in Figs. 3 and 4 are slightly different, the values for θ at the left and right extremes are $\theta_L = 0.40$ and $\theta_R = -0.30$ in Fig. 3 and $\theta_L = 0.36$ and $\theta_R = -0.34$ in Fig. 4.

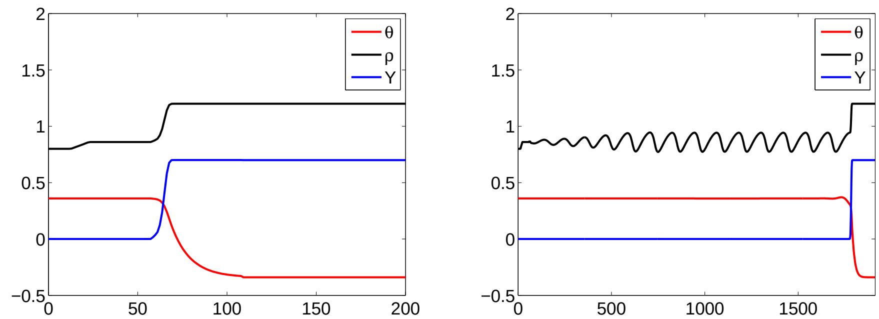

FIGURE 4. Initial condition is plotted on the left and simulation result at time 9000 on the right. Horizontal axis – variable x.

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