TRANSACTIONS OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 304, Number 1, November 1987

TRAVELING WAVES IN COMBUSTION PROCESSES WITH COMPLEX CHEMICAL NETWORKS

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ABSTRACT. The existence of traveling waves for laminar flames with complex chemistry is proved. The crucial assumptions are that all reactions have to be exothermic and that no cycles occur in the graph of the reaction network. The method is to solve the equations first in a bounded interval by a degree argument and then taking the infinite domain limit.

0. Introduction. In this paper we establish the existence of traveling waves for premixed laminar flames with complex chemical networks. We consider the case of vanishing Mach number i.e. the flame speed is much smaller than a typical gas velocity.

The resulting equations were solved by H. Berestycki, B. Nicolaenko, B. Scheurer [**1**] for a single step irreversible reaction. Here we discuss a class of exothermic acyclic chemical networks. In [**2, 3**] P. Fife and B. Nicolaenko used a somewhat weaker condition on the network than ours for a formal asymptotic analysis in the limit of high activation energy. For mathematical reasons we can only handle the case of exothermic, i.e. irreversible reactions.

In the first section we introduce the notations and derive the traveling wave equations from the thermodynamic conservation laws. In §2 these equations are solved in a finite domain by a mapping degree argument and then shown to converge in the infinite domain limit.

The third section treats some examples to which the existence theorem can be applied.

1. Notations and derivation of the traveling wave equations. Let Y_i be the mass functions of n chemical species A_i reacting in an infinite tube and depending on time t and one space variable ξ. A chemical network consisting of r reactions may be symbolically written as

$$R_j\colon \sum_{i=1}^{n} \nu_{ij} A_i \to \sum_{i=1}^{n} \mu_{ij} A_i, \qquad j = 1, \ldots, r,$$

where $\nu_{ij}, \mu_{ij} \in \mathbf{N} \cup \{0\}$ represent the stöchiometric coefficients and for every j there exist i and k with $\nu_{ij}, \mu_{kj} > 0$. Each reaction proceeds at a rate

$$\omega_j = \rho \prod_{i=1}^{n} Y_i^{\nu_{ij}} B_j(T) \exp\left(-\frac{E_j}{RT}\right). \tag{1.1}$$

Received by the editors July 16, 1986 and, in revised form, December 17, 1986.
1980 *Mathematics Subject Classification* (1985 *Revision*). Primary 35K40; Secondary 80A25.
Key words and phrases. Traveling waves, combustion, complex chemistry.
This work has been supported by the Deutsche Forschungsgemeinschaft.

Here T is the absolute temperature, E_j the activation energy, R the gas constant and $B_j(T) > 0$ for $T > 0$. The mass action law gives the product over the mass fractions and the Arrhenius kinetic the exponential factor. Next we introduce some notation. Let

$$\begin{aligned}
U &= (T, Y_1, \ldots, Y_n) \in \mathbf{R}^{n+1}, \\
Q_j &= \text{heat release of reaction } j, \\
d_0(U) &= \text{heat conductivity}, \\
d_i(U) &= \text{diffusion coefficient of species } i, \\
\rho &= \text{density}, \\
p &= \text{pressure}, \\
\frac{D}{Dt} &= \frac{\partial}{\partial t} + v\frac{\partial}{\partial \xi} = \text{convective derivative with } v \text{ as the velocity}, \\
c_p &= \text{specific heat at constant pressure.}
\end{aligned}$$

Using the notations

$$F_0(U) = \sum_{j=1}^{r} Q_j \omega_j(U),$$

$$F_i(U) = \sum_{j=1}^{r} (\mu_{ij} - \nu_{ij})\omega_j(U)$$

the balance laws of mass, momentum, energy and mass fractions for zero Mach number and no viscosity can be written in the form

$$\frac{D\rho}{Dt} + \rho\frac{\partial v}{\partial \xi} = 0, \tag{1.2.a}$$

$$\rho\frac{Dv}{Dt} = 0 \Leftrightarrow \frac{\partial p}{\partial \xi} = 0, \tag{1.2.b}$$

$$\rho c_p \frac{DT}{Dt} - \frac{\partial}{\partial \xi}\left(d_0 \frac{\partial T}{\partial \xi}\right) = F_0(U), \tag{1.2.c}$$

$$\rho\frac{DY_i}{Dt} - \frac{\partial}{\partial \xi}\left(d_i \frac{\partial Y_i}{\partial \xi}\right) = F_i(U).$$

Additionally the state equation for an ideal gas holds:

$$p = R\rho T \tag{1.2.d}$$

This approximation implies a constant pressure.

For the description of a flame moving to the left with constant velocity v_0 let $x = \xi + v_0 t$ be the single independent variable. (1.2.a) then gives with $d/dx = (\ ')$

$$v_0\rho' + (\rho v)' = 0 \quad \text{or} \quad \rho(v_0 + v) = c$$

Here c is the mass flux. If (1.2.d) is substituted in (1.2.c) and $B_j(T)$ is redefined by $(p/RT)B_j(T)$ one arrives at

$$-(d_0 T')' + cT' = F_0(U), \quad -(d_i Y_i')' + cY_i' = F_i(U). \tag{1.3}$$

Notice that c_p disappears after scaling.

Introduce the reaction vector $V_j = (\mu_{1j} - \nu_{1j}, \ldots, \mu_{nj} - \nu_{nj})$ and let $K_j = (Q_j, V_j)$. Now (1.3) may be written in the vector form

$$-(D(U)U')' + cU' = F(U) \tag{1.4}$$

where $D = \operatorname{diag}(d_0, \ldots, d_n)$ and $F = (F_0, \ldots, F_n)$. For a detailed formal derivation from the thermodynamic conservation laws see [5]. As boundary conditions we prescribe $T^- = T(-\infty) > 0$ and $Y_i^- = Y_i(-\infty) \geqslant 0$ where not all Y_i^- vanish.

Since we consider only exothermic reactions U^- is in general not an equilibrium point of (1.4), i.e. $F(U^-) \neq 0$. Therefore we introduce an artificial ignition temperature $\theta > T^-$ and redefine $F(U)$ as 0 for $T < \theta$. This cutoff of F is discussed in [1]. F is now discontinuous and (1.4) should hold in the following sense

$$-D(U)U' + c(U - U^-) = \int_{-\infty}^{x} F(U(s))\, ds \tag{1.5}$$

with $U \in C^1(\mathbf{R})$. At $x = +\infty$ we demand $U = U^+$ with $T^+ > \theta$. Hence $F(U(s))$ is C^1 near infinity and $F(U^+) = 0$ must hold. (1.5) gives the compatibility condition

$$c(U^+ - U^-) = \int_{-\infty}^{\infty} F(U(s))\, ds. \tag{1.6}$$

Given U^- we seek a positive solution of (1.5) for some c and U^+.

2. The main existence theorem. With the notations of §1 we state

THEOREM 1. *Suppose that the following assumptions hold*:

(i) *Let* $U^- \in \mathbf{R}_{+0}^{n+1} = \{U \in \mathbf{R}^{n+1};\ U_i \geqslant 0,\ i = 0, \ldots, n\}$ *be given. Assume* $U_0^- > 0$ *and that there exists* j^* *such that* $\nu_{ij^*} > 0$ *implies* $U_i^- > 0$.

(ii) *The ignition temperature* θ *should satisfy* $0 < \theta - U_0^- \leqslant R$ *where* R *is a constant which depends only on* U^- *and* K_j.

(iii) *The reaction rates have the form*

$$\omega_j(U) = \begin{cases} \prod_{i=1}^{n} U_i^{\nu_{ij}} B_j(U_0)\exp(-E_j/U_0) & \text{for } U_0 > \theta, \\ 0 & \text{for } U_0 < \theta. \end{cases}$$

(iv) *All reactions are exothermic, i.e.* $Q_j > 0$.

(v) *For the reaction vectors* V_j *there exists* $L \in \mathbf{R}_{+0}^{n}$, *such that* $L \cdot V_j < 0$ *for* $j = 1, \ldots, r$.

(vi) *The diffusion coefficients* $d_i(U)$ *are differentiable in* $\{U \in \mathbf{R}_{+0}^{n+1};\ U_0 \geqslant U_0^-\}$ *and strictly positive for* U *bounded*.

Then there exists $c > 0$; $U^+ \in \mathbf{R}^{n+1}$ *and a function* $U \in C^2(\mathbf{R} \setminus \{0\}) \cap C^1(\mathbf{R})$ *with values in* $\mathbf{R}_{+0}^{n+1}$ *such that*

$$-(D(U)U')' + cU' = F(U) \quad \text{in } \mathbf{R}\setminus\{0\}, \tag{2.1}$$

$$U(-\infty) = U^-; \quad U(+\infty) = U^+; \quad U_0(0) = \theta, \tag{2.2}$$

$$U_0'(x) > 0.$$

Furthermore U^+ *satisfies* $F(U^+) = 0$ *and there exist* $\alpha_j \geqslant 0$, $j = 1, \ldots, r$, *with*

$$U^+ = U^- + \sum_{j=1}^{r} \alpha_j K_j. \tag{2.3}$$

REMARKS ON THE ASSUMPTIONS. (i) guarantees the positivity of at least one reaction rate.

(ii) is needed for the estimate of c from below. It is also reasonable to choose $\theta - U_0^-$ small to diminish the cutoff error in ω_j.

(iv) yields the monotonicity of U_0, which implies the existence of $\lim_{x\to\infty} U(x)$.

(v) gives a priori bounds for U.

(v) is equivalent to the following (see Proposition 6): $\alpha_j \geqslant 0$ and $\sum_{j=1}^r \alpha_j V_j \in \mathbf{R}^n_{+0}$ imply $\alpha_j = 0$. In **[2, 3]** the weaker condition $\sum_{j=1}^r \alpha_j V_j = 0$ is used for an asymptic analysis at high activation energy. But the network $A \to 2B$; $B \to 2A$ shows the nonexistence of a boundary condiiton U^+ with the necessary conditions (2.2), (2.3). Reaction cycles are characterized by the existence of $\alpha_j \geqslant 0$ where not all α_j vanish, s.t. $\sum_{j=1}^r \alpha_j K_j = 0$; but the latter is excluded by (v). This seems reasonable because we consider only exothermic reactions.

FURTHER REMARKS. (a) Besides positivity and differentiability for $U_0 > \theta$ we need no condition on the temperature dependence of the reaction rates ω_j.

(b) If U^- is given U^+ is in general not unique (compare the examples in §3). Also if only one U^+ is possible no uniqueness of c or U^+ is asserted.

SUMMARY OF THE PROOF. (1.5) is first solved in a bounded domain with "false" boundary conditions to insure that the temperature is monotone increasing. A priori estimates establish the infinite domain limit. The monotonicity of U_0 gives the existence of $\lim_{x\to\infty} U(x) = U^+$ with the properties in (2.2), (2.3).

Solution in a finite domain. In the interval $(-a, a)$ we seek a positive solution of

$$-D(U)U' + c(U - U^{a-}) = \int_{-a}^{x} F(U(s))\,ds \tag{2.4}$$

with boundary conditions

$$\begin{aligned} -D(U)U' + cU &= cU^{a-} \quad \text{at } x = -a, \\ U(a) = U^{a+}, &\quad U_0(0) = \theta, \end{aligned} \tag{2.5}$$

where

$$U_i^{a-} = \begin{cases} U_i^- & \text{if } U_i^- > 0, \\ \dfrac{1}{a} & \text{if } U_i^- = 0, \end{cases} \tag{2.6}$$

and

$$U_0^{a+} > \theta \quad \text{will be chosen later independent of } a,$$

$$U_i^{a+} = 0 \quad \text{for } i = 1, \ldots, n. \tag{2.7}$$

This will imply $U_i(x) > 0$ and $U_0'(x) > 0$. First we show that for a solution of this problem the discontinuity of $F(U)$ occurs only once.

PROPOSITION 1. *Let $U \in C^1((-a, a))$ be a nonnegative solution of* (2.4), (2.5) *and $c > 0$. Then $U_0(x) = \theta$ for some x equivalent to $x = 0$.*

PROOF. $U_0(0) = \theta < U_0^{a+}$ implies the existence of a maximal $x_0 \in [0, a)$ with $U_0(x_0) = \theta$. Since for $x > x_0$ $U(x)$ is $C^2((x_0, a))$ and not constant the strong maximum principle **[6]** applied to $(d_0(U)U_0')' - cU_0' \leqslant 0$ gives

$$U_0'(x_0) > 0. \tag{2.8}$$

Suppose another $x_1 < x_0$ with $U_0(x_1) = \theta$. Because of (2.8) x_1 may be chosen maximal and $U_0(x) < \theta$ holds in (x_1, x_0). From $F(U(x)) \equiv 0$ in (x_1, x_0) it follows that $U_0(x) \equiv \theta$ in (x_1, x_0), a contradiction. □

By shifting U_0 we may assume $\theta = 0$ and $U_0^- < 0$. According to the proposition the problem is reduced to finding a function $U \in C^2(I, \mathbf{R}_+^{n+1})$ in the interval $I = (0, a)$ such that

$$(2.9)\qquad \begin{aligned} -\left(D(U)U'\right)' + cU' &= F(U) \quad \text{in } I,\\ -D(U)U' + c(U - U^{a-}) &= 0 \quad \text{at } x = 0,\\ U(a) = U^{a+},\quad U_0(0) &= 0. \end{aligned}$$

Next we construct a compact operator, whose fixed points are the solutions of (2.9).

Let $R > 0$ and Ω_R be the following open subset of $C^1(\bar{I}, \mathbf{R}^{n+1})$:

$$\Omega_R := \left\{U \in C^1(\bar{I}, \mathbf{R}^{n+1}) \colon |U|_{C^1(\bar{I})} < R;\ U_i > 0 \text{ on } I \text{ for all } i;\ U_0(0) = 0;\right.$$
$$\left. U_0'(0) > 0;\ U_0(a) > 0;\ U_i(0) > 0;\ U_i(a) = 0;\ U_i'(a) < 0 \text{ for } i \geqslant 1\right\}.$$

Assumption (vi) in Theorem 1 gives a constant $\alpha(\Omega_R)$ s.t. $d_i(U) \geqslant \alpha > 0$ for all $U \in \Omega_R$. Define $D_t(U) := tD(U) + \alpha(1 - t)\mathbf{1}$, $0 \leqslant t \leqslant 1$, with $\mathbf{1}$ the unit matrix. Further let $0 < \underline{c} \leqslant \bar{c}$. For $W \in \bar{\Omega}_R$; $c \in [\underline{c}, \bar{c}]$ we define

$$K_t(W, c) := \left(U, c + W_0(0)\right)$$

where U is a solution of the linear boundary value problem

$$(2.10)\qquad \begin{aligned} -\left(D_t(W)U'\right)' + cU' &= tF(W) \quad \text{in } I,\\ -D_t(W)U' + cU &= cU^{a-} \quad \text{at } x = 0,\\ U(a) &= U^{a+}. \end{aligned}$$

It is easy to check that K_t is well defined, continuous and compact with values in $C^1(I, \mathbf{R}^{n+1}) \times \mathbf{R}$. Observe that the fixed points of K_1 have the desired properties. Now a priori estimates are given to insure that K_t has no fixed points on $\partial(\Omega_R \times (\underline{c}, \bar{c}))$ for suitable R, $\underline{c}$ and $\bar{c}$.

PROPOSITION 2. *Let the assumptions of Theorem 1 hold. If U_0^{a+} is sufficiently large then there exist constants $R, \underline{c}, \bar{c}$ s.t. K_t has no fixed point on $\partial(\Omega_R \times (\underline{c}, \bar{c}))$ for $0 \leqslant t \leqslant 1$. In particular $(U, c) \in \bar{\Omega}_R \times [\underline{c}, \bar{c}]$ and $K_t(U, c) = (U, c)$ imply $|U|_{C^1(I)} < R$; $U(x) \in \mathbf{R}_+^{n+1}$ for all $x \in I$ and $\underline{c} < c < \bar{c}$. Additionally we have for $t = 1$ that $|U|_{C^2(I)}$ and $\bar{c}$ are bounded independent of a for $a > a_0$. Furthermore $U_0'(x) > 0$ holds.*

PROOF. Assume that (U, c) is a fixed point of K_t in $\bar{\Omega}_R \times [\underline{c}, \bar{c}]$. We have to prove that $(U, c) \in \Omega_R \times (\underline{c}, \bar{c})$ for suitable $R, \underline{c}, \bar{c}$ and U_0^{a+}. For fixed R assumption (vi) in Theorem 1 gives that $d_{it}(U)$ is uniformly positive. Hence the maximum principle can be applied. We divide the proof into several steps.

(i) First we verify the positivity of U_i in I and the boundary conditions specified in Ω_R. Proposition 1 gives $U_0(x) > 0$ in I. From (2.7), (2.9) we get $U_0(0) = 0$; $U_0'(0) > 0$; $U_0(a) > 0$. $F(U)$ is continuous for $U_0 > 0$ and hence

$$(2.11)\qquad -\left(D_t(U)U'\right)' + cU' = tF(U)$$

holds.

Now let $i \geqslant 1$. If $V_{ij} := \mu_{ij} - \nu_{ij}$ is negative then $\nu_{ij} > 0$ and $\omega_j(U)$ contains U_i as a factor. So $F_i(U)$ may be decomposed as

$$F_i(U) = -h_i(U)U_i + \sum_{V_{ij} > 0} V_{ij}\omega_j(U)$$

with $h_i(U) = -(1/U_i)\Sigma_{V_{ij} < 0} V_{ij}\omega_j(U)$ positive because $U_i \geqslant 0$. From (2.11) we derive

$$\left(d_{it}(U)U_i'\right)' - cU_i' - th_i(U)U_i \leqslant 0.$$

The maximum principle gives $U_i > 0$ in I and $U_i'(a) < 0$ because $U_i \equiv$ constant would violate the boundary conditions in (2.9). $U_i(0) > 0$ follows now from the b.c. at $x = 0$.

(ii) Next we derive an upper bound for $|U|$. By Theorem 1(v) there exists a vector $L \in \mathbf{R}^{n+1}_{+0}$ such that $L \cdot V_j < 0$, $j = 1, \dots, r$. Hence $L_0 Q_j + L \cdot V_j \leqslant 0$ for some $L_0 > 0$, i.e. $(L_0, L) \cdot K_j \leqslant 0$ and $(L_0, L) \cdot F(U) \leqslant 0$. Multiply (2.11) by (L_0, L) and integrate:

$$\sum_{i=0}^{n} L_i d_{it} U_i' \geqslant c \sum_{i=0}^{n} L_i\left(U_i - U_i^{a-}\right) \quad \text{in } I.$$

Choose now $U_0^{a+} > U_0^- + (1/L_0)\Sigma_{i=1}^n L_i U_i^{a-}$ and use $U_i(a) = 0$; $U_i'(a) \leqslant 0$ for $i = 1, \dots, n$ to conclude that $U_0'(a) > 0$.

Observe that U_0^{a+} is independent of the domain if $a > a_0$. If we would have $U_0'(x_0) = 0$ for some $x_0 \in I$ then the equation for U_0 would imply $U_0''(x_0) < 0$ and thereof $U_0' < 0$ in (x_0, a) which contradicts $U_0'(a) > 0$. Thus $U_0' > 0$ and $0 < U_0 < U_0^{a+}$ in I. Using the monotonicity of U_0 we get

$$\begin{aligned} c\left(U_0^{a+} - U_0^-\right) &\geqslant -d_{0t}U_0'(x) + c\left(U_0(x) - U_0^-\right) = t\int_0^x F_0(U(s))\,ds \\ &\geqslant tQ_j \int_0^x \omega_j(U(s))\,ds \end{aligned}$$

and for $i \geqslant 1$ it follows with some $R_1 > 0$:

$$-d_{it}U_i' + c\left(U_i - U_i^{a-}\right) = t\int_0^x F_i(U(s))\,ds \leqslant cR_1$$

since F_i is a linear combination of ω_j. This and $U_i(a) = 0$ give

$$|U|_{C^0(I)} \leqslant \max_{1 \leqslant i \leqslant n}\left(U_i^{a-} + R_1, U_0^{a+}\right) =: R_2$$

independent of a for $a > a_0$.

We remark that R_2 depends only on $U^{a\pm}$ and K_j. Now choose constants such that for all $U \in \{U \in \mathbf{R}^{n+1}_+;\ |U| < R_2\}$, $0 < \alpha \leqslant d_i(U) \leqslant \beta$; $|\nabla_U d_i| \leqslant \gamma$; $|F(U)| \leqslant M$ holds. Since R_2 is independent of $\overline{\Omega}_R \times [\underline{c}, \bar{c}]$ so are the other constants.

(iii) Now we prove a C^2-estimate for U. From $-D_t(U)U' + c(U - U^{a-}) = t\int_0^x F(U(s))\,ds$ we obtain

$$|U'| \leqslant (1/\alpha)c\left(R_2 + R_1 + |U^{a-}|^0\right) =: cR_3$$

and from (2.11)

$$|U''| \leqslant (1/\alpha)\left(\gamma R_3^2 c^2 + c^2 R_3 + M\right) =: R_4(c).$$

(iv) To derive an upper bound for c let $w(x) = U_0^- - U_0(x)$ and apply the lemma of Gronwall [7] to

$$-d_{0t}U_0' + c(U_0 - U_0^-) \leqslant tMx$$

and conclude

$$w(a) \leqslant w(0)e^{ca/\beta} + \frac{tM}{\alpha}\int_0^a se^{c/\beta(a-s)}\,ds.$$

Thus

$$-U_0^- e^{ca/\beta} \leqslant U_0^{a+} - U_0^- + (M\beta^2/\alpha c^2)e^{ca/\beta} \qquad (U_0^- < 0).$$

If $c^2 > -2M\beta^2/\alpha U_0^- =: c_1^2$ then

$$\frac{-U_0^-}{2e^{ca/\beta}} \leqslant U_0^{a+} - U_0^- \quad \text{or} \quad c \leqslant \frac{\beta}{a}\ln\left(2\frac{U_0^{a+} - U_0^-}{-U_0^-}\right) =: c_2.$$

Now choose $\bar{c} > \max(c_1, c_2)$ and $R > R_2 + R_3\bar{c}$. Observe that for $t = 1$ and $a > a_0$ one can estimate c and consequently the C^2-norm of U independently of a.

(v) Concerning the lower bound for c use $F_0(U) \geqslant 0$ and Gronwall's Lemma applied to $-d_0(U)U' + c(U - U^-) \geqslant 0$ to get

$$U_0^{a+} - U_0^- \leqslant -e^{ca/\beta}U_0^- \quad \text{or} \quad c \geqslant \frac{\alpha}{a}\ln\left(\frac{U_0^{a+} - U_0^-}{-U_0^-}\right) >: \underline{c} > 0$$

which gives all the desired estimates. □

Next we use the mapping degree to show that K_1 has a fixed point.

PROPOSITION 3. *There exist U_0^{a+} such that for any given domain $I = (0, a)$ the problem* (2.8) *has a solution $(U, c) \in C^2(I, \mathbf{R}_+^{n+1}) \times \mathbf{R}_+$.*

PROOF. Take $\Omega_R \times (\underline{c}, \bar{c})$ as above. By Proposition 2, $\deg(\mathrm{id}_{\Omega_R \times (\underline{c}, \bar{c})} - K_t(\cdot, \cdot))$ with respect to $(0, 0) \in C^1(I) \times \mathbf{R}$ is independent of t. The degree of $\mathrm{id} - K_0$ is easily seen to be 1. Consequently K_1 has a fixed point. □

The infinite domain limit. Let (U_a, c_a) be a solution of (2.9) in $(0, a)$. According to Proposition 2 there exist $R, \bar{c} > 0$ such that $|U_a|_{C^2((0,a))} < R$ and $0 < c_a < \bar{c}$ independent of a for $a > a_0$.

It remains to bound c_a from below independent of a.

PROPOSITION 4. *Under the assumptions of Theorem* 1 *let (U_a, c_a) be a solution of* (2.9) *in* $(0, a)$. *If U_0^{a+} is sufficiently large then $c_a > \underline{c} > 0$ for all $a > a_0$.*

PROOF. In the proof we omit the subscript a. Since $U_0' > 0$ and $F_0(U) \geqslant 0$ we get from (2.9)

$$\int_0^a F_0(U(s))\,ds \leqslant c(U_0^+ - U_0^-), \qquad 0 < \alpha U_0' \leqslant d_0(U)U_0' \leqslant c(U_0^+ - U_0^-).$$

This yields with U_0 as the independent variable

$$\int_0^{U_0^+} F_0(U(U_0))\,dU_0 \leqslant \frac{c^2}{\alpha}(U_0^+ - U_0^-)^2.$$

Thus it suffices to estimate $F_0(U(U_0))$ on a fixed U_0-interval from below. For that purpose we estimate one ω_j. Choose j^* according to assumption (i) in Theorem 1 and consider i with $\nu_{ij^*} > 0$. Hence $U_i^{a-} = U_i^- > 0$. Let V_{ij} be the ith component of V_j. Since $Q_j > 0$ we can find $\tilde{L}_i$ for all such indices i with $Q_j + \tilde{L}_i V_{ij} \geqslant 0$ and therefore $F_0(U) + \tilde{L}_i F_i(U) \geqslant 0$. Now add to the equation for U_0 the equation for U_i multiplied by $\tilde{L}_i$ and integrate:

$$d_0 U_0' + \tilde{L}_i d_i U_i' \leqslant c(U_0 - U_0^- + \tilde{L}_i(U_i - U_i^-))$$

or

$$\begin{aligned} d_0 U_0' + \tilde{L}_i(d_i U_i)' &\leqslant c(U_0 - U_0^- + \tilde{L}_i(U_i - U_i^-)) + \tilde{L}_i(\nabla_U d_i \cdot U')U_i \\ &\leqslant c(U_0 + (\tilde{L}_i(1 + \gamma R_3)/\alpha) d_i U_i - U_0^- - \tilde{L}_i U_i^-) =: cW \end{aligned}$$

where γ, α, R_3 are as in the proof of Proposition 2. With $U_0' > 0$ and $\alpha/(1 + \gamma R_3) \leqslant d_0(U)$ we get

$$\frac{\alpha}{1 + \gamma R_3} W' = \frac{\alpha}{1 + \gamma R_3} U_0' + \tilde{L}_i(d_i U_i)' \leqslant cW. \tag{2.12}$$

Now choose $U_0^+ \geqslant U_0^- + \tilde{L}_i U_i^-$ for all i with $\nu_{ij^*} > 0$. Since $U_i(a) = 0$ we have $W(a) > 0$ and by (2.12) $W(x) \geqslant 0$ throughout $[0, a]$. Hence

$$U_i(x) \geqslant \frac{\alpha}{\beta(1 + \gamma R_3)} \frac{(U_0^- + \tilde{L}_i U_i^- - U_0(x))}{\tilde{L}_i}.$$

Now let $-U_0^- < \tilde{L}_i U_i^-$ for all i with $\nu_{ij^*} > 0$ (see Theorem 1(ii)). Thus U_i is bounded from below by a positive function of U_0 on the U_0-interval $[0, \min_{\nu_{ij^*} > 0} \tilde{L}_i U_i^- + U_0^-]$. So the same is true for $\omega_{j^*}(U)$ and $F_0(U)$ and we are done. Now we can pass to the limit $a \to \infty$. $\square$

PROPOSITION 5. *Problem* (2.1) *has a nonnegative solution* $U \in C^2(\mathbf{R} \setminus \{0\}) \cap C^1(\mathbf{R})$ *such that* $\lim_{x \to \infty} U(x) =: U^+$ *exists and for which* (2.2), (2.3) *is satisfied. Furthermore* $U_0' > 0$ *holds.*

PROOF. The C^2-norm of a solution U^a in the finite domain $(0, a)$ is uniformly bounded. So by selecting a subsequence, as $a \to \infty$ U_a converges to U locally uniformly in $C^1(\mathbf{R}, \mathbf{R}^{n+1}_{+0})$ and $c^a \to c > 0$ since $\underline{c} < c^a < \bar{c}$.

U satisfies the boundary condition at $x = 0$ by (2.6) $U_0'(0) > 0$ and $U_0'(x) \geqslant 0$ imply $U_0(x) > 0$ in $\mathbf{R}^+$. Hence $F(U)$ is continuous and

$$\int_0^x F(U^a(s))\, ds \to \int_0^x F(U(s))\, ds \quad \text{for any fixed } x \text{ as } a \to \infty.$$

So U solves the integrated equation (1.5) and by continuity of $F(U)$ also (2.9). Therefore $U \in C^2(\mathbf{R}^+, \mathbf{R}^{n+1}_{+0})$.

The maximum principle gives $U_i > 0$ whenever $U_i^- > 0$. Since U_0 is bounded, nondecreasing and $U_0'(0) > 0$ $\lim_{x \to \infty} U_0(x) =: U_0^+ > U_0(0) = 0$ exists.

Let $W := D(U)U'$ and Γ the ω-limit set of (U, W). Note that

$$\Gamma \subset \left\{(\tilde{U}, \tilde{W}) \in \mathbf{R}^{2n+2};\ \tilde{U}_0 = U_0^+,\ \tilde{U}_i \geqslant 0\right\}.$$

Γ is compact, invariant and connected by the boundedness of (U, W) **[4]**. The flow on Γ is described by

$$(2.13) \qquad \tilde{U}' = D(\tilde{U})^{-1}\tilde{W}, \quad \tilde{W}' = cD(\tilde{U})^{-1}\tilde{W} - F(\tilde{U}).$$

$\tilde{U}_0 = U_0^+$ gives $\tilde{W}_0' = \tilde{W}_0 \equiv 0$, $F_0(\tilde{U}) \equiv 0$ and consequently $\omega_j(\tilde{U}) \equiv 0$ for all j. Since F_i is a linear combination of ω_j, $F_i(\tilde{U})$ vanishes for all i. Thus the only bounded solution of (2.13) in Γ is $\tilde{U} \equiv$ constant and $\tilde{W} \equiv 0$. Hence $\lim_{x\to\infty} U(x) =: U^+$ exists and $\lim_{x\to\infty} U'(x) = 0$, $F(U^+) = 0$. From the equation for U_0 we conclude

$$\int_0^\infty F_0(U(s))\,ds = c\left(U_0^+ - U_0'\right)$$

and $\int_0^\infty \omega_j(U(s))\,ds =: \alpha_j c$ exists with $\alpha_j \geqslant 0$. Thus $U^+ = U^- + \sum_{j=1}^r \alpha_j K_j$.

Now if $U_i^- > 0$ for $i \geqslant 1$ the maximum principle applied to any finite interval gives $U_i(x) > 0$; so at least $\omega_{j^*}(U(s)) > 0$ where j^* is as in Theorem 1(i) and consequently $F_0(U(s)) > 0$. If $U_0'(x) = 0$ for some x then $U_0''(x) = 0$ since U_0 is nondecreasing. This contradicts $F_0(U) > 0$. Hence U_0 is strictly monotone increasing. For solving the equation in $(-\infty, 0)$ take $U(0)$, $U'(0)$ of the solution in $(0, \infty)$ as initial data. Since $F(U) \equiv 0$ for $x < 0$ it is easy to see that $\lim_{x\to-\infty} U = U^-$ and $U_i > 0$ holds. This completes the proof of Theorem 1. $\square$

3. Simple existence criteria and examples. First we will give some equivalent conditions to Theorem 1(v), in order to characterize the class of admissible chemical networks.

PROPOSITION 6. *Let $V_1, \ldots, V_r \in \mathbf{R}^n \setminus \{0\}$. Then the following conditions are equivalent*:

(i) *There exists a vector $L \in \mathbf{R}^n_{+0}$ such that $L \cdot V_j < 0$ for all $j = 1, \ldots, r$.*

(ii) $\alpha_j \geqslant 0$, $j = 1, \ldots, r$, *and* $\sum_{j=1}^r \alpha_j V_j \in \mathbf{R}^n_{+0}$ *imply* $\alpha_j = 0$, $j = 1, \ldots, r$.

(iii) *Let C the positive cone spanned by V_j and $-C$ the negative cone. Then $C \cap \mathbf{R}^n_{+0} = \{0\}$ and $C \cap -C = \{0\}$.*

PROOF. (i) $\Rightarrow$ (ii). Multiply $\sum_{j=1}^r \alpha_j V_j$ by L and conclude $\alpha_j = 0$.

(ii) $\Rightarrow$ (iii) Let $X \in C \cap \mathbf{R}^n_{+0}$ i.e., $X = \sum_{j=1}^r \alpha_j V_j \in \mathbf{R}^n_{+0}$ with $\alpha_j \geqslant 0$. Then (ii) gives $\alpha_j = 0$.

Let $X \in C \cap -C$, i.e., $X = \sum_{j=1}^r \alpha_j V_j = -\sum_{j=1}^r \beta_j V_j$, with $\alpha_j, \beta_j \geqslant 0$. Hence $\sum_{j=1}^r (\alpha_j + \beta_j) V_j = 0$ and $\alpha_j = \beta_j = 0$ follows from (ii).

(iii) $\Rightarrow$ (i).

(iii) implies the existence of a $n - 1$ dimensional hyperplane that separates C and $\mathbf{R}^n_{+0}$ strictly. A normal vector L to this hyperplane may be chosen such that $L \cdot X < 0$ for $X \in C \setminus \{0\}$ and $L \cdot X > 0$ for $X \in \mathbf{R}^n_{+0} \setminus \{0\}$. By setting $X = V_j$ and X the basis vectors in $\mathbf{R}^n$ respectively we obtain (i). $\square$

REMARKS. (a) (ii) is the dual condition to (i); cf. the Fredholm-alternative for systems of inequalities. (ii) means that we cannot have reaction chains in the graph of the network whose beginning is part of its end. As an example the network $A \to 2B$; $B \to A$ or as a chain $A \to 2B \to 2A$ is excluded.

As a special case reaction cycles are not admissible.

(b) The networks $A \to B$; $B \to A$ and $A \to 2B$; $B \to 2A$ show that in general no condition in (iii) can be omitted. In this sense the condition is also necessary for exothermic networks.

Simple examples. For some simple reaction mechanisms, which occur as parts in many networks we check the above conditions for existence and give the possible boundary conditions U^+. U^+ satisfies $F(U^+) = 0$; $U^+ \in \mathbf{R}^{n+1}_{+0}$ and $U^+ = U^- + \sum_{j=1}^{r} \alpha_j K_j$ for some $\alpha_j > 0$.

(a) *Sequential reaction.*

$$A_1 \xrightarrow{R_1} A_2 \xrightarrow{R_2} \cdots \xrightarrow{R_{n-1}} A_n.$$

This gives

$$V_j = (0, \dots, 0, \overset{j}{-1}, 1, 0, \dots, 0) \in \mathbf{R}^n.$$

$L = (n, n-1, \dots, 1) \in \mathbf{R}^n_{+0}$ satisfies $L \cdot V_j = -1 < 0$. If $U_1^- > 0$ we have existence.

It turns out that U^+ is unique:

$$U_0^+ = U_0^- + \sum_{j=1}^{n-1} \sum_{K=1}^{j} Q_j U_K^-,$$

$$U_i^+ = 0, \qquad i = 1, \dots, n-1,$$

$$U_n^+ = \sum_{i=1}^{n} U_i^-.$$

Analogously for general stöchiometric coefficients.

(b) *Branching reactions.*

$$A_1 \xrightarrow{R_j} A_{j+1}, \qquad j = 1, \dots, n-1,$$

$$V_j = (-1, 0, \dots, 0, \overset{j+1}{1}, 0, \dots, 0) \in \mathbf{R}^n.$$

With $L = (1, 0, \dots, 0)$, $L \cdot V_j < 0$ holds. For U^+ we get

$$U_0^+ = U_0^- + \sum_{j=1}^{n-1} \alpha_j Q_j, \quad U_1^+ = 0,$$

$$U_i^+ = U_i^- + \alpha_{i-1}, \qquad i = 2, \dots, n,$$

under the constraint $\sum_{j=1}^{n-1} \alpha_j = U_1^-$. Hence $n-2$ of the α_j are not determined. This is the extreme case of nonuniqueness and typical for branched networks since there exist several reaction paths for reaching equilibrium. Which path actually is observed depends on the initial data of the time depending problem.

(c) *Radical reaction.*

$$R_1 : A_1 + A_2 \to A_3 + A_4$$
$$A_2 + A_3 \to A_5.$$

In [3] this describes a simplified global two step mechanism for a hydrocarbon flame, with

$$
\begin{array}{ll}
A_1 \mathrel{\hat{=}} C_nH_m & \text{hydrocarbon} \\
A_2 \mathrel{\hat{=}} O_2 & \text{oxygen} \\
A_3 \mathrel{\hat{=}} CO & \text{radical} \\
A_4 \mathrel{\hat{=}} H_2O & \text{product} \\
A_5 \mathrel{\hat{=}} CO_2 & \text{product}
\end{array}
$$

For simplicity we assumed the stöchiometric coefficients to be 1.

For $V_1 = (-1,-1,1,1,0)$ and $V_2 = (0,-1,-1,0,1)$ we may take $L = (0,1,0,0,0)$. Let $U_1^-, U_2^- > 0$ and $U_3^- = U_4^- = U_5^- = 0$. For calculating U^+ we have to distinguish two cases:

(i) $2U_1^- \geqslant U_2^-$ (fuel rich flames) which gives

$$
\begin{aligned}
&U_0^+ = U_0^- + (tQ_1 + (1-t)Q_2)U_2^-;\\
&U_1^+ = U_1^- - tU_2^-; \quad U_2^+ = 0; \quad U_3^+ = (2t-1)U_2^-;\\
&U_4^+ = tU_2^-; \quad U_5^+ = (1-t)U_2^-
\end{aligned}
$$

for some $t \in [\frac{1}{2}, \min(U_1^-/U_2^-, 1)]$.

(ii) $2U_1^- < U_2^-$ (oxygen rich flame) in which case

$$
\begin{aligned}
&U_0^+ = U_0^- + (Q_1 + Q_2)U_1^-, \quad U_1^+ = U_3^+ = 0,\\
&U_4^+ = U_5^+ = U_1^-, \qquad U_2^+ = U_2^- - 2U_1^-.
\end{aligned}
$$

This examples shows that uniqueness of U^+ depends also on U^-.

4. Concluding remarks. The essential restriction in the existence theorem was that all reactions have to be exothermic. It would be desirable to treat also reversible reactions, for they are present in any realistic combustion process. The effect would be that the final temperature and the flame speed would decrease. This can indeed be proven for a reversible one-step reaction with equal diffusion rates. In general the temperature will not be monotone. But this monotonicity was essentially used in this work. Therefore our method does not apply in this case. Whether there exist travelling waves then depends on the relative magnitude of forward and backward reaction.

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