Extinction and Spread of Isothemale Flame Balls in An Autocatalytic Chemical Reaction

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Where in this world is College of William and Mary?

1. College of William and Mary is in Williamsburg, Virginia, USA, about 200 km south of Washington DC.
2. College of William and Mary is 2nd oldest university in USA, founded in 1693. William and Mary were the king and queen of UK at that time, and they donated 120 pounds to build the school.
3. Williamsburg was capital of Virginia before America revolution, and George Washington lived there for some time when he served the senator of Virginia State. Thomas Jefferson was a law student in College of William and Mary.
4. College of William and Mary is ranked number 6 among all public universities (30 over all) by US News, only behind U Virginia, UC Berkeley, U Michigan, U North Carolina, and UCLA(?). Remember that there are more than 4000 universities in USA!
An isothermal autocatalytic chemical reaction:

\[ A + pB \rightarrow (p + 1)B. \]

\( a(x, t) \): the concentrations of the reactant \( A \)
\( b(x, t) \): the concentration of the autocatalyst \( B \)
\( p \geq 1 \): the order of the reaction w. r. t. autocatalytic species
\( D_A, D_B \): diffusion constants
\( k \): reaction rate

Reaction-diffusion system of chemical reaction:

\[
\begin{align*}
\frac{\partial a}{\partial t} &= D_A \Delta a - kab^p, \\
\frac{\partial b}{\partial t} &= D_B \Delta b + kab^p, \quad t > 0, \quad x \in \mathbb{R}^n, \quad (1)
\end{align*}
\]

Initial condition: \( a(x, 0) = a_0(x), \) and \( b(x, 0) = b_0(x), \) \( x \in \mathbb{R}^n. \)

Boundary condition: \( \lim_{|x| \to \infty} a(x, t) = a_0 > 0, \) and \( \lim_{|x| \to \infty} b(x, t) = 0. \)
**Autocatalysis**: A chemical is involved in its own production (modeling the feedback control in biological systems)

[Lokta, 1920] [Belousov, 1951] [Zhabotinskii, 1964]
[Prigogene-Lefever, 1968] [Gierer-Meinhardt, 1972]
[Schnackenberg, 1979] [Gray-Scott, 1983, 1986]

(more famous) Gray-Scott Model:
\[ A + 2B \rightarrow 3B, \ B \rightarrow C, \] constantly feeding \( A \) and removing \( B \) and \( C \)

\[
\frac{\partial a}{\partial t} = D_A \Delta a - kab^2 + f(1 - a), \quad \frac{\partial b}{\partial t} = D_B \Delta a + kab^2 - (f + q)b,
\]

Equ. (1): Gray-Scott model when \( f = q = 0 \) [Gray-Scott, 1990]
[Merkin-Needham, 1989-] [Berlyand-Xin, 1995] [Li-Qi, 2003]
Numerical Observations and Formal Arguments:

A. (Threshold phenomenon) When \( p \) is large, there is a critical size \( R_* > 0 \) such that when radius of the localized input of autocatalyst is smaller than \( R_* \), no traveling wave can be initialized (reaction fails); but traveling wave can be established when \( R > R_* \) (reaction succeeds).

B. (Flame ball) When \( p \) is large, there are non-trivial steady state solutions. [Ouyang-Shi, 1998] [Tang, 2000]

Our goal: establish mathematical results for these phenomena

Dimensionless Equation:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \Delta u - uv^p, & \frac{\partial v}{\partial t} &= D\Delta v + uv^p, & t > 0, & x \in \mathbb{R}^n, \\
\lim_{|x| \to \infty} u(x, t) &= 1, & \text{and} & \lim_{|x| \to \infty} v(x, t) &= 0.
\end{align*}
\]

(2)

We will assume: \( D = D_B/D_A = 1, \ p > 1 \)
\[
\begin{cases}
    u_t = \Delta u - uv^p, \quad v_t = \Delta v + uv^p, \\
    u(x, 0) = u_0(x) \geq 0, \quad v(x, 0) = v_0(x) \geq 0, \\
    \lim_{|x| \to \infty} u(x, t) = 1, \text{ and } \lim_{|x| \to \infty} v(x, t) = 0, \\
    \lim_{|x| \to \infty} u_0(x) = 1, \text{ and } \lim_{|x| \to \infty} v_0(x) = 0.
\end{cases}
\]

where \( n \geq 3 \), \( p > 1 \).

Flame ball extinction: (reaction fails)
\[
\lim_{t \to \infty} u(x, t) = 1, \quad \text{and} \quad \lim_{t \to \infty} v(x, t) = 0,
\]

Flame ball spread: (reaction succeeds)
\[
\lim_{t \to \infty} u(x, t) = 0, \quad \text{and} \quad \lim_{t \to \infty} \inf v(x, t) > 0.
\]

If \( p \leq (n + 2)/n \), flame ball always spreads.

[Aronson-Weinberger, 1978]
Steady State solutions:

\[
\begin{cases}
\Delta u - uv^p = 0, & \Delta v + uv^p = 0, \\
\lim_{|x| \to \infty} u(x) = 1, \text{ and } \lim_{|x| \to \infty} v(x) = 0.
\end{cases}
\]  

(4)

Let \( h = u + v \). Then \( \Delta h = 0 \) and \( \lim_{|x| \to \infty} h(x) = 1 \), thus \( h(x) \equiv 1 \).

Scalar steady state equation:

\[
\Delta v + (1 - v)v^p = 0, \quad v(x) > 0, \quad x \in \mathbb{R}^n, \quad \lim_{|x| \to \infty} v(x) = 0.
\]

(5)

**Theorem 1:** [Ouyang-Shi, 1998] Let \( p_* = \frac{n + 2}{n - 2} \).

(A) (5) has no solution when \( p \leq p_* \);

(B) When \( p > p_* \), (5) has a family of radial solutions \( v_d(x) \) such that \( \max v_d(x) = v(0) = d \) for any \( d \in (0, d_1] \) and \( 0 < d_1 < 1 \).

(C) When \( p > p_* \), the equation in (5) has radial solution \( v_d(x) \) such that \( \max v_d(x) = v(0) = d \) and \( v(x) = 0 \) when \( |x| = R(d) > 0 \) for any \( d \in (d_1, 1) \). (This is called crossing solution.)
The bifurcation diagram: (left: \( p \leq \frac{n + 2}{n - 2} \), right: \( p > \frac{n + 2}{n - 2} \))

\[
\begin{align*}
\text{Theorem 2: \cite{Tang, 2000}} & \quad \text{When } p > \frac{n + 2}{n - 2}, \\
\text{(A) The solution } v(r, d_1) & \quad \text{is the unique fast decaying solution such that } v(r, d_1) r^{n-2} \to \text{a constant when } r \to \infty. \\
\text{(B) For } d \in (0, d_1), & \quad v(r, d) \text{ is slow decaying solution such that } v(r, d_1) r^{2/(p-1)} \to L \text{ when } r \to \infty.
\end{align*}
\]

Question: Can we prove all solutions on \( \mathbb{R}^n \) are radially symmetric? For \( \Delta u + u^p = 0 \), \cite{Zou, 1995}, \cite{Guo, 2002}.
Hair-Trigger effect

Theorem 3: [Shi-Wang, 2005] Assume \( p_* < p < p_c \), and \( (u_d(x), v_d(x)) \) is a radial steady state solution with \( u_d(x) + v_d(x) \equiv 1, (u_d(0), v_d(0)) = (1 - d, d) \) and \( d \in (0, d_1) \).

(A) If \( v_0(x) \geq v_d(x) \), \( u_0(x) + v_0(x) \geq 1 \), but not \( \equiv \) simultaneously, then

\[
\lim_{t \to \infty} u(x, t) = 0, \quad \lim_{t \to \infty} v(x, t) = 1, \quad \text{(spread)} \tag{6}
\]

uniformly for any bounded subset of \( \mathbb{R}^n \) as \( t \to \infty \).

(B) If \( v_0(x) \leq v_d(x) \), \( u_0(x) + v_0(x) \leq 1 \), but not \( \equiv \) simultaneously, then

\[
\lim_{t \to \infty} u(x, t) = 1, \quad \lim_{t \to \infty} v(x, t) = 0, \quad \text{(extinction)} \tag{7}
\]

uniformly for \( \mathbb{R}^n \) as \( t \to \infty \). Here \( p_* = \frac{n + 2}{n - 2} \),

\[
p_c = \begin{cases} 
\frac{(n - 2)^2 - 4n + 4\sqrt{n^2 - (n - 2)^2}}{(n - 2)(n - 10)} & \text{when } n \geq 11, \\
\infty & \text{when } 3 \leq n \leq 10.
\end{cases}
\]
History of \( p_c (1) \):

\[
\begin{cases}
\Delta u + \lambda (1 + u)^p = 0, & x \in B^n = \{|x| < 1\}, \\
u(x) = 0, & x \in \partial B^n.
\end{cases}
\]  

[Joseph-Lundgren, 1973]

(A) When \( n \leq 2 \), or \( n \geq 3 \) and \( p \leq p_* \), the bifurcation diagram has exactly one turning point.

(B) When \( 3 \leq n \leq 10 \) and \( p > p_* \), or \( n \geq 11 \) and \( p_c > p > p_* \), the bifurcation diagram has countably infinite many turning points.

(C) When \( n \geq 11 \) and \( p \geq p_c \), the bifurcation diagram is monotone increasing.

Later work:

[Mignot-Puel, 1980] [Brezis-Vazquez, 1997] [Cabré, 2003]

extremal solution (the one at the 1st turning point) is always in 
\( H^1_0(B^n) \) but is not in \( L^\infty(B^n) \) if \( n \geq 11 \) and \( p \geq p_c \).
Fujita-type equation

\[
\begin{cases}
\frac{\partial w}{\partial t} = \Delta w + w^p, & t > 0, \ x \in \mathbb{R}^n, \\
w(x, 0) = w_0(x) \geq 0, & x \in \mathbb{R}^n.
\end{cases}
\] (9)


(A) If \(1 < p \leq \frac{n+2}{n} \) and \(w_0 \geq (\neq) 0\), then \(w(x,t)\) blows up in finite time; if \(p > \frac{n+2}{n}\), there is the threshold phenomenon: if \(w_0\) is “small”, then \(w(x,t) \to 0\) as \(t \to \infty\); and if \(w_0\) is “large”, then \(w(x,t)\) blows up in finite time.

(B) When \(p > \frac{n}{n-2}\), singular steady state \(w_s(x) = L|x|^{-2/(p-1)}\).

(C) When \(p < p_*\), no radial regular steady state; when \(p \geq p_*\), there is a family of radial regular (slow decaying) steady states \(w_d(x)\) with \(\max w_d(x) = w(0) = d\) for any \(d > 0\).
(D) When $3 \leq n \leq 10$ and $p > p_*$, or $n \geq 11$ and $p_c > p > p_*$, any two slow decaying steady states (including the singular one) intersect each other infinitely many times.

(E) When $n \geq 11$ and $p \geq p_c$, any two slow decaying steady states (including the singular one) do not intersect.

(D) is also true for slow decaying solutions of $f(u) = u^p(1-u)$, but (E) is not known for that case.

Conjecture: There exists $d_2 \in (0, d_1)$ such that when $d \in (0, d_2)$, any two slow decaying steady states do not intersect, but when $d \in (d_2, d_1)$, they do intersect.
History of $p_c$ (2):

[Gui-Ni-Wang, 1992, 2001]: when $n \geq 11$ and $p \geq p_c$, each radial steady state of $u_t = \Delta u + u^p$ is stable in some sense.

[Herrero-Velázquez, 1994, preprint] [Matano-Merle, 2004]:

(A) when $n \geq 11$ and $p > p_c$, $u_t = \Delta u + u^p$ has type II blowup (blowup rate faster than $u_t = u^p$)

(B) when $n \geq 3$ and $p \leq p_*$, $u_t = \Delta u + u^p$ has type I blowup (blowup rate as $u_t = u^p$).

(C) when $p_* < p < p_c$, the blowup rate is still unknown.
Recall: **Hair-Trigger effect**

**Theorem 3**: [Shi-Wang, 2005] Assume \( p_* < p < p_c \), and \((u_d(x), v_d(x))\) is a radial steady state solution with \( u_d(x) + v_d(x) \equiv 1 \), \((u_d(0), v_d(0)) = (1 - d, d)\) and \( d \in (0, d_1)\).

(A) If \( v_0(x) \geq v_d(x), u_0(x) + v_0(x) \geq 1 \), but not \( \equiv \) simultaneously, then

\[
\lim_{t \to \infty} u(x, t) = 0, \quad \lim_{t \to \infty} v(x, t) = 1, \quad \text{(spread)} \quad (10)
\]

uniformly for any bounded subset of \( \mathbb{R}^n \) as \( t \to \infty \).

(B) If \( v_0(x) \leq v_d(x), u_0(x) + v_0(x) \leq 1 \), but not \( \equiv \) simultaneously, then

\[
\lim_{t \to \infty} u(x, t) = 1, \quad \lim_{t \to \infty} v(x, t) = 0, \quad \text{(extinction)} \quad (11)
\]

uniformly for \( \mathbb{R}^n \) as \( t \to \infty \). Here \( p_* = \frac{n + 2}{n - 2} \),

\[
p_c = \begin{cases} 
\frac{(n - 2)^2 - 4n + 4\sqrt{n^2 - (n - 2)^2}}{(n - 2)(n - 10)} & \text{when } n \geq 11, \\
\infty & \text{when } 3 \leq n \leq 10.
\end{cases}
\]
Idea of the proof:
1. first deal with scalar equation $v_t = \Delta v + v^p(1 - v)$
2. construct suitable supersolution/subsolution

Lemma: For $u_t = \Delta u + f(u)$, $u(0) = u_0$ in $\mathbb{R}^n$

(A) If $u_0(x)$ is a supersolution but not solution, then $u(x, t)$ is strictly decreasing in $t$.

(B) If $u_1(x)$ and $u_2(x)$ are both supersolutions, then $\min(u_1, u_2)$ is also a supersolution.

Idea: If $v_0(x) \leq v_d(x)$, a steady state, we can assume $v_0(x) < v_d(x)$ from strong maximum principle. Define $\bar{v}(x) = v_{d'}(x)$ when $|x| < z(d')$, and $\bar{v}(x) = v_d(x)$ when $|x| > z(d')$, where $z(d')$ is the intersection of $v_d$ and $v_{d'}$ for $d' < d$ and close to $d$. Then $\bar{v}$ is a supersolution such that $\bar{v} > v_0$. But $z(d')$ must exist and stay bounded when $d' \rightarrow d$. 
Key ingredient: the crossing property of the radial steady states.

Crossing property implies that for the solution $\phi(r)$ of

$$
\begin{cases}
\phi'' + \frac{n-1}{r} \phi' + f'(v_d(r))\phi = 0, & r \in (0, \infty), \\
\phi(0) = 1, \quad \phi'(0) = 0,
\end{cases}
$$

where $f(u) = u^p$ or $f(u) = u^p - u^{p+1}$, $\phi(r)$ changes sign in $(0, \infty)$.

Need to prove: $\phi(x)$ changes sign.

**Theorem 3-a:** The result of Theorem 3 still holds if $n \geq 11$ and $p > p_c$, and $d = d_1$ (so $v_d(x)$ is the fast decaying solution.)
A weak instability result (History of $p_c$ (3)):
Suppose that $u(x)$ is a solution of $\Delta u + f(u) = 0$ in $\mathbb{R}^n$. Then $u(x)$ is stable if for any $\eta \in C_0^\infty(\mathbb{R}^n)$, $\int_{\mathbb{R}^n} (|\nabla \eta|^2 - f'(u)\eta^2) \, dx \geq 0$.
[Berestycki-Caffarelli-Nirenberg, 1998]

Lemma 4: Suppose that $f \in C^1(\mathbb{R})$.
(A) [Ghoussoub-Gui, 1998] $u(x)$ is stable if and only if there exists $\phi(x) > 0$ in $\mathbb{R}^n$ such that $\Delta \phi + f'(u)\phi = 0$.
(B) [Cabr´ e-Capella, 2004] If $u(x)$ is radially symmetric, $|u'(x)| = O(r^{-\beta})$ and $\beta > \frac{n - 2 - 2\sqrt{n-1}}{2}$, then $u(x)$ is unstable.

1. Any non-constant radial solution is unstable if $n \leq 8$ or $n = 9, 10$ but $f'(v)$ is a power-like function at any critical point of $f$.
2. Any fast decaying solution is unstable.
3. Slow decaying solution when $n \geq 11$ and $p < p_c$ is unstable.
4. Some slow decaying solutions when $n \geq 11$ and $p > p_c$ are stable.
Weak instability implies strong instability:

**Lemma 5**: [Shi-Wang, 2005] Suppose that $f \in C^1(\mathbb{R})$, and $u(x)$ is an unstable solution of $\Delta u + f(u) = 0$ in $\mathbb{R}^n$. Let $v(x,t)$ be the solution of $v_t = \Delta v + f(v), v(x,0) = v_0(x)$ for $x \in \mathbb{R}^n$.

(A) If $v_0(x) \leq u(x)$, then $v(x,t)$ is either unbounded as $t \to T$ (life span of the solution), or $\limsup_{t \to \infty} v(x,t) \leq u_1(x)$, a radial steady state such that $u_1(x) < u(x)$.

(B) If $n \leq 10$, then $u_1(x)$ is constant.

**Conditions of spread**: $v_0(x) \geq v_d(x), u_0(x) + v_0(x) \geq 1$

$u_0(x) + v_0(x) \geq 1$ implies $u(x,t) + v(x,t) > 1$ for $t > 0$

Thus the system can be compared with the scalar equation
Theorem 6: [Shi-Wang, 2005]
When \( n \geq 11, \ p \geq p_c, \) and \( 0 < d < (p - 1)/p. \)

(A) If \( v_0(x) \leq \lambda v_d(x) \) for some constant \( \lambda \in (0, 1), \) and
\( u_0(x) + v_0(x) \leq 1, \) then the flame ball extinguishes;

(B) If \( v_0(x) \geq \lambda v_d(x) \) for some constant \( \lambda \in (1, \infty), \) and
\( u_0(x) + v_0(x) \geq 1, \) then the flame ball spreads.

(Note: we can show that \((p - 1)/p < d_1\) by Pohozaev’s identity.)

Recall
Theorem 1: [Ouyang-Shi, 1998] Let \( p_* = \frac{n + 2}{n - 2}. \)

(C) When \( p > p_*, \) the equation in (5) has radial solution \( v_d(x) \) such that
\( \max v_d(x) = v(0) = d \) and \( v(x) = 0 \) when \( |x| = R(d) > 0 \) for any
\( d \in (d_1, 1). \)

\[
\begin{array}{c}
\text{1} \\
\text{d_1} \\
R_* \\
\end{array}
\quad
\begin{array}{c}
R(d) \\
\end{array}
\]
Theorem 7 [Shi-Wang, 2005]

When \( p > 1 \),

\[
v_0(x) \geq \begin{cases} 
v_d(|x|), & |x| < R(d); \\
0, & |x| \geq R(d), 
\end{cases}
\]  \hspace{1cm} (13)

for some \( d \in (d_1, 1) \) (\( d_1 \) is understood to be 0 if \( p \leq p_* \)), and \( u_0(x) + v_0(x) \geq 1 \), then the flame ball spreads.

In fact, for \( R > R_* \), there are exactly two \( d \in (d_1, 1) \) such that \( R(d) = R \), say \( d_a > d_b \), then \( v_{da}(x) > v_{db}(x) \) for \( |x| < R \). Thus Theorem 7 still holds if \( v_0(x) > v_{db}(x) \) (the lower steady state).
Future work:

1. Threshold manifold: so the steady state solutions are on the threshold set (separatrix) between the basins of attraction of \((0, 1)\) and \((1, 0)\), but what else are also on the threshold set? [Shi-Wang, in progress] for Fujita equation [Mizoguchi, 2002] [R.Suzuki, 2003]

2. Threshold when \(\frac{n + 2}{n} < p < \frac{n}{n - 2}\): no steady state (even singular one) for Fujita equation

3. Stability of slow decaying solution when \(p > p_c\).
Future work:

4. Structure of the radially symmetric solutions of $\Delta u + u^p + u^q = 0$ when $1 < p < q$ and $q > \frac{n + 2}{n - 2}$.

[Lin-Ni, 1988] [Bamon-del Pino-Flores, 2000] [Flores, 2004]

5. What happens when $D = D_A/D_B \neq 1$? And what about if $B$ also decays?

$$\frac{\partial a}{\partial t} = D_A \Delta a - kab^p, \quad \frac{\partial b}{\partial t} = D_B \Delta b + kab^p - qb, \quad t > 0, \quad x \in \mathbb{R}^n, \quad (14)$$


6. Equation on bounded domain:

Dirichlet boundary condition $a(x) = a_0 > 0$, and $b(x) = b_0 \geq 0$

The bifurcation diagram of steady states when the domain is a ball $(n = 1, 2)$ is $S$-shaped if $b_0 > 0$

[Kay-Scott, 1988] numerical [Shi-Wang-Zhao, in progress]