Dangerous failure of scientific process: A Case of Collective Amnesia

How collaboration between mathematicians and chemical engineers can save lives

Rowena Ball

Conference themes: Case Studies, Other

Outline

1. Introduction: The existence of thermochemical oscillators is denied, then affirmed. I get suspicious.

2. What is the first question we should ask of an open thermoreactive system?

3. Flawed critical conditions: Case studies I and II.

4. Collective amnesia, and how to cure it.

5. The field of thermochemical oscillators finds its muse.

An emphatic denial!

July 2011: Seminar I gave at expert colloquium at UC Irvine, CA on the role played by a thermochemical oscillator in the Bhopal disaster — comment from learned member of audience:

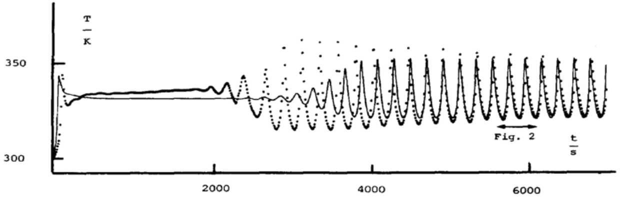
❝ I can't believe there exists a thermal instability that I haven't heard of, so as far as I'm concerned your equations must be WRONG. ❞

- My equations, and results derived from them, were subsequently peer-reviewed and published unchanged.[†]
- I first begin to suspect some kind of failure of research integration and implementation in this field over a whole generation or more!

[†] R. Ball, Oscillatory thermal instability and the Bhopal disaster, Process Safety & Environmental Protection 89 317–322, 2011.

Thermochemical oscillators

- A thermochemical oscillator is a thermally reacting system that gives a periodic, quasiperiodic or chaotic temperature response.
- Experimental observations made since the 1960s.



- **Violent thermal runaway (or explosion) via a temperature oscillation has been observed.**

Thermal runaway: the **first** question

- In specifying thermal stability criteria for an open thermoreactive system, **Question 1** is

  ❝ Will a small perturbation to the temperature grow uncontrollably, or decay harmlessly? ❞
- Answering this question necessarily involves stability analysis using the well-founded mathematics of stability theory.
- Prompted by my first suspicions, I reviewed the refereed literature and found two recent cases where **Question 1** was *completely* disregarded.
- The evidence is irrefutable that ignorance of oscillatory thermal instability has become widespread, in circles where knowledge of it counts most.
- We are looking at a **dangerous** knowledge gap, a **dangerous** failure of research integration and implementation between mathematics and chemical engineering.

Case study I: Synthesis of RDX explosive

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Available online at www.sciencedirect.com

SCIENCE DIRECT

Journal of Loss Prevention in the Process Industries 18 (2005) 1–11

Journal of Loss Prevention in the process industries

www.elsevier.com/locate/jlp

Critical runaway conditions and stability criterion of RDX manufacture in continuous stirred tank reactor

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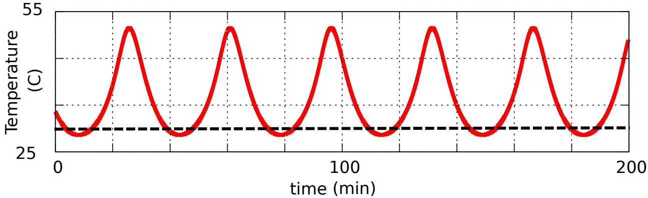
- The authors purported to determine ‘critical runaway conditions’ and recommended ‘safe operating conditions’ for industrial synthesis of an explosive, but **completely** ignored stability.

Ignoring stability could lead to catastrophe



- This steady state occurs at 28°C. According to Lu et al. (2005) it is 'safe'.
- However, **stability analysis** tells us that the steady state is **unstable** and that the temperature will oscillate around it.
- The amplitude is **dangerously** high.†
- Operation of the industrial RDX synthesis at these conditions is likely to ***blow the factory up!***

†At $\gtrsim$ 35°C exothermic side-reactions can take over.

Case study II

PROCESS SAFETY AND ENVIRONMENTAL PROTECTION 86 (2008) 37–47

available at www.sciencedirect.com

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journal homepage: www.elsevier.com/locate/psep

The kinetic parameters and safe operating conditions of nitroglycerine manufacture in the CSTR of Biazzi process

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- ‘Safe’ operating conditions were prescribed for synthesis of nitroglycerine but stability analysis **not** carried out.
- **Correct** application of **Question I** shows the ‘safe’ state is actually a **dangerous** oscillatory spike.

- *These papers may have already cost human lives: serious and fatal thermal runaways and explosions in factories are alarmingly common in Asian and developing nations, but rarely make it into the Western press or process safety incident databases.*

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2 women killed in chemical factory explosion in city

TNN Aug 19, 2011, 04.32am IST

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HYDERABAD: Two daily-wage workers died in an explosion at a chemical unit in Amberpet on Thursday morning.

The two victims were identified as Venkata Lakshmi, 45, and Kalpana, 30, of Venkatapuram Colony, who were working at Nagamani Chemicals owned by B Nanda Gopal from Bapu Nagar in Amberpet. The incident took place at 11.30am when the two workers were mixing hydrogen peroxide, methyl ethyl ketone and sodium sulphate to produce a chemical substance used in the manufacturing of asbestos sheet moulds and coolants. The high intensity of the explosion damaged a portion of the chemical unit's roof and severely injured both Venkata Lakshmi and Kalpana.

News item from The Times of India, Aug 19, 2011.

A case of collective amnesia?

- Ignorance of stability analysis and oscillatory thermal instability extended, at least, to
  - The authors of Case I and Case II;
  - Subject editors of **two** leading chemical engineering journals;
  - Some of the referees used by these journals;
  - An unknown number of the journals' readers, since no-one publicly queried these papers until 2013†;
  - My expert commentator at UC Irvine colloquium (who runs his own explosives lab and consults for industry).
- Since all these people are sincerely concerned with thermal process safety, we are looking at **systemic** problems or **failure-of-process** in research, collaboration and education.

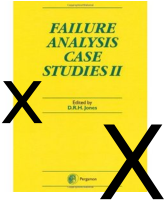
† *Ball, R., Gray, B.F., Thermal instability and runaway criteria: The dangers of disregarding dynamics. Process Safety & Environmental Protection 91, 221–226, 2013.*

A dangerous failure of scientific process

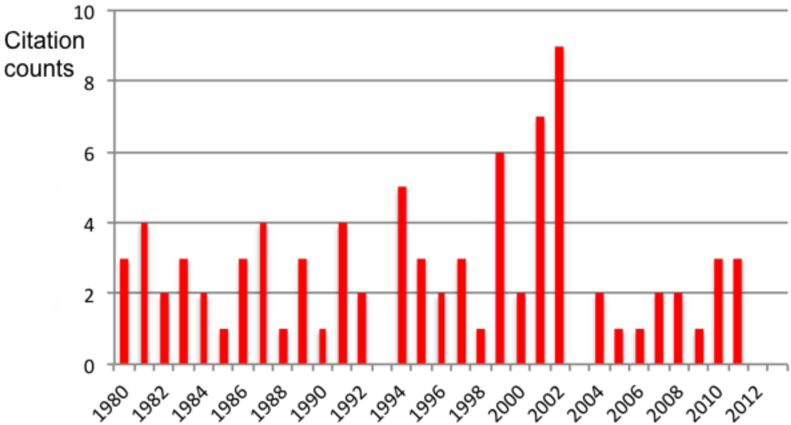
- Thermochemical oscillators were **well**-known to chemical engineers from the mid 1950s to the 1990s, and a great many theory, modelling and experimental papers were published on the topic in the **mainstream** chemical engineering literature during that period.

- Therefore it is of great concern that **three decades** of research on a hazardous thermal instability seems to have been forgotten or ignored in some sectors of the community which deal with reactive thermal hazards and runaway criteria.

- How could this **systemic failure of process** have happened?
- Books on failure analysis were no use on this question.
- I decide to investigate.

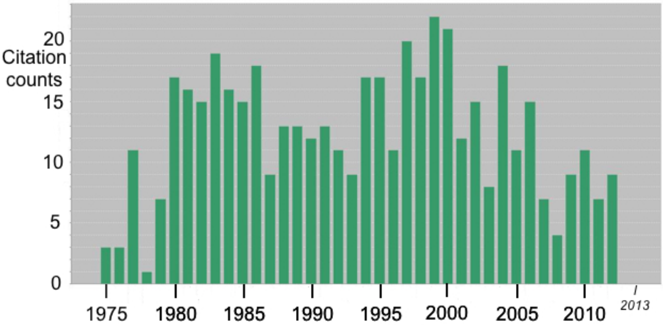


Bibliometric data I



- Citations to the experimental works crashed after 2002.

Bibliometric data II

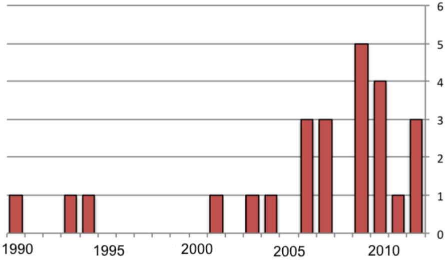


- Citations to relevant theoretical and modelling works on thermochemical oscillators decline after 1999.†

Oscillatory thermal instability, and knowledge of the serious hazard it presents, seems to have almost faded from the collective memory of chemical engineers.

† *Citation data for most highly cited paper on thermochemical oscillators: A. Uppal, W. H. Ray, A. B. Poore, On the dynamic behaviour of continuous stirred tank reactors, Chemical Engineering Science 29 (1974) 967Ð985.*

Bibliometric data III



- Number of papers in relevant journals[†] having author with mathematical affiliation is very low.
- Collaboration between chemical engineers and mathematicians is low in an area that would benefit most: thermal process safety and thermal hazards.

[†] *Process Safety & Environmental Protection and Journal of Loss Prevention in the Process Industries*

Other possible contributing factors

- Although chemical engineers from the mid 1950s to the 1990s can take credit for driving real-world applications of **dynamical systems and stability theory**, this subject is typically taught by mathematicians as a full semester later year course.
- Few chemical engineering majors would take such a course as an elective.
- Imperatives to incorporate biotechnology and nanotechnology, which essentially have no thermal dynamics, into teaching & research may have crowded out thermal stability studies.
- The ever-growing obsession with computational fluid dynamics necessarily ignores stability.

Other possible contributing factors

- The sociology of science — the system failed me:
  - I was forced to work in a very different research area for 10 years post graduation, as I had to put family obligations first.
  - If I could have continued working on thermochemical instabilities, most likely the offending papers advocating dangerous process conditions would have come to me for refereeing. I would have sent them to the bottom of the harbour and enlightened their authors!
    - My own work and publications and attendances at appropriate international forums and international networking would have kept the topic at the forefront of the field.
    - A great many serious thermal process incidents would not have occurred.
- You know not what damage may ensue unintentionally when a person is forced to drop a research field.
- This is perhaps an issue for ‘research integration and implementation’ to respond to.

How to fix it

- Current research strategy is to raise awareness of the dangers of oscillatory thermal instability by developing a suite of novel, useful and relevant applications:
  1. Explosives detection;
  2. The ‘methanol economy’ is back!
  3. Renaissance of firestick farming;
  4. A sitting duck: Exploit the existence of canard cycles;
  5. The origin of life in the primordial soup!!
- Resulting increased collaborations between mathematicians and chemical engineers will restore and re-embed stability analysis firmly into the very same areas which pioneered its use in the 1950s then forgot it: thermal process engineering, design and safety.
- Recent developments in research integration and implementation science will help create conditions for such collaborations to thrive, e.g., through improved assessment mechanisms for crossdisciplinary grant applications.

" A little learning is a dangerous thing;
Drink deep, or taste not the Pierian spring.[†]
There shallow draughts intoxicate the brain,
And drinking largely sobers us again."

Alexander Pope, An Essay on Criticism, 1709

[†] In Greek mythology, the sacred Pierian Spring was the metaphorical source of knowledge of art and science

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First Global Conference on Research Integration and Implementation, 8–11 Sep 2013, Canberra, www.I2Sconference.org

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