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Danckwerts Memorial Lecture

The art of mixing with an admixture of art: viewing creativity through P. V. Danckwerts's early work[1]

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Dedicated to the memory of my father

Abstract

P. V. Danckwerts's work provides a springboard for an examination of issues dealing with creativity in research and acceptance of new viewpoints. When is a concept ready to be embraced and to what extent can an advance be premature? I argue that the visual arts offer thought-provoking analogies and examples are used to illustrate various points. © 2000 Elsevier Science Ltd. All rights reserved.

1. PVD's oeuvre and objectives of this work

PVD's work provides a springboard for a discussion about creativity.

The Danckwerts Memorial Lecture provides an opportunity to look at the past and project into the future. It is honor to be invited to attempt to do this. The key issue is: In what possible ways may I provide some illuminating viewpoint?

It would be foolish to attempt to place P. V. Dankwerts's (PVD's) oeuvre in perspective. This was done by Neal Amundson, the first Danckwerts's Lecturer, in 1986 (Amundson, 1986), by PVD himself in his "Insights into Chemical Engineering" (Danckwerts, 1981), and by Rutherford Aris in 1990 in both, a pithy review of PVD's Insights as well as in his own Danckwerts Memorial Lecture in 1991.

PVD had already written some of the most influential papers before I was in my teens and was still at it when I wrote my first paper in Chemical Engineering Science. My research connections and indebtedness, however, are too obvious to miss. In Insights PDV broke his research output into four sections, including one that he called RTD and Related Topics, and another, Mixtures and Mixing, covering mixing measures and the like. I tend to view these two areas as brackets: The RTD concept succinctly capturing in one stroke the bare elements of the process (and often the only thing one needs to know), the quantification of mixing, on the other, forming a separate chapter that is far from being closed.

I will use this opportunity for an examination of issues dealing with creativity in research and acceptance of new viewpoints, using the mixing theme to anchor a few concepts. When is a concept ready to be embraced and to what extent can an advance be premature? The example of Osborne Reynolds (1842–1912) — foreshadowing chaos before the work of Poincaré formed part of the accepted mathematical vocabulary — provides a striking example. Two examples from my own work — chaotic mixing of fluids and the self-organization of segregating granular materials — are used to highlight issues having to do with modeling and theory. Visual arts analogies are used throughout to illustrate the various points. The paper concludes with a summary of "lessons" distilled from the examples presented in the work.

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[1] Note to the Reader: The fact that someone may do work that may be regarded as creative does not mean that one should be aware of the process of creativity itself. I have been, however, seriously interested in visual arts, and to a lesser extent, in general aspects of creative processes, for far longer than I have been doing chemical engineering. To paraphrase PVD, the title of this presentation is somewhat pretentious, but a title was needed, and I hope that readers will find the ideas presented thought-provoking. The research examples are from my own work; quite certainly they are not the most transparent in illustrating points but are cases whose historical genesis I am most familiar with. The scope of the comparisons between Art/Science is limited in the sense that the majority of the parallels presented focus in the time-frame 1890–1950. In any case I appreciate the opportunity to air my views here.

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Fig. 1. Pablo Picasso (Spanish, 1881–1973). Baboon and Young (Vallauris, 1951). The head consists of two toy cars, the ears were ceramic pitcher handles, and the large belly was a large pot. The objects, once combined, cannot be seen independent of the whole. Bronze (cast 1955), after found objects, (53.3 × 33.3 × 52.7 cm). The Museum of Modern Art, New York. Mrs. Simon Guggenheim Fund. © The Museum of Modern Art, New York. © 2000 Estate of Pablo Picasso/Artists Rights Society (ARS), New York.

2. Creativity views

Defining a few terms to provide a setting.

There are hundreds of books, ranging from the highly scholarly to the eminently practical, as to what creativity is and who possesses it. Opinions range from the German philosopher Immanuel Kant (1724–1804), for whom not even Isaac Newton qualified as creative — "Science is ephemeral, art is permanent", he said — to organizational behavior views, where creativity is supposed to be possessed, to a degree or another, by most individuals (Amabile, 1996) and where creativity is seen to lie at the intersection of motivation, creative ability, and knowledge. What is pertinent here is scientific and technological creativity. Without making any claim to completeness let us consider some of the main issues.

Much has been written about creativity and the creative processes, and there is a considerable body of literature scattered over several intellectual domains addressing the related topics of invention, creation, and discovery.[2] Hamlet was created, the telephone was invented, and the structure of DNA was discovered. Which one is more personal? Many will argue that Artistic Creation is: Without Picasso Baboon and Young would not exist (see Fig. 1); on the other hand, the

[2] The number of work in this area by chemical engineers is small. Exceptions are the articles of John Prausnitz and Val Haensel (e.g. Prausnitz, 1986; Haensel, 1994).

argument goes, if Thomas Edison had not lived someone would surely stumbled into the light bulb, and "Newton's laws" would have been discovered, probably not by Newton, but inevitably, though possibly in a different form (think of calculus and Newton and Leibnitz or the progressively more sophisticated views of mechanics, "Lagrangian" (after Lagrange, 1736–1813), "Hamiltonian" (after Hamilton, 1805–1865), and so on). Unquestionably all this has to do with the issue of uniqueness; with the personal stamp of the creator.

Are creative thinking processes in different disciplines — art, science, and technology — in different classes? Is one a more profound act of creativity than the other?

Jacob Bronowski's definition is all-embracing: "There exists a single creative activity, which is displayed alike in the arts and in the sciences ... the scientist or the artist takes two facts or experiences which are separate; he finds in them a likeness which had not been seen before, and he creates a unity by showing the likeness." (Bronowski, 1958). His views extend to the uniqueness issue; *a scientific theory can bear the stamp of his creator*, Bronowski opines, and I concur.

Let us make one more observation contrasting science and technology. Let us assert that science is explaining or *unveiling* — revealing what was already there — whereas technology is making and building. It then follows that in science the final result is inevitable and that creativity enters in the construction of the path leading to the unveiling of the result. But it would be hard to argue that technology is inevitable. In this case creativity enters in both, the product and the path.

But what about the creative individuals themselves? Are there common traits and characteristics? Herbert Simon's views on this issue are particularly clear (Simon, 1983). Creative individuals show:

(i) A willingness to accept vaguely defined problem statements and gradually structure them.
(ii) A continual preoccupation with problems over considerable periods of time.
(iii) Extensive background knowledge in relevant and potentially relevant areas.

Attribute (i) is critical, and in my opinion is often lacking in people over-trained with analytical tools (PVD had opinions on this issue; more on this later). Creative activities involve exploring unstructured and uncharted territory, and linear and sequential thinking simply does not work. Two (of the many) observations by George Polya (1887–1985) in the context of reasoning in (pure) mathematics are particularly revealing: "Demonstrative reasoning is safe, beyond controversy, and final. Plausible reasoning is hazardous, controversial, and provisional". Also "Demonstrative reasoning penetrates the sciences just as far as mathematics does, but it is in itself (as mathematics is in itself) incapable of yielding essentially new knowledge about the world around us" (Polya, 1954a, b).

Point (ii) in Simon's list is uncontroversial, though, I believe, people tend to overrate the mythical sudden flashes of genius rather than the more mundane aspect of the value of persistence in creative work. Point (iii), however, is less obvious than may appear at first glance. What does exactly constitute a *related* field? Who in 1950 would have called diffraction an essential tool in the toolkit of biologists? (think of James Watson and Francis Crick and the discovery of DNA; Watson, 1968). And what about computer science, which has recently invaded molecular biology to the point that molecular biology is regarded by some as a subset of information science? Having the right tool at precisely the right time — think of mathematics in chemical engineering in the 1950s or a combination of computer science/molecular biology now — allows one to solve problems that may remain hidden to others.

But creativity is not just about solving problems. It is about creating them. Einstein supports this view: "the formulation of a problem is often more essential than its solution, which may be merely a matter of mathematical or experimental skill ... to raise new questions ... requires creative imagination ... ".

Creative ideas involve departing from the canonical picture, the standard picture of the times. Normal training in science involves learning the canonical picture, the established techniques accepted in an intellectual domain. Creativity is needed to deviate from normal science and create a new paradigm (Kuhn, 1962). The key is to learn the canon without falling captive to it. Most of the great names in science posed a big question and solved the simplest problems first.

Creativity does not exist in isolation; a work is regarded as creative when it is judged as such by a *domain* (Kuhn, 1962; Csikszentmihalyi, 1996). The most significant creative ideas are those that affect a domain; in fact, some of them may re-shape the domain or create an entirely different one. An idea accepted by a domain constitutes innovation.

A reputation can be built by solving a specific problem that everybody knows but no one knows how to solve (think of Fermat's theorem, measuring the speed of light, determining the charge of the electron) or, *and this is the high pay-off activity*, opening a new conceptual framework and paving the way to new vistas and territories. Think of the beginnings of quantum mechanics, Newtonian mechanics, celestial mechanics, or, somewhat closer to us, the seminal work in chemical engineering in the 1960s in reaction engineering and transport or the fast-paced days of polymer physics in the early 1970s. The initial work is about asking questions and solving the easy problems first.

These opinions are hardly uncontroversial. A scholarly view into scientific creativity is provided by Gerald

Holton, a historian of science from Harvard. Holton considers three kinds of creativity: visual, analogical, and thematic (Holton, 1996). *Visual imagination* — exemplified in juxtaposing the astronomical investigations of Thomas Harriot (1560–1621) (the *No*-side) and Galileo Galilei (1564–1642) (the *Yes*-side) — finds proponents in Albert Einstein (1879–1955) and Richard Feynman (1918–1988). To this list we may add David Hilbert (1862–1943); commenting on one of Hilbert's books the French mathematician Jacques Hadamard (1865–1963) said: "diagrams appear in every other page". But Werner Heisenberg (1901–76) is decidedly on the *No*-side ("The progress of quantum mechanics has to free itself first from all these intuitive pictures") and, I suspect, Joseph Louis de Lagrange (1736–1813) and Karl Weierstrass (1815–1897). "You may leaf through all his books without finding a figure", Poincaré said of Weierstrass (Hadamard, 1945, p. 111). The *analogical imagination*, something fitting with Bronowski's view of connecting seemingly unrelated subjects, is exemplified by Holton by the light/sound analogy of Thomas Young (1773–1829), the wave-particle duality, and Newton's clockwork Universe. The *thematic imagination*, possibly the harder to grasp, refers to the scientist's willing suspension of disbelief in judging the merits of two contrary themata leading to two conflicting viewpoints. Holton offers Robert Millikan (1868–1953) — 1923 Physics Nobel Prize, the person who measured the charge of the electron — as his example of this trait. We shall say more about measurement and quantification, later on in the talk.

The creative act seems magical because we rarely see its evolution; we see the final picture and not the perspiration. This is particularly true in science. We are interested in the final product and rarely in the processes that led to the result. But this is not the case in Art. Think of art retrospectives. Curators earn a living by displaying genesis and revealing evolution. This is not true in science and clearly not in Mathematics, where Karl Friedrich Gauss (1777–1855) and Bernhard Riemann (1826–1866) left no trace of the scaffold that lead to their final results. "I did not succeed in compacting the proof as to make publishable", Riemman said, and simply stated four properties of the "Riemann" function. It took Hadamard 30 years to prove the first three (Hadamard, 1945).[3]

A great painting does not happen in flash. There are many documented examples of this. Picasso made 45 sketches for Guernica (there are seven photos by Dora Marr) and, remarkably, we know this fact. We know the sketches for Matisse's La danse, for Seurrat's La grande jatte. The sketches are themselves regarded as works of art. Etchings are unique in showing the evolution of an idea; we know what Rembrandt did first and what he did last. The sketches of Picasso's bull series are unique in showing how an idea evolves from complex to simple (Fig. 2).

[3] Aesthetic considerations may play a strong role in this process: George Hardy's dictum: "there is no place in world for ugly mathematics", Hardy (1967), encapsulates a pure mathematician's point of view.

3. Growth through creativity

New enterprises start with a burst of creativity.

In reviewing PVD's Insights Rutherford Aris wrote that "[creativity involves] moments ... when a new concept emerges clearly from the mass of material ... or a new relationship is perceived between to hitherto disparate subjects" and, "Danckwerts may have experienced many such moments", Aris said (Aris, 1982). This fits Bronowski's view of creativity and may undoubtedly be true. Speaking of his RTD paper, PDV said in Insights: "Like most conceptual advances, it represents a crystallization of ideas that at the time were scattered or and ill-defined". But it is undoubtedly true that PVD's creativity had another component, a keen sense of awareness of the times he lived in.

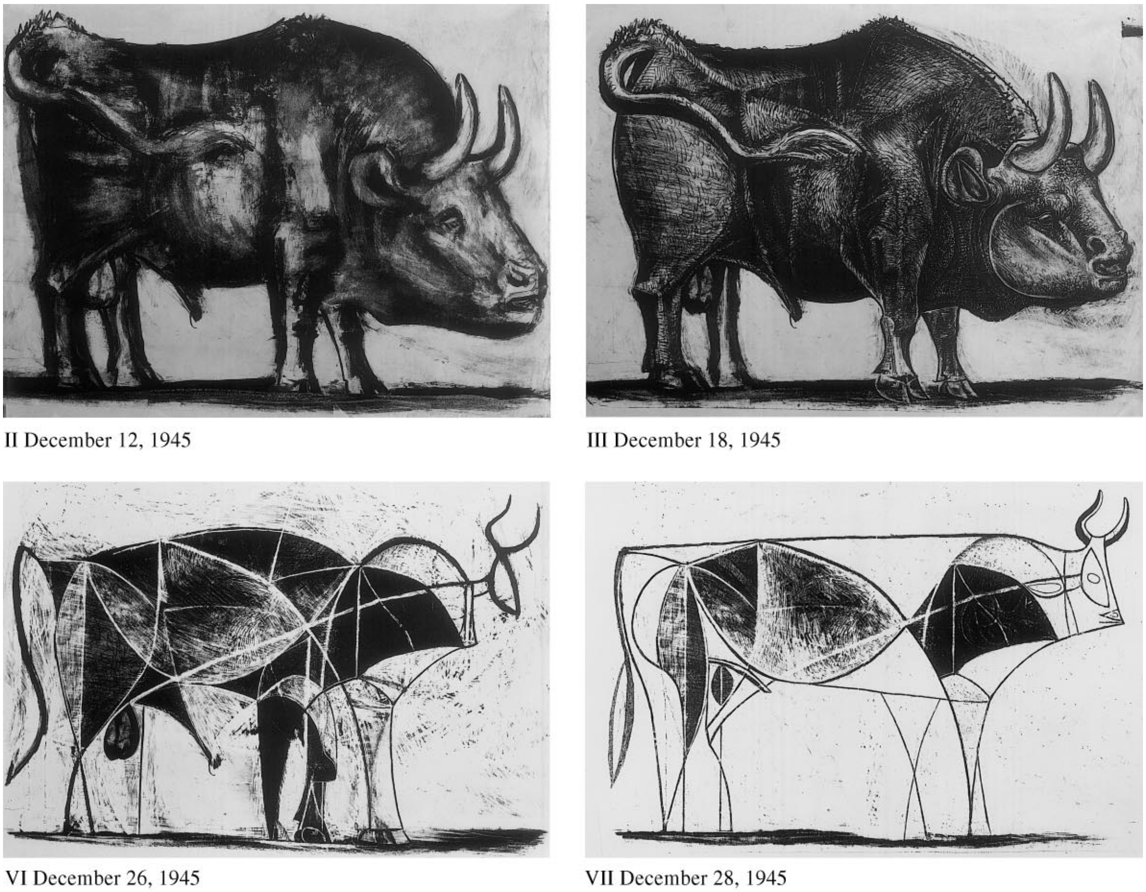
"In the sphere of Chemical Engineering, creative inspiration remains always the real source of progress". This appeared in the very first paragraph of the very first article in the very first issue of Chemical Engineering Science (Cathala, 1952). Who could possibly argue with this, even half a century after? The reason this is important is that the initial building of a discipline starts with a creative burst (see Fig. 3). That was the environment PVD found himself in. "We had an almost virgin field to plough ... ", PVD said (Danckwerts, 1981).

Of course there was such a thing as "ChE Science" before CES and PVD, but it was scattered (the AIChE J had in fact been started a few years earlier, in March, 1955). But a lot of the engineering science was going elsewhere; Lapidus and Amundson were publishing in the Journal of Chemical Physics and Denbigh was publishing in the Transactions of the Faraday Society. What CES provided was an important nucleus; what PVD provided was a style.

4. Uniqueness and inevitability

Could PVD's work been done by someone else?

"Continuous flow systems. Distribution of residence times"; this was PVD's first paper in CES (Danckwerts, 1953b). It was a defining paper. Danckwerts himself declares — in Insights into Chemical Engineering — "[this paper] is my most influential contribution to chemical engineering ... ". It is hard to disagree. The paper has received the ultimate accolade; it has become an unquoted primary reference. However, as indicated by PVD himself, not everything in this paper is new. Turner (1983) reviews the history of RTD and goes back to earlier work in pipes (Bosworth, 1949). But things did not gel until PVD's work. The strength of PDV's paper is its air of completeness — it was all there, compact and unadorned.



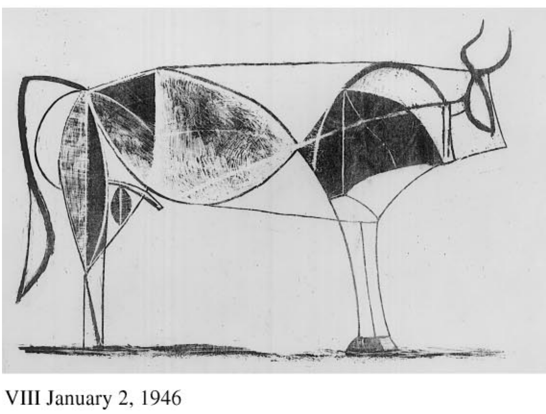


Fig. 2. From complexity to simplicity. Picasso's Bull series, done in the time span December 5, 1945–January 17, 1946, shows the evolution of an idea. The complete series is 11 lithographs; here we reproduce five of them: Stage II (The Bull (Le Tarreau), December 12, 1945; 32.1 × 42.9 cm), III (The Bull (Le Tarreau), December 18, 1945; 31.4 × 48.1 cm), VI (The Bull, December 26, 1945; 30.5 × 44.4 cm), VII (The Bull, December 28, 1945; 32.1 × 41.6 cm), VIII (The Bull, January 2, 1946; 31.1 × 43.8 cm). In the last stage, XI (corresponding to January 17, 1946), the bull gets reduced to just a few lines. The Museum of Modern Art, New York, Mrs. Gilbert W. Chapman Fund. Photograph © 2000 The Museum of Modern Art. The © 2000 Estate of Pablo Picasso/Artists Rights Society (ARS), New York.

It appealed to two constituencies: it was immediately practical but at the same time it left opportunity for academic continuation. Was it inevitable? Perhaps yes. But things could have taken a different shape had they not been put in a style that was worthy of imitation.

5. Questions of style

What was PVD's style?

"… I was a mathematical formalist, PVD was an idea person" Neal Amundson said of Danckwerts in his PVD Lecture "PV Danckwerts — His research career and its significance". That may be true, but what kind of idea person was PVD? What was PVD's style? Again, people have looked into the issue of academic research styles, even associating it with different cultures (Galtung, 1981), a dangerous proposition as noted by Hadamard as early as 1945.

PVD seems hard to classify. It is clear that he had analogical imagination; this is evident in the work he did on mixing measures when he brought in ideas from turbulence (Danckwerts, 1952). And it is clear that he could balance contrary themata. How after having done

one thing (the RTD work) could he do the other (mixtures)? But most of all, I think, PVD was balanced. The blend of Oxford Chemistry and MIT Practice School may undoubtedly have something to do with it.

Recently, Donald Stokes developed a model of scientific research (Stokes, 1997). His objective was to provide a framework for scientific public policy but his observations fit our objectives here. Stokes's model is a four-quadrant picture (see Fig. 4). One of the axis is "consideration of use", the other "quest for fundamental understanding". Each of the axes is divided into "yes" and "no". Niels Bohr, Thomas Edison, Louis Pasteur are archetypical of the three modes of research modes. PVD, it appears to me, is a clear exponent of Pasteur's Quadrant. He did fundamental work but was always guided by ultimate applicability.

6. Recognizing our times; the "myth" of the lonely genius

Greatness does not imply infallibility.

For an idea to flourish it has to fit with the canonical knowledge of the time. But being attuned with a field at some point does not guarantee life-infallibility. Fields have the nasty habit of evolving making earlier modes of thinking obsolete. There are many examples of great minds missing the big picture; it is remarkably easy to misjudge one's times. Think of the case of Albert Michelson (1852–1931), America's first Nobel Prize winner in science (for designing the interferometer to measure the speed of light). In 1894, on the occasion of the dedication of a physics laboratory in Chicago, noting that the more important physical laws had all been discovered, Michelson remarked: "Our future discoveries must be looked for in the sixth decimal place". Things had surely changed even as he was receiving his Nobel Prize in 1907.

I do not subscribe to the romantic notion of the unrecognized genius. Examples notwithstanding — Van Gogh (1853–1890) in painting, Evàriste Galois (1811–1832) in mathematics — the unrecognized genius is mostly a myth: Death is not a good career move. The converse seems closer to the truth; reputations diminish after death. Carlo Marata (1625–1713), the last of Raphael's line, and after the death of Giovanni Lorenzo Bernini (1598–1680), possibly the most important European artist of his time, is an early example; Victor Vasarely (1908–1997) a more recent one. The jury is out for Roy Lichtenstein (1923–1997) and the last few years of Willem de Konning (1904–1997) [Kimmelman, 1998]. It happens in science as well. Johan Poggendorff (1796–1877) was arguably one of the most influential physicists of his time. His influence waned after his death.

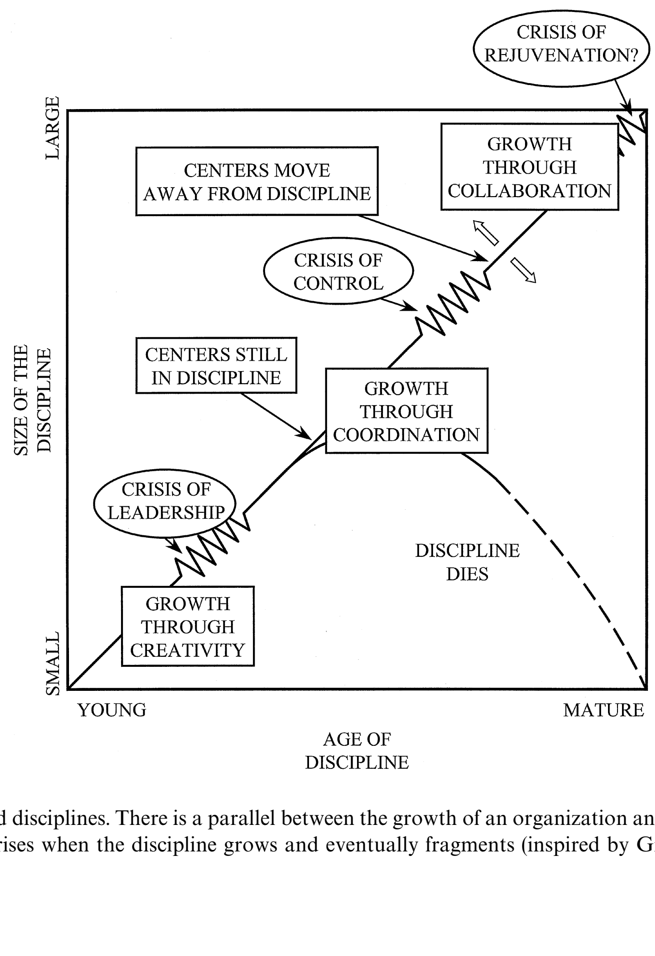


Fig. 3. Evolution of organizations and disciplines. There is a parallel between the growth of an organization and the growth of a discipline. Both start with a creative burst and there are crises when the discipline grows and eventually fragments (inspired by Greiner, 1998).

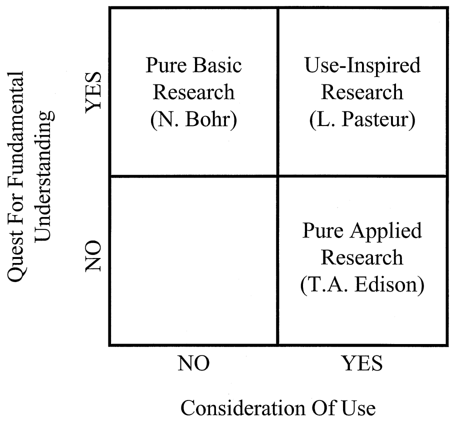


Fig. 4. In Stokes's view (Stokes, 1997), Niels Bohr (1922–), Thomas Edison (1847–1900), and Louis Pasteur (1822–1895) typify the three archetypical research styles.

It is easy, however, to misjudge part of a body of work without the perspective of time. Consider the obituary of Jules Henri Poincaré (1854–1912). He was clearly admired in his time. "…the contribution of Poincaré to celestial mechanics not only brought new life to a subject which showed signs of becoming stale…". But referring to the three-body problem the obituary states "…that he did not succeed in solving it, either in the old or *modern sense* [my italics], is no criticism of his achievement…it is sufficient to say that he opened the way and explored a new region by routes which may ultimately lead to the final goal — a demonstration of the stability or instability of the solar system" (Nature, 1912, pp. 353–356). But this misses the point. In fact, Poincaré had already shown that the three-body problem has no solution (in the *classical* sense; more on this later).

These two examples, Michelson and Poincaré, share a common link: *quantification*. Prior to 1900 science was measuring and precision — "all the laws had been discovered… ." as Michelson said — what was needed was precision. And mathematics was about calculation, and it certainly was not qualitative. It was assumed that all problems — the three-body-problem included — had solutions that could be written down. Poincaré's result, foreshadowing homoclinic tangles (Moser, 1973), was a large qualitative deviation from this belief; so large, in fact, that did not become part of the canonical knowledge of his time.

Much has been said about the parallel Science/Art, and it is worth repeating a few aspects again though it is important to remark that progress is far from rectilinear (see Figs. 5 and 6). Both intellectual domains went through a metamorphosis between 1900 and 1910: Art went from figurative and life-like, "rendering reality as it is" to abstraction, cubism and the like (though complete abstraction had to await for Vassily Kandinsky (1866–1944)). Correspondingly, science went from quantification and measuring things more precisely (e.g. speed of light, charge of the electron) to abstraction and structure, to how a theory is built and how it fits together or even how two different views of the world — quantum mechanics and relativity — could mesh with each other (still an open question today).

How did PVD fare in the pronouncements category? He was not shy in making his views known. History shows he was more or less correct. "I have felt for some years that chemical engineering is weighted-down with more mathematics it can support…" he declared in 1982 (Danckwerts, 1982); this view seems supported by events. The science content has certainly not decreased but nowadays the discipline is decidedly tilted towards applications.

7. Peaking too early; Reynolds's paper

An example of competing paradigms; an idea that did not take root.

Osborne Reynolds, of the Reynolds number fame, had the right idea about mixing, one that potentially could have revolutionized fluid mechanics and also physics and nonlinear analysis and mathematics. In 1894 Reynolds advocated in a Friday night lecture demonstration in the Royal Institution that the process of fluid mixing, when stripped of details, was essentially stretching and folding (Reynolds, 1894). Reynolds's key point was that of folding. That Reynolds regarded his idea as obvious is clear. However, he also understood why people might not actually "see it", to the point that he felt compelled to introduce it by drawing a parallel with Edgar Allan Poe's[4] (1809–1849) "The Purloined Letter", the short story where Auguste Dupin — Sherlock Holmes was just on his way — finds a hidden letter in the most obvious of all places, on top of a desk. Reynolds's concerns turned out to be right; his idea was forgotten, and waned and died. In fact, Reynolds himself might have brought its demise.

Why was that? An obvious reason was that the idea was premature, in the sense that it did not connect with the canonical thinking of its times. In fact, the climate was to be inhospitable for the next 80 years or so. The intellectual framework that surrounded fluid mixing and turbulence until recently was primarily statistical. It is now standard to visualize the internal motion of fluids by deformation of "coloured bands", as Reynolds called them in his 1894 paper, and it also has become standard to apply geometrical thinking to rationalize internal motions of fluids, including the once forbidden turbulent

[4] Coincidentally, Edgar Allan Poe (see Poe, 1966) described in amazing detail what one would now call lamellar structures in mixed fluids. Lamellar structures are generated by Reynolds's mechanism of stretching and folding.

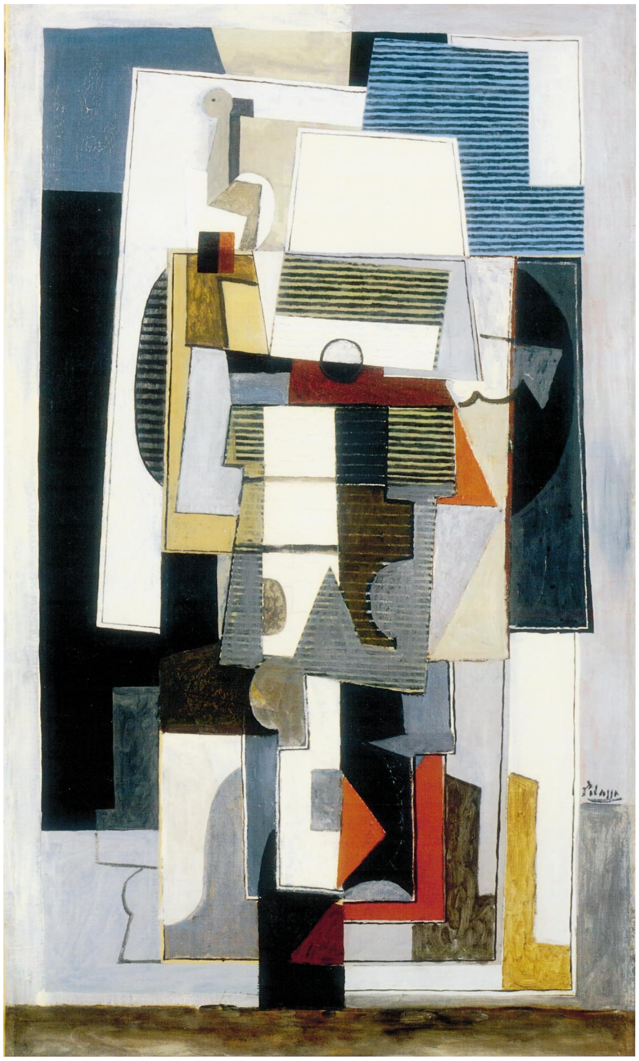


Fig. 5. Pablo Picasso (Spanish, 1881–1973). Table, Guitar, and Bottle (La Table). 1919. Oil on canvas. Smith Museum of Art, Northampton, Massachusetts. Purchased, Sarah J. Mather Fund, 1932. © 2000 Estate of Pablo Picasso/Artists Rights Society (ARS), New York.

flows (Sreenivassan, 1991). But the prevalent picture of turbulence during the 1950–1960s decades was one, as aptly described by Theodorsen (1955), of "a perfectly random motion of particles [where] no basic pattern should or could exist." Similar comments applied to mixing, the conceptual pictures relying mostly on eddy diffusivities and the like. Geometry played little role.

It is somewhat ironic that the statistical view can be traced back, most clearly, to Reynolds himself and his averaged Navier–Stokes equations (Reynolds, 1895). The two mixing paradigms could not co-exit. But this is hardly surprising. The method of colored bands was not couched in a quantitative format — just like the ideas of Poincaré missed in Nature's obituary were the most qualitative ones — and in those days quantification was king. Lord Kelvin (1824–1907) is credited with "unless an idea can be quantified the knowledge is of a meager kind". Moreover, it was impossible to see how Reynolds's ideas could be couched in mathematical terms. The necessary mathematics had not yet been created.

It is hard to resist pointing out further link associated with the Reynolds–Poincaré connection, and I have commented on this issue before (Ottino, Jana & Chakravarthy, 1994). In the introduction of his 1894 Nature paper Reynolds stated that "in respect of the mental effort involved, or the scientific importance of the results (referring to work dealing with motion of fluids) goes beyond that which resulted in the discovery of Neptune". Why Neptune?

Neptune's discovery was the result of unbounded faith in Newtonian mechanics and determinism. Uranus was not behaving as it should; 30 s of arc deviation from Newtonian Predictions was unacceptable, and the idea of a trans-Uranian planet took shape. The discovery of the reason for these deviations — after dispensing with explanations, such as an incorrectly calculated mass for Uranus, as proposed by Friederich Bessel (1784–1846) — took the form of finding an as yet undiscovered, *trans*-Uranian planet. This laborious task was completed almost simultaneously by Jean Leverrier (1811–1877) in France and John Couch Adams (1819–1892) in England, and unveiled what we now call Neptune. This was going to be the crowning triumph of determinism, and, in some sense, it would be its last. Propelled by an unbounded faith in the existence of a solution for the motion of planets, a sort of race took place to find out the first closed-form analytical solution for the three-body problem (a prize was established by the King of Sweden; see Moser (1973)). The answer, as it turned out, was anticlimactic, and it was most clearly not what people were looking for. Jules Henri Poincaré showed that no solution could possibly be written down; three bodies interacting via gravitational forces were enough to produce chaos. We have thus come full circle: The reasons for this chaos are what we now call homoclinic intersections, the mechanism being exactly equivalent to *stretching and folding* in phase space. This was precisely the idea advocated by Reynolds to explain fluid mixing.[5] That Poincaré's three-body-problem effort was not fully appreciated in his lifetime is clear from the obituary in Nature. Coincidentally, just a few months earlier, Reynolds's own obituary had appeared in Nature. It is a praising account but, as may be expected from the foregoing discussion, there was nothing on the method of colored bands. Tellingly, there was little also on the work that will be his major triumph (Reynolds, 1895), the beginnings of turbulence article, the article that

[5] The concept of stretching and folding of stretching and cutting can be captured by means of the so-called baker's transformation (see Ottino, 1989). It is noteworthy that Danckwerts included a picture of the baker's transformation in his 1953 review of mixing and mixtures (Danckwerts, 1953a).

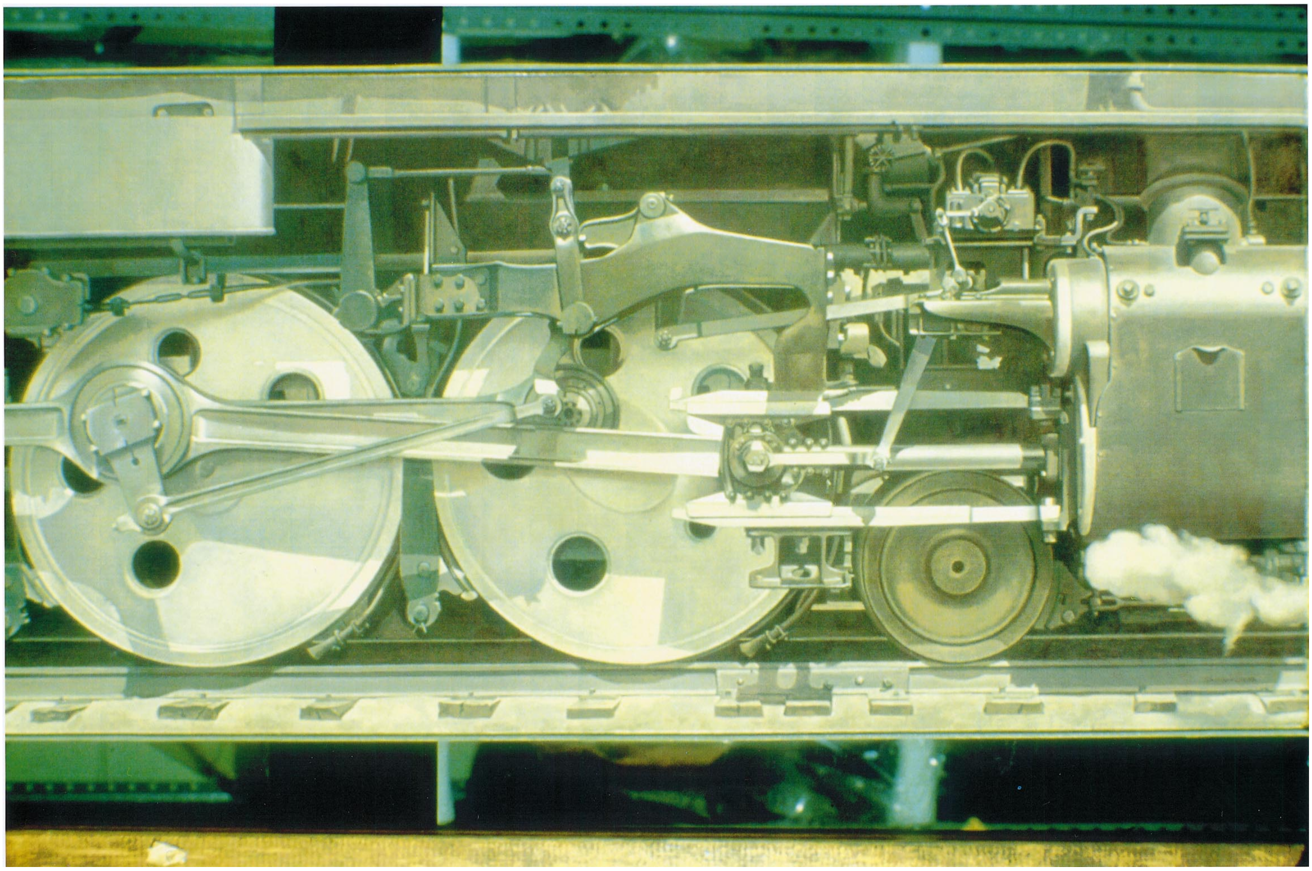


Fig. 6. Progress and progression. Charles Sheeler (American 1883–1965). Rolling Power, 1939. Oil on canvas. Smith Museum of Art, Northampton, Massachusetts. Purchased, Drayton Hillyer Fund, 1940. Art does not move in a rectilinear fashion, even within the production of a single artist. Compare Picasso's Fig. 5 (1919), cubism, and Fig. 11 (1921), showing Picasso's own brand of neoclassicism, with Sheeler's intense realism, and de Kooning's, abstract expressionism, Fig. 10 (1950).

dethroned the "coloured bands" for the mixing paradigm. With this view Reynolds was also ahead of his times, by about 40 years or so.

A long time passed before stretching and folding made a final and permanent entrance again. Stretching and folding as the fingerprint of chaos formally appeared in the literature in the late 1960s (Smale, 1967) through the horseshoe map of Smale and the connection between fluid mixing, stretching, and folding, and Smale horseshoes was pointed out in 1986 (Khakhar, Rising & Ottino, 1986). Reynolds's thought experiment became a real experiment also in 1986 (Chien, Rising & Ottino, 1986; Chaiken, Chevray, Tabor & Tan, 1986). Unfortunately, I did not become aware of Reynolds's paper until three–four years afterwards.

Anybody could have done Reynolds experiment in the last hundred years — something that a computer would have had difficulty in mimicking until the mid 1960s. The result would have been a remarkable visual demonstration of the complexities of mappings in the plane. Nonlinear mathematics could have been affected in a mayor way.

8. Modeling and theory

Modeling entails the reduction of complexity; a complex problem is broken down and reassembled in terms of known time-honored building blocks. There is certainly art in doing this. The final picture, very much like a painting, rests on an underlying sketch which hopefully contains the most important aspects of the problem. It may be argued that a theory is, in essence, a similar thing: a sketch which hopefully contains the most important aspects of, say, the physics. But there is a big difference though. Modeling is convergent, its goal is to get to an answer. The goal of *theory*, on the other hand, is divergence and generality; a well-formulated theory opens new avenues, it forms the generating sketch for a variety of images. The stretching and folding idea of Reynolds, for example, fulfills that role in mixing. True, most mixing processes are more complicated, but this simple picture captures the essence of the problem.

Too much detail clouds the picture, in either modeling or theory. Irineo Funes, the character in one of Jorge Luis Borges (1899–1986) short stories (Borges, 1974,

p. 485) may be an extreme example of this. Funes lives in Fray Bentos, Uruguay, and is a case of prodigious memory. Cyrus the Great (?–529 BC) purportedly remembered all the names of all the soldiers in his armies. Funes's memory was even more prodigious. Funes remembered the shapes of all the clouds he had seen; he could remember an entire day, but it took him an entire day to reconstruct it, he even tried to devise a catalog of all the images he had seen (the English philosopher John Locke (1632–1704) in the 17th century proposed and refuted a similar concept). A running horse now and an instant afterwards were for Funes two different horses. Funes was unable to discover essences or rules; he could not grasp the concept of tree; he could not even grasp the concept of the first bull in Picasso's series nor see how the images relate to one another (see Fig. 2). Musical idiot savants have no problem with Edward Grieg (1843–1907); there are rules in Grieg. Béla Bartok (1881–1945), on the other hand, is much harder to distill.

Having a selectively myopic view is often of help. There are many examples of this in science, the belief in the essential validity of a theory, even if parts or data do not seem to fit the picture (the negative consequences of this trait are too obvious to point out). The kinetic theory of gases developed by James Clerk Maxwell (1831–1879) predicted that the viscosity was independent of the density, and that the specific heats were constant. Maxwell was troubled by this, and wrote to G.G. Stokes (1819–1903) and learned from him that there was (only) one experiment made in 1892 by a fellow of name Edward Sabine that suggested that the viscosity or air does vary with the density. This disagreement was mentioned by Maxwell in his kinetic theory paper. The case of the specific heats was more problematic — it was clear that the kinetic theory could not account for the variation with temperature. Maxwell made this point clear at the 30th Meeting of the British Association for the Advancement of Science: "[the theory] being at variance with experiment… overturns the whole hypothesis [the molecular hypothesis], however satisfactory the other results may be" (see Brush, 1974). The issue of viscosities is an interesting one for another reason. Maxwell conducted experiments and found that the viscosity was nearly constant over a wide range of densities; this, in fact, became one of the stringiest arguments in favor of the kinetic theory (Sabine's experimental results had assumed that the viscosity would vanish at low densities). Had it not been for Maxwell's theory this (rather "natural") assumption would have remained uncontested for a long time. Fortunately, in spite of these two conflicts, constant viscosity, constant specific heats, Maxwell decided to push ahead developing the kinetic theory of gases and inspired others to follow him (Brush, 1971, 1974). It would have been hard to develop in one stroke a theory accounting for all these facts. The essential merit of Maxwell's theory is given by the fact that it is still part of the standard curriculum in physical chemistry courses.

9. The mixing of fluids

An inevitable problem.

Uncovering the connection between stretching and folding and mixing enters in the category of inevitable. Anybody could have been able to do the critical experiment before 1986. The diversity of scenarios may, however, cloud the thinking. Fluid mixing might involve miscible or immiscible fluids, diffusive or non–diffusive substances that might be reacting or not. The problem here is one of not being derailed by unimportant details and framing the problem in the most natural way. Consider as an example the case of mixing of a passive tracer in a Newtonian flow. The equations governing the physics have been known for long time; still the problem was regarded as intractable. Clearly this is not where the problem resides.

An example may be educational. Consider a particle of mass m with coordinate $Y(t)$ under the action of a force F. The motion of the particle is governed by

$$m\mathrm{d}^2 Y/\mathrm{d}t^2 = F.$$

This implicitly assumes that t is the independent variable. On the other hand, if Y is regarded as the independent variable, now $t(Y)$, and Newton's law becomes

$$F + m(\mathrm{d}Y/\mathrm{d}t)^3\, \mathrm{d}^2 t/\mathrm{d}Y^2 = 0.$$

The underlying physics is the same but viewing variables in a different way has made the problem unnecessarily harder (Corrsin, 1966).

Similarly, viewing mixing in x, y, z Eulerian coordinates makes things needlessly complicated. The key idea is to be able to follow identifiable elements of fluid, Reynolds's colored bands, and this requires a Lagrangian viewpoint. The elementary mixing action is stretching and folding. The flow has to be capable of stretching a region of the flow and returning it — stretched and folded — to its original location. The repetition of the operation leads to a layered structure — very much like puff pastry — consisting of folds within folds (Fig. 7). The chaos however, is confined; where folds do not invade islands of poor mixing form. Islands appear and within islands more folds are possible, in a Kafkaesque succession, ad infinitum. The key question then is what flows to examine, what mechanisms to put in evidence, and how complete, compelling, and inspiring the presentation of ideas is, it is going from simple to complex in Fig. 2. The stretching and folding mechanism provides a springboard for more elaborate examples — going from time-periodic to spatially-periodic. Fig. 8 shows the time evolution of two dye-streams in a continuos flow chaotic

Fig. 7. Stretching and folding revealed. In a turn of events, the byline in the cover of Scientific American inverts the relationship between mathematics and understanding of physical systems ["Patterns of complexity that emerge in the mixing of fluids have began to yield insight into nonlinear physics"; Ottino (1989)]. Reproduced with permission from Scientific American.

flow. The model corresponding to this system was first published in these pages (Khakhar, Franjione & Ottino, 1987).

10. A complex system — mixing of solids; getting lost in details?

A problem in the category of modeling.

Some of the simplicity of mixing of fluids carries over to mixing of solids. But this problem is more complicated on several levels. First, there is new physics: flowing granular materials quickly segregate. Small differences in either size or density lead to *flow-induced segregation*; this is a complex and imperfectly understood phenomenon. The second problem is the absence of a clear starting point. In fluids, in the simplest case, the Navier–Stokes equations are the conventional point of departure. In solids things are much less clear and several alternative viewpoints are possible: continuum and discrete descriptions (particle dynamics, Monte Carlo simulations, cellular automata computations). Moreover, the continuum and discrete descriptions of granular flows are regime dependent and this may require adopting different subviewpoints (Ottino & Khakhar, 2000). Granular mixing — as opposed to the fluid case described before — requires *modeling*.

Tumbling in a pseudo-two-dimensional clockwise rotating container provides a simple starting point. Under suitable conditions, easy to achieve in the laboratory, the flow of *non-cohesive* granular materials moves in a continuous flow, the so-called *rolling* regime. The flow is confined to the top free surface in the form of a thin shear-like flat layer whereas the rest of the material moves in solid-like rotation with the mixer walls. Material is fed into the flowing layer $-L < x < L$ with thickness $\delta(x)$ for $x < 0$ and leaves the layer for $x > 0$. The simplest case is a circle rotating at a constant speed ω. In this case L, δ, and streamlines are time-invariant (Fig. 9a). If the flow is steady, as in the case of a cylinder, the streamlines coincide with the pathlines and the flow is non-chaotic. However, if the container is *non-circular*, the flow is time periodic, and the flowing layer grows and shrinks in time. The system is now referred to as having one-and-a-half degrees of freedom and chaos is possible. Experimental studies using colored tracer particles in mono-disperse granular materials show that increased mixing rates occur in non-circular containers.

Surprisingly, a continuum description works remarkably well and a Lagrangian formulation is useful for interpreting this behavior of the system. Constitutive models for mixtures of different sized particles can be incorporated into advection–diffusion computations. Once a modeling viewpoint has been adopted the elements of theory become evident. Granular mixing offers experimental prototypes of the competition between order and disorder. It is convenient to start with the simplest case: mixing of cohesionless granular materials in quasi two-dimensional rotating containers half-filled with solids in the so-called continuous flow regime when the flow comprises a thin cascading layer at the flat free surface, and a fixed bed which rotates as a solid body.

Chaotic advection interacts in non-trivial ways with segregation and leads to unique structures that serve as prototypes for systems displaying organization in the midst of disorder (see Fig. 9). These structures are relatively easy to investigate experimentally and can be mimicked by a continuum flow model that incorporates collisional diffusion and density-driven segregation. Under certain conditions, the structures never settle into a steady shape (Hill, Khakhar, Gilchrist, McCarthy & Ottino, 1999). The problem is clearly divergent. This is the beginning rather than the end.

11. Lessons

What lessons can we extract?

Distilling lessons about creative processes is a dangerous undertaking. Nevertheless, in the interest of demystifying the process, let us make some general observations.

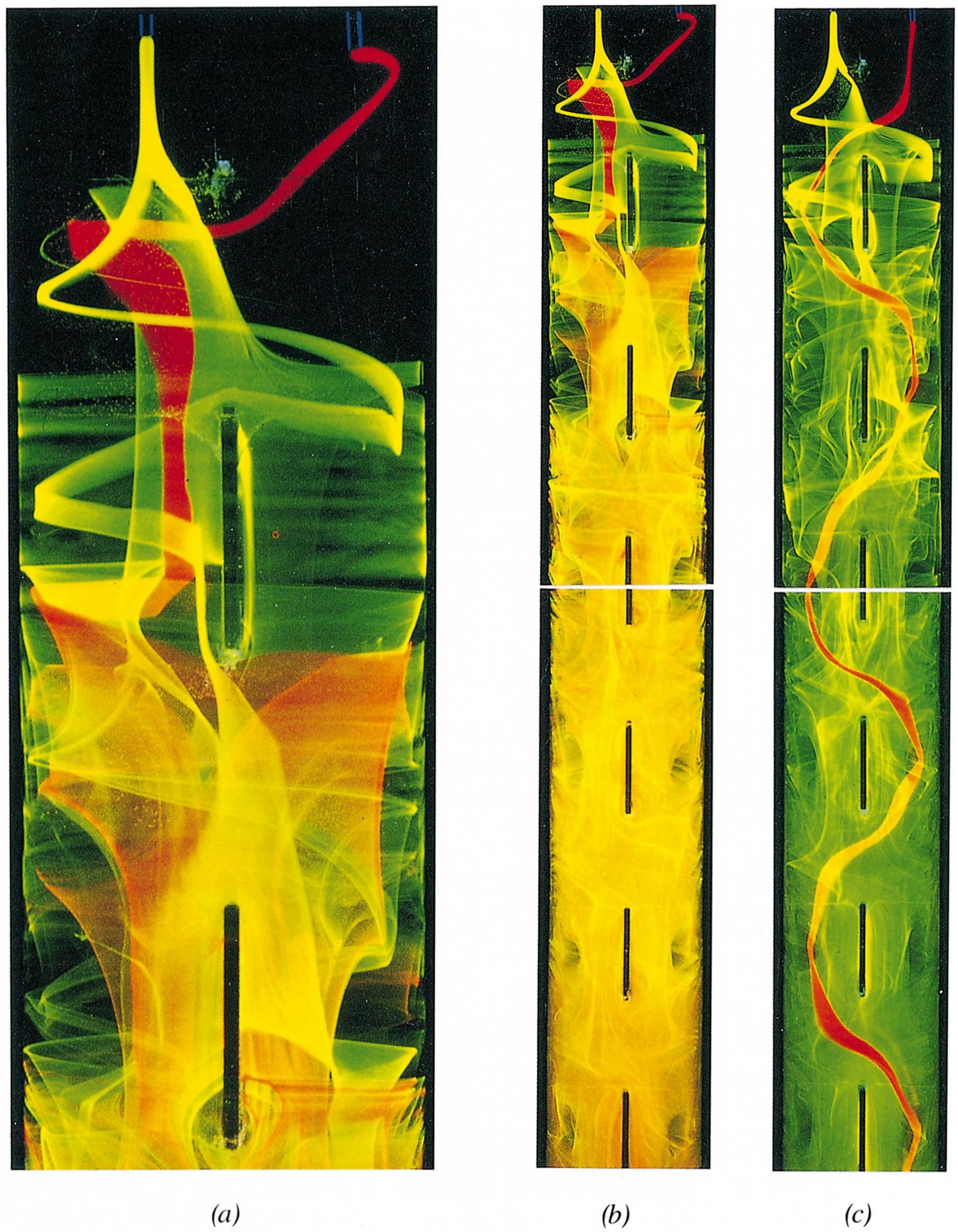


Fig. 8. Coexistence of chaos and order in a spatially periodic viscous flow (the "partitioned pipe mixer", Khakhar et al., 1987; Kusch and Ottino, 1992). The system consists of an array of plates fixed orthogonally to each other inside a rotating tube. The left image (a) shows a magnified view of the top of the central figure. In (b) both dyes undergo chaotic advection whereas in (c) the inlet position of the reddish stream has been changed, revealing regularity within the system (KAM tubes). Note that the pattern of the yellow–green dye is nearly identical in (b) and (c). Reproduced with permission, Journal of Fluid Mechanics, Cambridge University Press.

- *Start with a solid grounding*

Creativity requires effort. This is clear when one has access to the evolution of a work, the arc of creation that generates the final product. Things are surely changing now but up to 1960 or so even the most revolutionary artists learnt by copying the classics; consider the "before" and "after" of Willem de Kooning (Fig. 10). This is transparent in art but is an unseen part in science and engineering. We rarely get to see the training exercises of great scientists. Only once in a great while we see the editing processes of a great paper (e.g. the manuscript of Einstein containing the celebrated $E = mc^2$), or a great book with annotations and markings of another towering figure (e.g. Newton's *Principia* with the markings by Leibniz).

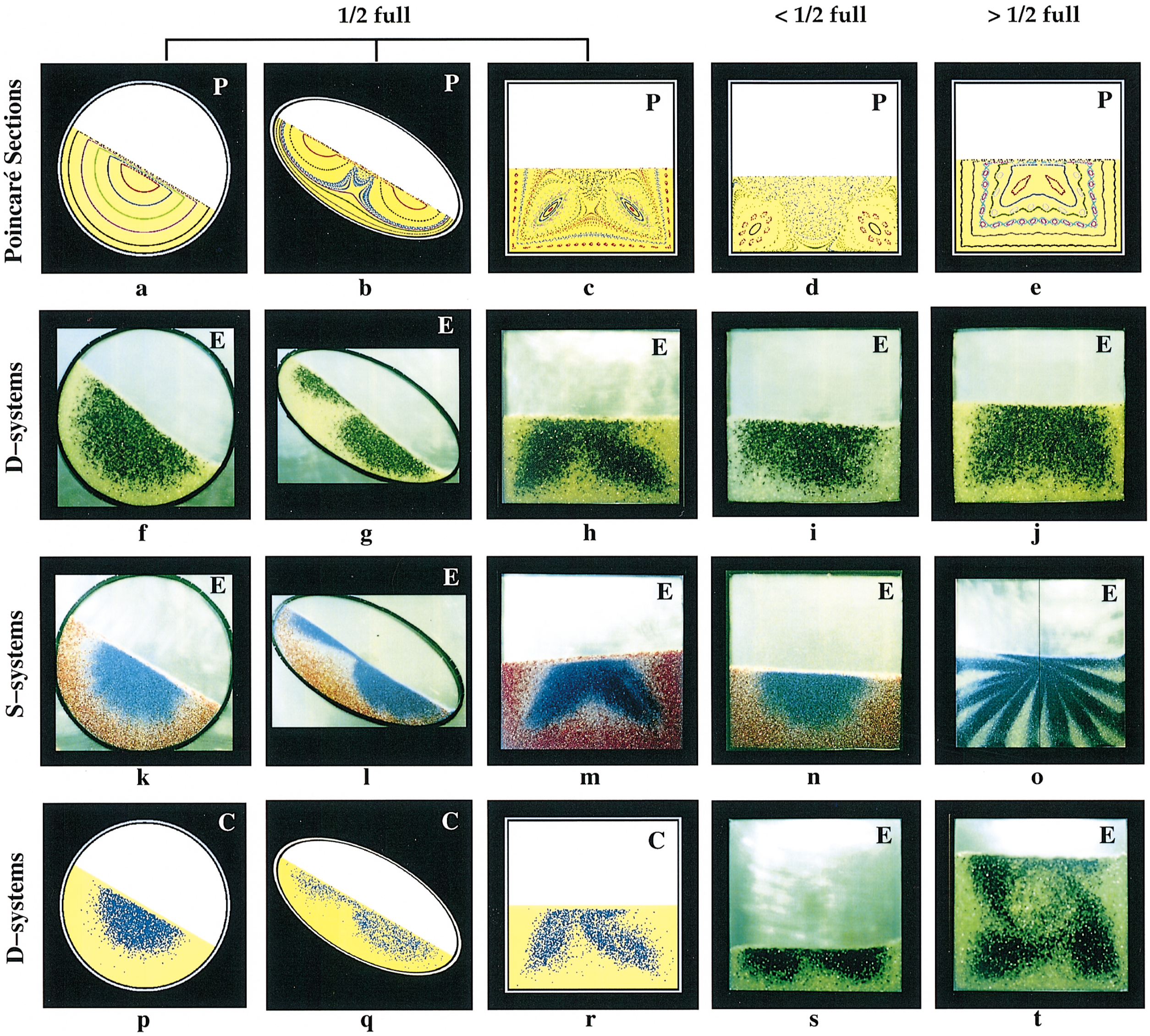


Fig. 9. Mixing and segregation of solids highlights self-organization in systems where there is a competition between order (the tendency for the materials to segregate) and disorder (brought by chaotic advection). "E" denotes experimental results; "C" denotes computational results and "P" denotes computationally obtained Poincaré sections for a system of equal size and density particles. All images are taken while the mixer is rotated, though the images of the square are rotated counter-clockwise by $\sim 30°$ to maximize the use of space. The mixtures consist of binary D-systems (2 mm glass and steel spheres) and ternary S-systems (0.8 mm blue, 1.2 mm clear, and 2.0 mm red glass spheres). The volume fraction of steel : glass beads in the D-system is $\frac{1}{4}:\frac{3}{4}$, and the volume fraction of the small : medium : large beads in the S-system is $\frac{1}{4}:\frac{3}{8}:\frac{3}{8}$. Computational results correspond to binary mixtures of D-systems (p, q, r). A comparison of the fourth and fifth rows shows the variations in structures obtained as the degree of filling is changed from the half-full case (third row). D-systems and S-system behave similarly (h, m; i, n). The 55% full S-system, (o), never reaches a final segregated pattern, but instead shows changing patterns of streaks as opposed to the compact structure (j) obtained in D-systems. Increased filling of the S-system (o) results in a structure similar to (t) for D-systems (from Hill et al., 1999). Reproduced with permission, Proceedings of the National Academy of Sciences of the United States of America.

Without solid grounding we learn trivia. PVD may have been apologetic about his lack of formal math training, but he made excellent use of it. Having technique is simple not enough. In the worst cases it just gets in the way and forces viewing through a single lens. Problems are fitted to techniques rather than attacked with an open mind. Over reliance on technique can have a paralyzing effect.

- *Take time to reflect*

"I recommend my colleagues the practice of academic indolence", PVD said. This is sound advice. And he goes on to mention the example of the discovery of the benzene ring structure by August Kekulé (1829–1896) and his own insights into the RTD concepts during tea time at Cambridge. Moving and doing does not imply progress. It is healthy to step back and look the big

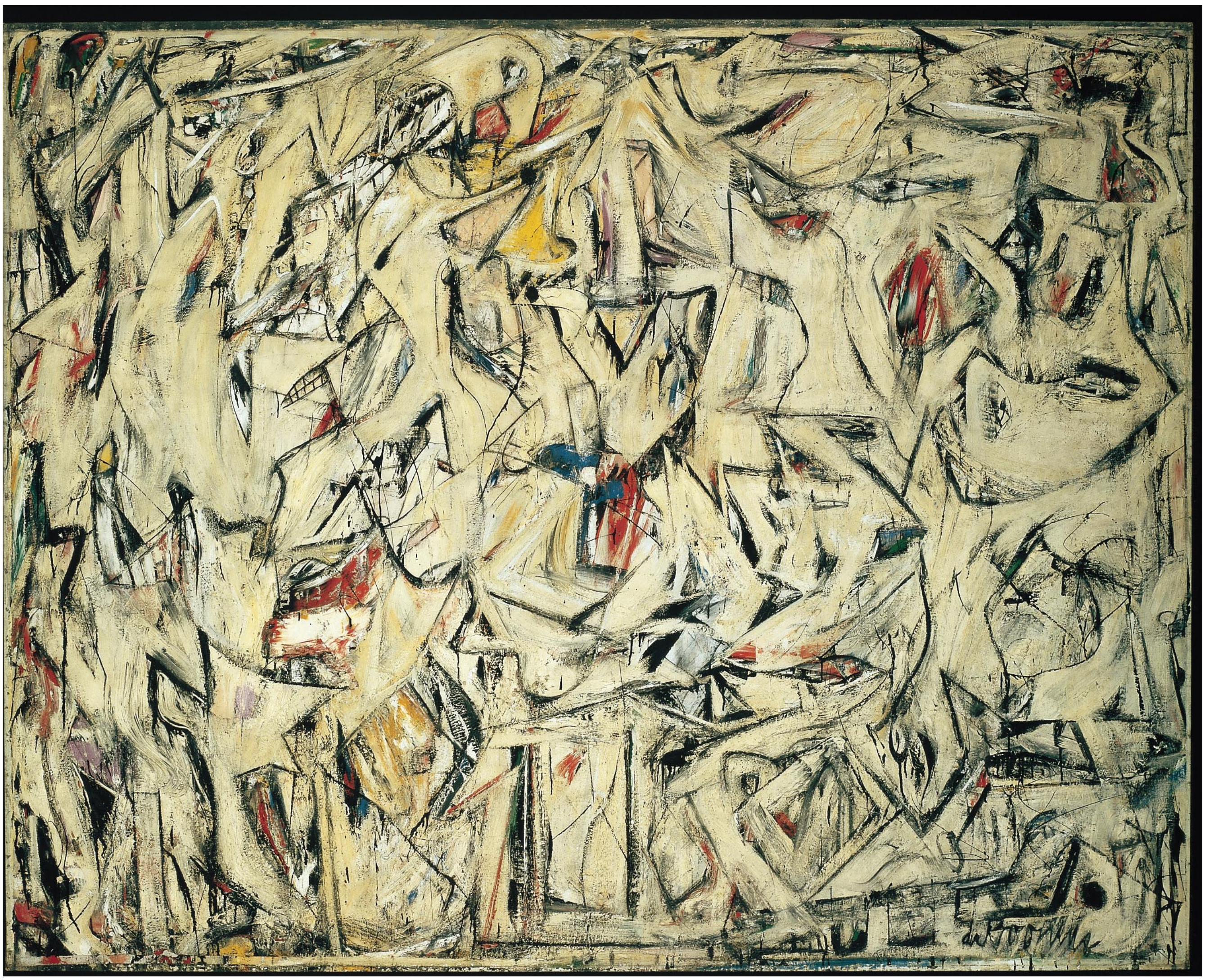


Fig. 10. Even the most revolutionary artists started from the classics. Willem de Konning (American, b. the Netherlands, 1904–1997). Portrait of Elaine, charcoal, 1940–1942, private collection. Excavation, oil on canvas, 1950. 206.2 × 257.3 cm, Mr. and Mrs. Frank G. Logan Purchase Prize; gift of Mrs. Noah Goldowsky and Edgar Kauffmann, Jr., 1952.1. The Art Institute of Chicago.

Fig. 11. Pablo Picasso, Spanish, 1881–1973. Mother and Child, oil on canvas, 1921, 142.9 × 172.7 cm, Mary and Leigh Block Charitable Foundation; restricted gift of Maymar Corporation and Mrs. Maurice L. Rothschild; through prior gift of Mr. and Mrs. Edwin E. Hokin; Hertle fund, 1954.270 (shown with tacking margin exposed) with fragment at left. The Art Institute of Chicago.

picture. But this does not mean that one should wait for divine inspiration to struck. Picasso did not paint thinking that everyday he would come up with a masterpiece; he painted a lot. Anybody who has been to a retrospective sees that all great painters painted a lot (what survives of Leonardo being a singular exception).

- *Do not wait for divine inspiration*

If ideas do not come one should follow Jasper Johns dictum: "… do something, then do something else to it…" Do not wait for "the idea". Linus Pauling (1901–1994) sait it best: "the best way to get good ideas is to get lots of ideas...".

- *Do not converge too quickly*

The equivalent in problem solving is to solve the wrong problem. We have seen that great masterpiece may appear effortless, but may involve numerous unseen sketches. The time spent in the sketches and turning things around may be much more than the actual time of execution of the final piece.

- *Learn how to adapt*

Edison put it this way: "… and idea has to be original only in its adaptation to the problem at hand…". Moving ideas from turbulence to mixing measures as PVD did is surely one example. Recognizing that a problem in mass transfer was already "solved" in a heat conduction text (e.g. Carslaw and Jaeger) — is another.

- *Step back and look at the entire picture*

It is a mistake to fall in love with the "final" product; one should be willing to completely rethink and modify things at the end. Picasso provides a great example. The story is that William E. Hartmann, who was a senior partner at the architectural firm of Skidmore, Owens and Merrill of Sears Tower fame, was visiting Picasso in Mougens, France, and presented Picasso with a catalog of a 1968 Chicago exhibit where Picasso's "Mother and Child" appeared. The painting was originally different, Picasso reportedly said: "there was a bearded man holding a fish over the baby's head", and proceeded to give Mr. Hartmann the fragment that he had cut at the last moment from the left side of the painting. Both the fragment and the painting are now at the Art Institute of Chicago (see Fig. 11). How many of us are courageous enough to step back and take such a drastic action when things appeared to be almost finished?

- *Be conscious of repetition*

There is a style of doing science, in the same way that style is what allows a trained person to attribute a painting, that he or she may have not seen before, to a specific artist. In the final instance, style is what makes a scientific theory or a clever experiment unique. Style is good and one should be aware of it. Style, however, should never get in the way. There is an unavoidable all-too-human tendency to stick with a style, a way of doing things, way past its useful limit.

"Too many academics looking at too many non-problems", PVD said, and this is probably true of most disciplines at most times (with the possible exception of the beginning, just as a new discipline is starting to emerge, when there are many good open problems). An artistic example is useful. When Robert Rauschenberg won the 1st prize in the Venice Biennale in 1964, he telephoned a friend asking him to destroy his silk screens, thereby ensuring that he would not repeat himself and move to something new. Avoid becoming a caricature of yourself.

Further reading

See also Aris, 1991, 1997 and Ottino, 1988.

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