40 Principles – Chemical Illustrations

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Introduction

The origins of TRIZ are to be found in the analysis of engineering and utility patents of the former USSR. As such the 40 Principles of TRIZ were constructed to tackle engineering problems. Much work has been done attempting to extend the use of the principles into non-engineering situations, such as the ‘soft’ issues in business, personal or health. However, there has been less work published which aims TRIZ directly at chemistry and its applications. This paper is designed to initiate the discussion on how the 40 principles of TRIZ may be applied directly to chemical problems.

Background

In Ciba we have tried to apply TRIZ to chemical problems but have found it difficult to relate the 40 Principles to what happens in a chemical system. The main challenge we have experienced in applying TRIZ to chemistry is finding examples that can be used to explain the meaning of the 40 Principles in chemical terms. Most of the examples currently used are engineering systems that do not always have an obvious relevance to the molecular world.

In order to try to overcome this hurdle we have put together some illustrations based on chemistry and its applications rather than engineering. We have tried to use general chemical reactions or principles as far as possible, but coming from a pigment manufacturing background there are inevitably some examples which are specific to the colour industry. Full explanations of all examples given can be found in generally available chemical textbooks (see below) and most should be familiar to any chemist with a good general knowledge of the subject.

This list is not intended as an aid to the extension of TRIZ into chemistry, but rather as a teaching tool to help introduce TRIZ to chemists in terms they understand. We would be greatly interested in any other suggestions for illustrations, or any case studies involving chemical systems.

Chemical Illustrations of the 40 Principles of TRIZ

	Principle	**Illustration**
1	**Segmentation** Separation into smaller parts	Mass Spectrometry – molecules broken down determine structure Synergist/hyperdispersant*
2	**Extraction** Take out or separate something	Fractional distillation Chromatography

		Crystallisation Soxhlet extraction of natural products or additives.
3	**Local Quality** Different parts of an object carry out different functions	Surfactants – hydrophobic and hydrophilic parts Block copolymers – pigment anchoring and solvent compatible* Directing groups – change the reactivity of different sites. Charge transfer complexes.
4	**Asymmetry** Introduce, or increase the degree of, asymmetry	Chiral centres – biologically active materials are often a particular stereoisomer Surfactants
5	**Combination (Consolidation)**	One pot reactions Nitrocellulose – fuel and oxidant in the same molecule High throughput synthesis/combinatorial chemistry/parallel synthesis. Used for synthesis/screening/crystallization
6	**Universality** Use an object to perform several functions	Monomer used as solvent and reactant in UV inks Urea used as solvent and source of nitrogen in Copper Phthalocyanine synthesis.
7	**Nesting** Putting one thing inside another	Encapsulation Inclusion compounds Chelates – e.g. EDTA to mask transition metals
8	**Counterweight** Compensate for the weight of an object	Loosely equating boiling point with weight: vacuum distillation or rotary evaporation.
9	**Prior counteraction** Take action to prevent, or reduce, harmful effect	Drying of solvents for use in water sensitive reactions Use of blocking groups to prevent reaction at particular sites Use of secondary complexing agents in EDTA titration e.g. Zn will be precipitated at pH10 but we need this pH to titrate it with EDTA. Add Ammonium Chloride. The ammonia complex of Zn is soluble but does not interfere with the ZnEDTA chelate. (The NH$_4$CL also acts as a buffer – Principle 6 – Universality) Use of protecting groups in organic synthesis Reactions under argon/nitrogen Low temperatures to prevent side reactions

		Slow addition or defined order of addition to control side reactions Dean Stark apparatus to remove water in condensation reaction
10	**Prior action** Take action beforehand to ease an event	Back titration e.g. add excess of EDTA then back titrate the excess with Ca or Mg. Adding UV stabilisers to prevent sun damage Addition of seed crystals to control crystallisation Crystal engineering by addition of additives, choice of solvent/conditions etc.
11	**Cushion in advance** Prepare for things which may fail or go wrong	Explosion prevention system Use of EDTA in fount solution to prevent precipitation of citrates/tartrates. Bursting discs on pumps. Cold finger traps when distilling
12	**Equipotentiality** Avoid lifting or lowering an object	Catalyses and enzymes Activating groups Use of automated methods for addition e.g. syringe pumps
13	**Inversion** Do it the other way round	Back titrations Reverse chromatography to measure surface properties Poisoning of crystal to prevent growth Sublimation instead of crystallisation
14	**Spheroidality** Replace linear with a curve or a sphere	Non-linear gradient for solvent mix in HPLC Nono-tube graphite and fullerenes Slowing coupling reaction toward the end to achieve a better end point
15	**Dynamicity** Create systems which are able to cope with change and intrusions from the outside – separating parts, flexible connections etc.	Remove aromaticity, double bonds etc to make a molecule more flexibly. Increase chain lengths to increase flexibility Use of plasticiser PH and redox buffers
16	**Partial, overdone or excessive action** Achieve more or less of the desired effect	Take reaction to 90% and then clean up rather that try to get 100% Add excess of reactant to push an equilibrium in the desired direction. Refluxing reaction mixture
17	**Move to a new dimension**	Comb copolymers

	Go upwards, sideway, around corners, rotate object, change viewpoint	Cross-linking polymers Dendrimers Branched rather than linear hydrocarbons Multi-layer effect pigments Cyclic rather than linear aliphatics
18	**Mechanical vibration** Shaking, vibrating, sound waves, ultrasound	Sonochemistry Photoinitiators, thermal initiators IR. Spectroscopy
19	**Periodic action** Pulsed action	Non-intrusive mixing
20	**Continuity of useful action** Carry out actions without a break	Continuous vs batch production Citric acid cycle React and distil final product in same apparatus
21	**Rushing through** Do things at high speed to reduce time for problems to occur	Kinetically controlled reactions Drown out crystallisation to produce a thermodynamically unstable polymorph
22	**Convert harm into benefit**	Use waste heat to pre-heat reactants Recover and use by-products of a reaction Immunisation
23	**Feedback** Introduce. If it exists, change it	Buffered systems pH controlled pump Thin layer chromatography to monitor reaction progress. Distil or otherwise remove side or by products to monitor progress of reaction
24	**Mediator** Use an intermediary object to transfer or carry out an action	Photoinitiators Steam heating Synergists on pigment surface Dispersant on pigment Grignard reaction Catalyst Phase transfer catalyst
25	**Self-service** Can your device do things for itself	Photochromic glass
26	**Copying** Use a simple, cheap copy	Amplification reactions Electron microscopy Molecular modelling
27	**Inexpensive short life (Dispose)** Replace expensive object with a	Disposable pipettes

	cheap one	Use excess of less reactive but cheaper raw material.
28	**Replacement of a mechanical system** Replace a mechanical system with a field	Sonochemistry Microwave reactions Use of a radioactive source in a smoke detector or a chemical reagent in a CO detector as opposed to some mechanical means of measurement.
29	**Use of pneumatic or hydraulic systems**	Use pressure rise to detect a runaway reaction. Use hydraulics for power when using flammable solvents Filter press
30	**Flexible films or thin membranes**	Vapour deposition of Cr to dissipate charge in Scanning Electron Microscope Interference colours Surface treatments Paints and inks
31	**Use of porous materials**	Filtration Zeolites Chromatography e.g. GPC – small molecules enter pores and so take longer to elute Osmosis Crystal growth limited with a pore of say a zeolite
32	**Changing the colour**	Titration indicators Photochromic lenses Carbonless copying Thermochromic thermometers
33	**Homogeneity** Increase? Decrease?	Block copolymers, comb copolymers Replace solvent blend with single solvent with same solubility parameters Phase transfer reactions Is it necessary to have reagents in one phase? e.g. solid state reactions avoid solvent or reaction between a solid and a liquid.
34	**Rejecting and regenerating parts** When a part is used and no longer needed throw it away, restore it or recycle it	Catalysis Silica gel for drying Ammonia recovery Recycling solvents e.g. recovery of toluene in gravure printing

35	**Transforming physical or chemical states**	Separation by distillation Precipitation Crystallisation Drying/evaporation Gas phase reactions Sublimation
36	**Phase transitions**	a to ß Copper Phtalocyanine Allotropes of sulphur Synthesis of volatile derivatives for gas chromatography or gas phase reactions
37	**Thermal expansion**	Explosives
38	**Use of strong oxidisers**	Bleaches Oxidising agents Oxidation at electrodes
39	**Inert environment**	N_2 blanket Co-solvents or inert solvents Vacuum
40	**Composite materials**	Surfactants Copolymers Alloys Nanocomposites – clays mixed with nylon give improved properties

* The term synergist/hyperdispersant is familiar to anyone working in the ink or surface coating industry. In principle, a dispersion of pigment particles in a liquid medium will tend to flocculate unless there is some stabilisation mechanism. In non-aqueous systems, this is achieved by adsorbing a solvent soluble chain onto the pigment surface. This creates a barrier which prevents particles from approaching close enough to interact. However, if the adsorbing chain is soluble, it will stay in solution and not adsorb onto the pigment. What is needed is an insoluble soluble surface treatment. The principle of segmentation is used by having a two part system. One part, the “synergist”, is insoluble and strongly adsorbs onto the pigment. This synergist contains polar groups. The dispersant consists of a soluble chain, with a polar end group. Overall, the dispersant is soluble in the medium, but the polar end group interacts strongly with the synergist and so is held close to the surface of the pigment. The soluble chain of the dispersant sticks out into the medium and gives a barrier to flocculation.

An alternative approach is to use ABA block co-polymers. The A blocks consist of solvent soluble chains, whereas the B block is insoluble. The B block will sit on the pigment surface and hold the A blocks in position to create the barrier.

Bibliography

Kirk Othmer Encyclopaedia of Chemical Technology, 3rd Edition. 1982. Wiley Interscience.

The Printing Ink Manual, edited by R.H. Leach & R.J. Peirce, 5th Edition. 1993. Blueprint.

Color Chemistry, H. Zollinger. 2nd, Revised. 1991. VCH.

Perry's Chemical Engineers' Handbook, Robert H. Perry, Don Green, 6th Edition. 1984. McGraw Hill.

Chemistry - The Central Science, 9th Edition, Brown, LeMay, Bursten & Burdge. 2003. Prentice-Hall.