

# Practitioner's Section

## Sources of Information for Technology Intelligence in Chemical Formulation

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This article delineates the chemical formulation field and presents the sources of information, formal and informal, related with technological intelligence in the design of chemical formulations. Furthermore elements are provided for technology strategy integration through the formation of technological maps. In addition relevant databases and web sites were identified: scientific, intellectual property, as well as industry and enterprise specific databases. A technologist must have a panoramic view of the information available and an understanding for the databases structure to conduct the required tests by using Boolean Searching techniques and taking advantage of iterative search strategies. With this, a technologist can choose those sources that are pertinent to chemical product formulation research projects.

### 1 Introduction

Intelligence is defined as the capacity to obtain and analyze information which facilitates decision making (Cohen, 1999). Technology intelligence (TI) detects opportunities based on early identification of emerging technologies or white spaces pertinent to a company's business interests. Moreover, it surveys the competitive landscape to identify areas with limited or no competition, which corporate strategy can exploit. Competitive intelligence (CI) tracks competitor activities to spot threats early; competitive technical intelligence (CTI) blends elements of both. Porter (2005) described a "tech mining" approach to generate CTI. Tech mining addresses managerial issues by deriving empirical knowledge, primarily from patent and research publication abstract databases. This article extends the resource base to be mined to information from the suppliers, book editors, norms and regulations available through the internet.

Technological intelligence systems have become a fundamental tool for organizations that manage R&D and innovation projects. The UNE166006:2006 EX (standard-Management of R&D and innovation: technological surveillance systems) systematizes the manner in which this activity is set up within innovation organizations. Muñoz et al. (2006)

describe the main processes required for the efficient development of this activity by information management professionals.

For the technology intelligence focus on chemical formulation presented here, we refer the reader to two references: the first one is related to the chemical formulation domain (Aubry and Schorsch, 1999). The second one, related with the field of technology intelligence, is Benavides and Quintana (2006). In effect, to avoid useless repetitions, we will take for granted that the person that wants to be familiarized with the techniques of technology intelligence in chemical formulation already knows the mechanisms of the formulation on one side, and the principles and tools of technology Intelligence on the other. This focus will enable us to go in this article to the essential thing, and to present the strictly necessary complements for the specific sources of information and development of technology Intelligence in chemical formulation.

#### 1.1 Some considerations regarding surveillance and chemical formulation

Chemical formulation, still considered today to be an art, increasingly needs a great quantity of multidisciplinary knowledge and has a multisectorial application. The term "formula" here does not refer to the molecular structure but the composition of

a mixture of chemical components which is often complex. In fact the formulation consists of the combination of several "active agents", and some auxiliary components that allow the mixture to have the precise charges, to satisfy a need - real or created - of a consumer. In general, the chemical design problem starts with a basic definition of the product's requirements and sets out to identify a chemical candidate that satisfies a specified set of properties and property values (Cussler and Moggridge, 2001).

The design of chemical-based consumer products, such as specialty coatings, detergents, personal care products and cosmetics, can be largely characterized by efforts to satisfy a unique combination of factors. Several examples of chemical product design approaches can be found in the literature (Hill, 2004; Ng et al. 2007; Wibowo and Ng, 2002) that may include empirical modeling of product properties. Models and simulations may be available but in many cases the formulation process had to be carried out in a design space that is multi-dimensional and difficult to conceptualize.

In the practice, formulation was initially centered on the basis of natural products, but soon organic synthesis the manufacture of new products with very specific physical and chemical properties, which takes us to another function of technological intelligence in this field: the scouting the suppliers of ingredients.

Finally, other aspects should be taken in consideration, such as the price of the active and auxiliary (functional) materials, shelf life, and preparation time (as determined by physical processes of dispersion, mixture, heating or cooling, etc.).

### 1.1 Principal industrial fields included by chemical formulation

Structuring the chemical industry around two variables, tonnage and formulation (OPTI, 2004), chemical production is broken down into four groups (see Table 1). The Formulation Chemistry subsector comprises Branded Commodities and a large share of Specialty Chemicals (as shown in the green-

Table 1 Industrial Fields in the Chemical Industry

Type	Definition	Manufactured and sold in amounts	Prices
Fine Chemicals	Pure and defined chemical substances, both intermediate and active principles, of high added value.	Less than 10 or 20-ton drums and smaller capacity containers	usually over 3 €/kg
True Commodities	Chemical molecules, highly pure, usually manufactured by a continuous process (ethylene, polyvinyl chloride, sulphuric acid, sodium hydroxide, chlorine, etc.).	Bulk selling	Less than 3 €/kg
Branded Commodities	Mixtures of chemicals of known formulation sold in bulk (household detergents, ornamental paints, cars lubricants, etc.) and in general, products for chemistry consumers.	Sold in bulk	Less than 3 €/kg
Specialty Chemicals	Mixtures of chemical compounds of high value (added cosmetic products, resins, surfactants, additives, dyes, and perfumes, generally speaking) Mixtures of chemical products for use in different chemical industrial processes (textiles, tanning, paper, metallurgy, steel making, construction, water treatment, etc.) as well as other non-chemical processes	Less than 10-20 tons in drums and small capacity containers	In excess of 3 €/kg

shaded areas). This classification will serve as an approximation to the databases.

Specialty Chemicals, also called functional chemicals, are complicated systems and formulations consisting of various components that sell because of their application-relevant properties. As opposed to commodities and fine chemicals, the customer does not purchase molecules, but rather an application-relevant effect; the product performance is achieved by means of targeted design of molecule systems. As a result of this development, the customer is provided with a "high impact additive" which has a very good price-performance ratio and which provides the essential component of his product.

The customer's requirements dictate the development of products and therefore very special customer-specific solutions will be developed in close cooperation with the customer. Because of this, functional chemicals can be described as problem solvers. The products that are developed cannot simply be substituted with competitors' products; in other words, the cost and risks associated with product substitution are high for the customer. Decisive for the successful marketing of the products is the kind of technology applied, and the implementation of targeted development of a solution specifically tailored to the customer's needs.

The formulator may also routinely access databases in search of previous formulations as well as make use of mathematical models. Design for preformulation development includes statistical design of experiments, allowing simultaneous evaluation of multiple factors and evaluation of interactions between factors. It is crucial to use advanced biophysical characterization techniques to evaluate the conformational stability of large molecules in addition to traditional methods for evaluation of chemical stability.

The implementation of intelligent software can also lead to significant improvements in knowledge generation and protection of intellectual property, cost reduction, training consistency, and improved communication. Rowe and Roberts (1998) reviewed the applicability of expert systems, neural networks, genetic algorithms and other intelligent software in product formulation for applications ranging from agrochemicals and aluminum alloys to pharmaceuticals and textile finishings, including an explanation of the technology involved and examples of two commercial software packages specifically developed for product formulation.

Based on the preceding considerations we can suggest that the scouting will be much easier to perform if those in charge of executing it have already been employed in the area of chemical formulation. The necessarily implied analytical

effort, accounting for the available sources of information in one or more fields of application, will ensure, besides the basic principles, the functionalities that it is necessary to take in consideration.

In this way, in relatively classic services of intelligence, the specializing documentation can be an important contribution. In the case of chemical formulation, the technologists themselves must perform the searches. The role of their knowledge in selecting sources of information, recognizing weak signs, analyzing the patents, etc., acquires utmost importance. It is then a field where tacit knowledge plays an important role. This also means that in the organizations where this tacit knowledge could be transferred, it becomes favored within the frame of informal information.

## 2 Strategic technology intelligence

After choosing a narrowly defined, strategically important topic, this is constituted as a technological front. The technologist will then proceed to carry out the "exploration route or technological intelligence" to arrive at the available information upon said topic. The route of exploration includes the following steps (at least):

- A. Aim for a professional level of knowledge.
  - A1. Compiling the catalogues of suppliers and competitors.
  - A2. Identifying competitive advantage attributes.
  - A3. Finding out the pertinent national and international norms and regulations.
  - A4. Understanding the books and articles related to the front.
  - A5. Determining the suppliers' knowledge. With all this information the technologist would be able to draw a map with the main technological dimensions and its professional marks, and to set the technological position of the business with regard to the most capable international competitor in each dimension. (See Figure 1).
- B. Discern the limits of the knowledge frontier.
  - B1. Reviewing existing discussions around new international norms and regulations.
  - B2. Compiling and analyzing patents.
  - B3. Compiling scientific and technological articles and locating them on the map.
- C. Envision possible directions for knowledge advancement:
  - C1. Making inferences about the dimensions which technological advance is likely to affect.
  - C2. Consolidating the net of consultants, mainly with expert university research assistants
  - C3. Performing technology

Figure 1 Technology Map

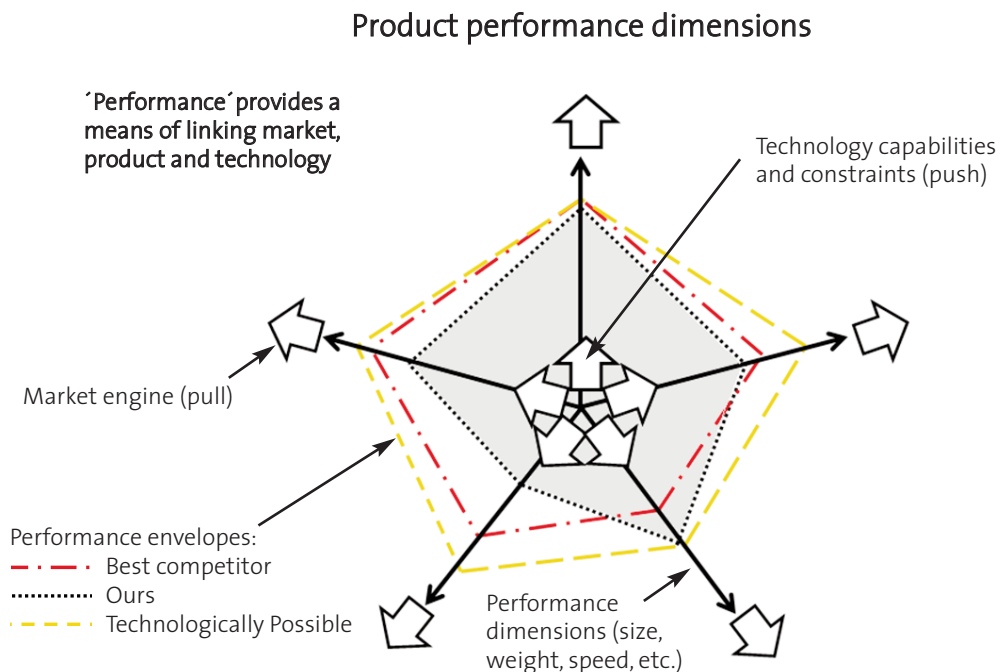
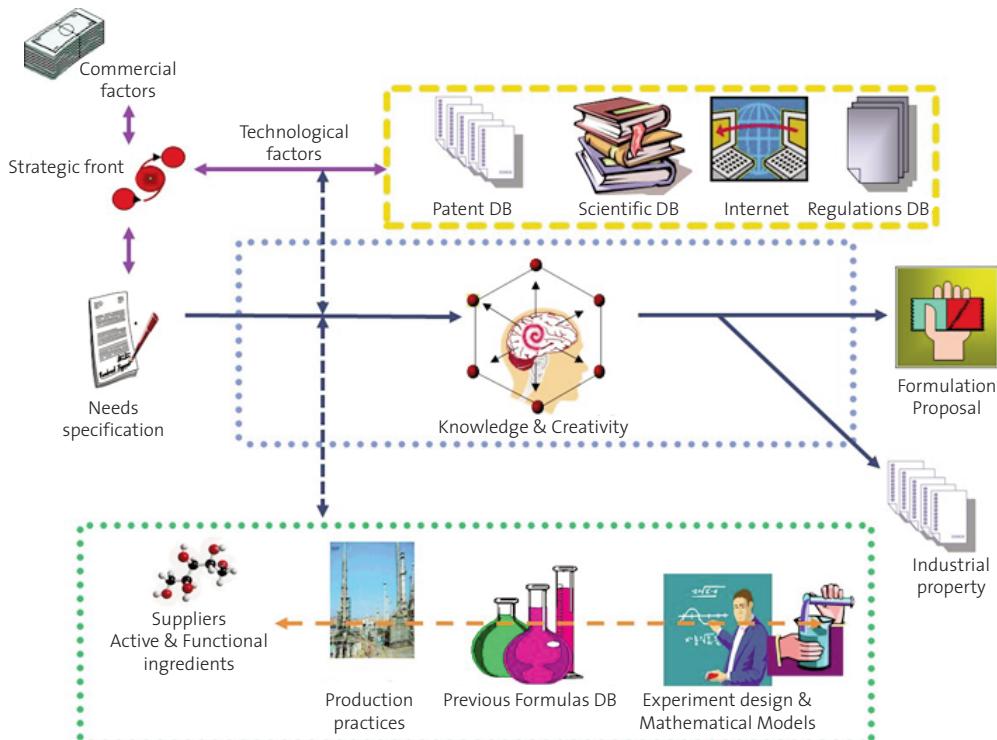


Figure 2 Chemical Formulation Information Flow



and market forecasts. C4. Simulating relationships among variables to increase the value of their dimensions, including finding relevant variables to measure and

to define their relation to one another so they can be manipulated to predict their behavior. C5. Carrying experiments to verify hypotheses.

Figure 2 illustrates the information flow in this process. The first step in knowledge acquisition is to collect all the potential sources of knowledge. These include written documents, i.e. books written specifically in the domain, research and technical reports, reference manuals, case studies, and even standard operating procedures and organizational policy statements.

### 3 Sources of formal information

#### 3.1 Scientific and technology publication databases (nonpatent)

Following is a non-exhaustive selection of the principal databases that are linked to chemical formulations. In order to exploit this list, it is necessary to relate each chemical specialization with a specific database. For a more advanced analysis, the reader should review in the catalog of that database its description, coverage, frequency of update, etc. For this, it is essential, starting from what we want to do, or the specific products investigated, or the physical-chemical interactions considered, to formulate one or various terms of search from different databases. From the results obtained a selection of the pertinent terms can be made. It should be borne in mind that the diversity of the formulation field and its transversality means that there is not a specific database in the area of formulation.

- CAS ([www.cas.org](http://www.cas.org)), a division of the American Chemical Society, is the most authoritative and comprehensive source for chemical information.
- The CrossFire Database Suite ([info.crossfiredatabases.com](http://info.crossfiredatabases.com)) consists of Beilstein, (organic chemistry), Gmelin (inorganic and organometallic chemistry), EcoPharm (pharmacology) and Patent Chemistry Databases.
- Based on The Landolt-Börnstein Database, Springer provides a resource for Physical and Chemical Data in Materials Science ([www.springermaterials.com](http://www.springermaterials.com)).
- Chemseer ([www.chemseer.com](http://www.chemseer.com)) offers a diary of chemistry conferences occurring

throughout the world. Also included are a number of valuable resource tools for chemists, including links to online chemistry and chemistry-related journals, links to some chemistry-related companies, chemistry related societies ([www.chemseer.com/societies/societies.shtml](http://www.chemseer.com/societies/societies.shtml)) and to UK academic establishments.

- CambridgeSoft's ChemFinder ([www.cambridgesoft.com/databases](http://www.cambridgesoft.com/databases)) searches hundreds of internet sites via a chemical name, CAS Registry Number, molecular formula, or molecular weight.
- There are many other sources of chemical information on the internet. Useful in discovering new ones are comprehensive guides to chemistry resources on the net, such as Chemdex ([www.chemdex.org](http://www.chemdex.org)) or ChemIndustry.com ([www.chemindustry.com](http://www.chemindustry.com)). Whereas the University of Liverpool's links for chemists ([www.liv.ac.uk/Chemistry/Links/links.html](http://www.liv.ac.uk/Chemistry/Links/links.html)) claims access to over 8000 sources. Knovel ([www.knovel.com](http://www.knovel.com)) provides information on a range of topics, including material selection and tolerances, heat transfer, coatings, corrosion, hazard related properties, environmental impacts, industrial hygiene and energy efficiency.

A selection of web sites with databases relating to the formulation of chemical products is:

[cds.dl.ac.uk/cds](http://cds.dl.ac.uk/cds)

[depth-first.com/articles/2007/01/24/thirty-two-free-chemistry-databases](http://depth-first.com/articles/2007/01/24/thirty-two-free-chemistry-databases)

[www.cambridgesoft.com/databases](http://www.cambridgesoft.com/databases)

[www.chemistryguide.org/chemical-databases.html](http://www.chemistryguide.org/chemical-databases.html)

[www.ddbst.com/en/online/Online\\_DDB.php](http://www.ddbst.com/en/online/Online_DDB.php)

[www.csa.com/e\\_products/databases-collections.php](http://www.csa.com/e_products/databases-collections.php)

[www.dialog.com](http://www.dialog.com)

[www.ovid.com/site/products/index.jsp?top=2](http://www.ovid.com/site/products/index.jsp?top=2)

[www.science.co.il/Chemistry-Databases.asp](http://www.science.co.il/Chemistry-Databases.asp)

[www.symyx.com/products/databases/index.jsp](http://www.symyx.com/products/databases/index.jsp)

[zusammen.metamolecular.com/2009/03/09/sixty-four-free-chemistry-databases-serialized](http://zusammen.metamolecular.com/2009/03/09/sixty-four-free-chemistry-databases-serialized)

We encourage the technologist to refer to other providers in order to obtain the corresponding list of databases and description.

It will be necessary to single out the databases that contain norms and regulations, especially those related to environmental issues, since they will limit the use of certain products in the formulation. We find in this list, besides types of chemical products, information about industrial, legislative, and environmental aspects of marketing and industrial property. We might also observe that if the databases are differentiated, there exist those linked to basic research (Chemical Abstracts, Inspec, Medline, Biosis Previews), and those linked to applications (Rapra for the polymers, Paperchem for the paper industries, WSCA for Coatings, etc.).

Sometimes it will be difficult to investigate the topic in the database. The following guide will save time in the search:

1. Begin with the Database subject guide.
2. Choose a subject area.
3. Start from the list of "key resources".
4. Read the database descriptions to decide which one to search. (Find out about update speeds, coverage, references format, if it provides summaries, keywords and descriptors.) Sometimes, you will have to search in two or three databases to find all the information you need.
5. When that is done, it is necessary to formulate keyword searches. From the obtained results a selection of the most pertinent databases could be done.

Example:

If one is interested in paints, the keyword "coating" may be used to search in the list of a commercial provider (for example Dialog <http://support.dialog.com/publications/dbcat>) for the databases that can respond to our search. We obtained, mainly:

- PRA's journals ([www.pra-world.com/business\\_services/journals](http://www.pra-world.com/business_services/journals)), specializing in up-to-date information on surface coatings worldwide.
- Encyclopedia of Polymer Science and Engineering ([onlinelibrary.wiley.com/book/](http://onlinelibrary.wiley.com/book/)

[10.1002/0471440264](http://10.1002/0471440264)).

- Smithers Rapra ([www.rapra.net](http://www.rapra.net)).
- TOXNET [toxnet.nlm.nih.gov](http://toxnet.nlm.nih.gov), providing access to a cluster of databases on toxicology.
- Advanced Polymers Abstracts ([www.csa.com/factsheets/ema-polymers-set-c.php](http://www.csa.com/factsheets/ema-polymers-set-c.php)).

### 3.2 A special database: Chemical Abstracts

Chemical Abstracts Service (CAS) is the world's most important abstracting and indexing service for chemistry and related disciplines. The main databases include Chemical Abstracts, which contains over 32 million document records from the chemical journal and patent literature, and the CAS REGISTRY, for substance information, which contains more than 54 million substance and 62 million sequence records.

SciFinder is integrated with STN's ChemPort Connection, which in turn links to the participating publishers' web sites for the full-text electronic journals<sup>1</sup>. It is the most thorough way of hunting for premium data because of the quality of their indexation and the coverage of the database. In fact, it systematically indexes most of the journals linked to formulation owing to its increasingly interdisciplinary nature. It takes into account chemical, physicochemical and sometimes biological aspects (for example Biosis).

Many electronic journal articles can also be accessed directly via the web from the references retrieved with SciFinder, provided the user is a subscriber to the journals. For more information on this subject it is necessary to consult the "Chemical Abstracts learning center" ([www.cas.org/products/scifindr](http://www.cas.org/products/scifindr); [www.cas.org/products/sfacad](http://www.cas.org/products/sfacad)).

### 3.3 Searching on databases

Databases are elaborated by different agents and therefore, the indexation methods, the key words used, and the codes, vary among them. Thus, it is often difficult to know all of them. By using Boolean Searching techniques, compounded with an understanding of database structure, and taking advantage of iterative search strategies, a searcher can use these systems to isolate technical intelligence which may otherwise be overlooked. Use of finder files is an essential part of a searcher's arsenal. In order to become confident in our surveillance,

<sup>1</sup>) The CAS Source Index (CASSI) Search Tool [cassi.cas.org](http://cassi.cas.org) is an online resource intended to support technologists and librarians who need accurate bibliographic information. Use this free tool to quickly identify or confirm journal titles and abbreviations for publications indexed by CAS since 1907, including serial and non-serial scientific and technical publications.

and especially to carry out tests, we advise to choose a body of pertinent references, then to dig up the same references in new databases by using different search strategies. Thus, by comparison, a good notion can be developed of how indexation works and of ways in which searches can be refined.

### 3.4 A special database: Chemical Abstracts

The patents are an essential information source in the domain of formulation. In fact, they allow connecting the research to the industrial plan. Bios provides a roadmap of U.S. Patent No. 5,723,765 ([www.bios.net/daisy/bios/204/version/live/part/4/data](http://www.bios.net/daisy/bios/204/version/live/part/4/data)) with explanatory text of the purpose and goals of each section. The U.S. patent is used as a model because of its well-ordered structure and because its format is similar to patents in other major jurisdictions (e.g., Europe).

The industrial property databases from commercial suppliers can become prohibitive for the small companies. In this perspective, usage of free databases on the internet is a better solution to facilitate the research and the downloading of the results. A directory of them is at [www.wipo.int/directory/en/urls.jsp](http://www.wipo.int/directory/en/urls.jsp). These free databases make it possible to run key term searches (an idea, a product's chemical name, data about a medicine) in an accessible manner. In our case, we generally use Espacenet ([ep.espacenet.com/?locale=en\\_EP](http://ep.espacenet.com/?locale=en_EP)) and PATENTSCOPE ([www.wipo.int/patentscope/en](http://www.wipo.int/patentscope/en)). But effective manual consultation of these databases is often long and does not allow to perform automatic analyses. For this reason (and to this effect), there exists software that affords automatic consultation of the databases (Porter and Cunningham, 2005 p.361), allowing for the creation of local data, and the simultaneous production of statistic representations.

The patents themselves do not feature any key words. Therefore, their interrogation is

special. For example, in the case of the Espacenet database, it is necessary to use terms that are present both in the title and in the abstract (always in English), classifications more or less truncated. The international classification of patents (IPC) is the most widely used. The European classification (EC) is more specific and it is rooted in the IPC (but uses more digits). One is often driven to use a mixture of classification and general terms, such as applicants, assignees, inventors, filing date, priority date and patent number.

The International Patent Classification (IPC)<sup>2</sup> system is organized hierarchically into sections, classes, subclasses and groups (main groups and subgroups), for the classification of patents and utility models, according to the different areas of technology to which they pertain. If one does not know the classes and wants to look for application domains, one can interrogate by using free terms from the summary or title and then obtain the relevant classes. There is an IPC natural language search at [www.wipo.int/tacsy](http://www.wipo.int/tacsy). Some advantages of using IPC searching are more complete results than text searching, independent of the language of the text and of changes in terminology. The main disadvantages are e.g. a more complex structure of classifications and the requirement of studying classification rules. We made a general search from the software PATENTSCOPE<sup>®</sup> Search Service ([www.wipo.int/patentscope/en](http://www.wipo.int/patentscope/en)). Table 2 shows the global IPC classes involved in the 147260 patents results of searching in PCT for: chemical AND formulation.

Patent information is downloaded from the USPTO and Espacenet databases. With this information, a local database of the project is produced. Software for patent analysis allows selections, presentations and possible correlations (histograms, graphs, charts and nets) to place the search in its context and to obtain the necessary information for the key patents. We show some accessible treatments

Table 2 Some Results from Patent Scope on the Search: Chemical and Formulation

Offices		MAIN IPC										
Name	No	Name	A61K	Co7D	Ao1N	Co7K	C12N	C11D	Co7C	Go1N	Co8G	C12Q
PCT	147260	No	50471	12927	6449	5793	4095	3858	3820	3023	2980	2281

<sup>2</sup> Assistance in the use of the Classification can be obtained in [http://www.wipo.int/export/sites/www/classifications/ipc/en/guide/guide\\_ipc\\_2009.pdf](http://www.wipo.int/export/sites/www/classifications/ipc/en/guide/guide_ipc_2009.pdf)

in the following paragraphs.

For example, applicant expertise correlation can be established if a matrix between applicants and IPC is built and a network of expertise is drawn from this matrix. In the same way, networks of applicants (when several applicants appear in the same patent) will show the related companies, etc. For instance, applicants may be correlated with IPC, which will produce a competency matrix, this allows determining the set of competencies of an applicant company in the field, or that of an applicant corporate group, determined by comparison of the common competencies and contrast between different ones.

A matrix of IPC against IPC will reveal the technological network of common patents; inventors with inventors will give the inventor network; and inventor with IPC will give the inventor competencies. Other comparisons can be made by cross-linking the set of available fields: applicants – inventors (what works and where), IPC - date of publication (technologies of the public domain), applicants - date of publication (applicants concerned with technologies of the public domain), etc. Working this way will also make it possible to develop other databases by keeping the original IPC and combining it with other terms such as different active ingredients or coadjuvants, etc. Dou (2004) shows how innovative thinking, comparisons, and value-maps can thus be achieved.

### 3.5 Chemistry books and journals related to chemical formulation

Journal abstracts from chemistry publishers such as Bentham, Elsevier, Springer and others, covering over 500 journals can be searched and accessed for free. Search by title and issue, or use the journal search engine for full-text search of abstracts across all journals ([www.chemweb.com/journals](http://www.chemweb.com/journals)).

The NIST Chemistry WebBook ([webbook.nist.gov/chemistry](http://webbook.nist.gov/chemistry)) contains data on gas chromatography, spectroscopic, ion energetic, thermophysical property, thermochemical for organic and small inorganic compounds, reaction thermochemistry for over 8000 reactions; IR, Mass, UV/Vis, Electronic and vibrational spectra. Data on specific compounds can be searched in the Chemistry WebBook by name, chemical formula, CAS registry number, molecular weight, chemical structure, or selected ion energetics and spectral properties.

Wiley presents information from Journals,

Backfile Collections, Online Books, Databases, and Reference Works, including the Encyclopedia of Life Sciences, Kirk-Other Encyclopedia of Chemical Technology and Ullmann's Encyclopedia of Industrial Chemistry ([www3.interscience.wiley.com/browse/?subject=CHEM](http://www3.interscience.wiley.com/browse/?subject=CHEM)), also available from Current Protocols® Laboratory Methods ([www.wiley.com/WileyCDA/Section/id-350192.html](http://www.wiley.com/WileyCDA/Section/id-350192.html)).

Other major editors with chemistry references are:

Cambridge University Press Chemistry  
([www.cambridge.org/us/chemistry](http://www.cambridge.org/us/chemistry))

Chapman & Hall/CRC Press  
([www.chemnetbase.com](http://www.chemnetbase.com))

Marcel Dekker  
([www.cplbookshop.com/glossary/G486.htm](http://www.cplbookshop.com/glossary/G486.htm))

Oxford University Press  
([ukcatalogue.oup.com/category/academic/chemistry.do](http://ukcatalogue.oup.com/category/academic/chemistry.do))

ScienceDirect Elsevier  
([www.sciencedirect.com](http://www.sciencedirect.com))

SciTopics  
([www.scitopics.com](http://www.scitopics.com))

Springer Verlag  
([www.springer.com/chemistry?SGWID=0-135-0-0-0](http://www.springer.com/chemistry?SGWID=0-135-0-0-0))

### 3.6 Chemistry books and journals related to chemical formulation

The chemical industry is a highly regulated sector which makes it necessary to be alert to new requirements continuously being incorporated in the formulation designs. The most important include the following:

- REACH is a new European Community Regulation on chemicals and their safe use. It deals with the registration, evaluation, authorisation and restriction of Chemical substances. The new law entered into force on 1 June 2007.
- The mission of the Environmental Protection Agency (EPA) is to protect human health and the environment (EPA's Laws & Regulations Quick Finder: <http://www.epa.gov/lawsregs>). The chemical and process information component of CTSA (Cleaner Technologies Substitutes Assessment) consists of nine data



gathering modules: Chemical Properties, Chemical Manufacturing Process & Product Formulation, Environmental Fate, Human Health Hazards, Environmental Hazards, Chemistry of Use & Process Description, Process Safety Assessment, and Market and International Information.

- The Food and Drug Administration (FDA) is responsible for protecting the public health by assuring the safety, effectiveness, and security of human and veterinary drugs, vaccines and other biological products, medical devices, food supplies, cosmetics, dietary supplements, and products that give off radiation. Of special interest is the Code of Federal Regulations (CFR), Title 21.
- National offices of standards and regulations, i. e. U.K. ([www.bsigroup.com](http://www.bsigroup.com)), Spain ([www.aenor.es](http://www.aenor.es)), France ([www.afnor.org](http://www.afnor.org)), Germany ([www.vde.de](http://www.vde.de) and [www.din.de](http://www.din.de)).
- Industrial Chemical Standards, i.e. ASTM ([www.astm.org/Standards/industrial-chemical-standards.html](http://www.astm.org/Standards/industrial-chemical-standards.html)), CENELEC ([www.cenelec.eu](http://www.cenelec.eu)), IEEE ([standards.ieee.org](http://standards.ieee.org)).
- The NIST Data Gateway ([srdata.nist.gov/gateway](http://srdata.nist.gov/gateway)) provides access to scientific and technical data produced by the US National Institute for Standards and Technology including free web databases, such as standards for chemical analysis, etc. The TRC Thermodynamic Tables - Hydrocarbons and the TRC Thermodynamic Tables - Non-Hydrocarbons are technical resources used extensively by the petrochemical industry. Authors in technical and scientific journals regularly cite the Tables as a reputable source of evaluated thermophysical and thermodynamic data ([trc.nist.gov/tables/trctables.htm](http://trc.nist.gov/tables/trctables.htm)).

While no method has emerged as dominant for evaluating and comparing chemical or material hazards, rather there exists a range of assessment methods and tools that are available for defining and comparing the hazards associated with chemicals. The Lowell Center's Chemicals Policy Initiative presents a comprehensive framework for alternatives assessment; and identifies tools and appropriate ways of assisting green chemistry innovation and safer supply chain management of chemicals ([www.chemicalspolicy.org/downloads/FinalAltsAssesso6.pdf](http://www.chemicalspolicy.org/downloads/FinalAltsAssesso6.pdf)).

#### 4 Informal Sources of Information

The domain of informal information is also

important. Nevertheless, we recommend to validate it before incorporating to intelligence reports. This domain comprises information from symposia, exhibitions, scientific meetings, workshops, reports of industrial corporations, advertisements, catalogs, etc.

##### 4.1 Scientific and technological associations

Scientific and technological associations are of great utility especially when there are approached complex or multidisciplinary fields, since it is possible to rest on sets of competitions. Scientific associations are a way of simultaneously obtaining information and personal contacts. There exist numerous scientific associations that organize congresses, jointly contribute information, produce scientific magazines, etc. Some of them are purely scientific, others have lucrative purposes. A large number of organisations are devoted to formulations—either making or analysing them, providing raw ingredients, manufacturing instruments to study them, creating jobs for formulation scientists, providing training, publishing literature, etc. At any rate, it is good to know them, to analyze their domains of competence and to take part or to monitor their production. Below are a few links from institutions that support or have formulation activities:

- The Societe Chimique de France (SCF), the Institute of Chemical Engineers (IChemE) and the Royal Society of Chemistry (RSC) have established new subject groups focusing on formulation to support both major businesses and the multitude of small businesses active in product formulation, process, design, and manufacture ([www.societechimiquedefrance.fr/fr/formulation.html](http://www.societechimiquedefrance.fr/fr/formulation.html), [www.icheme.org/communities/subject\\_groups/formulated%20product%20engineering.aspx](http://www.icheme.org/communities/subject_groups/formulated%20product%20engineering.aspx) and [www.rsc.org/Membership/Networking/InterestGroups/FSTG](http://www.rsc.org/Membership/Networking/InterestGroups/FSTG)).
- The DECHEMA Gesellschaft für Chemische Technik und Biotechnologie e. V. is distributing databases ([www.dechema.de/en/Publications/Databases.html](http://www.dechema.de/en/Publications/Databases.html)) covering different aspects of chemical technology, environmental protection and biotechnology. These systems are available as online and in-house databases.
- The Formulation School (UK) ([www.formulationschool.com](http://www.formulationschool.com)) and The Association of Formulation Chemists (US)

([www.afc-us.org](http://www.afc-us.org)) are a virtual cross-linking interface between industry and expertise within universities to help companies working in formulation to search for all the support services they need; contract research, contract manufacture, contract packaging, training, consultancy, analytical services etc.

#### 4.2 Information from suppliers

Many corporations that sell chemical products or mixtures of chemical products suggest various formulations which include their ingredients and additives. They put them to the service of their potential customers. Many examples exist: [www.happi.com/formulary](http://www.happi.com/formulary), [www.issa.com](http://www.issa.com), [www.cspa.org](http://www.cspa.org), BASF Formulation Assistance [www2.basf.us/performancechemical/bcperformulation\\_assistance.html](http://www2.basf.us/performancechemical/bcperformulation_assistance.html). Synapse information resources ([www.synapseinfo.com](http://www.synapseinfo.com)) constantly update a growing database which includes ingredients and additives of worldwide manufacturers.

#### 4.3 Free Internet Sources

There is a lot of available information on the internet. Note for example the information coming from laboratories of university researches, of special advertisings done for certain products, the forums of discussions, etc. This information, in contrast to the preceding one, will have to be validated.

Example:

The Indiana University School of Informatics built CHMINF-L, an Internet resource for keeping

up with new information products of interest to chemists and for getting answers to chemical information questions in general ([listserv.indiana.edu/cgi-bin/wa-iub.exe?Ao=chminf-l](http://listserv.indiana.edu/cgi-bin/wa-iub.exe?Ao=chminf-l)). There are still many examples of good web sites where reliable chemical information can be found at no cost: [www2.chemie.uni-erlangen.de/services](http://www2.chemie.uni-erlangen.de/services), <http://chem.sis.nlm.nih.gov/chemidplus> and [www.orgsyn.org](http://www.orgsyn.org).

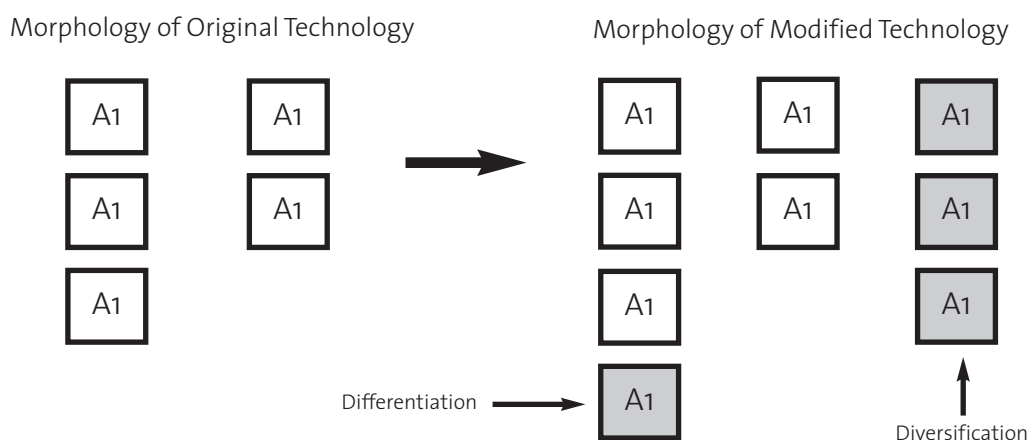
### 5 A creative use of technology intelligence

As we have seen, information is the essential ingredient for innovation. With this cognition the technologist will be able to think up ("incubate") other forms of classifying knowledge. Methodologies to apply creative thinking include the following (among others):

Quality Function Deployment (QFD) The procedure consists of five steps: First, the market research was conducted to determine the target segment. Second, the behavioral motives of the consumers in the target segment were analyzed. Third, product objective specifications were established through physico-chemical and instrumental methods. Fourth, sensory analyses were performed involving both consumer and trained panels. The last step of research relates to analysis of the mutual relations between technical and sensory measurements and integration of results in the House of Quality matrix (Seider, et. al 2009).

Systematic Inventive Thinking (SIT). Stern et al. (2006) describe case studies of the application of the SIT method, through the Function Follows Form work process, for the purpose of arriving

Figure 3 Morphology Analysis (Yoon and Park, 2005 p. 151).



at innovative product and technological solutions in the chemical industry.

Morphological analysis (Yoon and Park, 2005). The morphological analysis of claims in patents is based on the identification of occupied configurations on collected patents while the unoccupied configuration territory is suggested as a technology opportunity. Technologies can be analyzed to identify a technological breakthrough by revising the morphology of patents, which is achieved through two methods—differentiation and diversification. While differentiation is related with the extension of shapes, diversification is concerned with the extension of dimensions (see Figure 3).

Chemical formulation patents can be analyzed to identify ingredients in the protected formulation and the behavior (response) of such mixture (see Table 4). Furthermore, with data derived from technology intelligence, similar and substitutive ingredients can be proposed for the purpose of an innovative formulation with intellectual property possibility.

## 5 Conclusions

Even when we did not develop the technological intelligence within the frame of a specific formulation, a route to obtain desired information was determined as applied within the frame of chemical formulation. It is also necessary to point out that depending on the project that is going to be developed, or the ingredients to be used, the technologist will

have to re-cap the information and construct its data base constantly, because of the continuous evolution in this area.

In one sense, constant alertness should be exercised towards products offered by the suppliers of the ingredients, both actives and coadjuvants, as well as towards investigation work, and to competitors' products and packaging systems and applications, due to the fact that all of them have an important role to play in the product's marketing and usage plan.

The transdisciplinarity of the formulation sometimes requires expert feedback. This will in turn require at least two activities: consolidating a net of experts from chemical associations, and managing intellectual property in those cases where exchanging or sharing information is required.

We will do the same step for all the chemical terms in accordance with the schedule of conditions. According to the selected products, we will look at the toxic effects, etc. It should be noted also that it is necessary to search Chemical Abstracts to obtain the results upstream. But in this case the appropriate set of scientific vocabulary is required. We might use selected patents, and having retrieved them in Chemical Abstracts, move towards the fundamental one. It would also be necessary to test the commercial databases present in Dialog or DataStar in the domain of interest.

Technological alertness in the formulation domain will take time and might be relatively complicated, since it is evident that there is inevitable work to do, e.g. by selecting the most

Table 4 Methylene Chloride Free Paint Stripping Composition (US patent 7087565).

Halogenated hydrocarbon liquid, having more than one atom	Polar oxygenated organic liquid	Hydrogen bondable thickener
Conc. 40-90%	Conc. 0.1-20%	Conc. 0.01-20%
n-propyl bromide	hydroxilated alkanols	alkylated celluloses
1-chloro-2-methylbenzene	hydroxilated alkenols	alkylated silicas
1-chloro-4-methylbenzene	hydroxilated cycloalkanols	
1-chloro-4-(trifluoromethyl)-benzene	hydroxilated cycloalkenols	
1,2-dichloro-4-(trifluoromethyl)-benzene	ethers	
	ketones	
	esters	

important critical factors to monitor.

Last but not least, the competitors' products are a good information source. By reverse engineering their functionality, cost, etc. can be analyzed. While time-consuming, it may in certain cases be the least risky solution. The importance of the analysis and tacit knowledge of the specialists is then preponderant. The names of the different ingredients that are present in the product considered are also a precious assistance. In fact the legislation, in the domain of the food processing, cosmetics, pharmaceuticals, sanitary products, regulate the use of ingredients.

Creating Coincidental Product Evolution Case Studies of the Application of the Systematic Inventive Thinking® (SIT) Method in the Chemical Industry, *Journal of Business Chemistry*, **3** (1), p. 13-21.

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