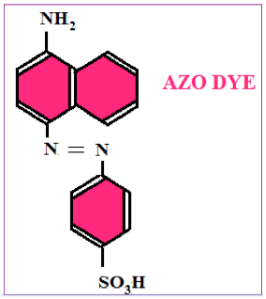
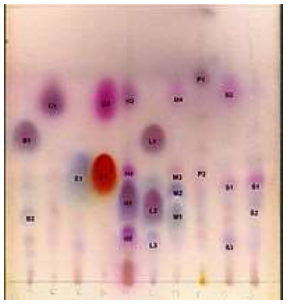
Irish Chemical News

The Journal of the Institute of Chemistry of Ireland

Feature Articles:-

Chemistry, the Law, Justice and the Maguire Seven





Improving Processes With Statistical Models

Irish Chemical News

The Institute of Chemistry of Ireland

PO Box 9322, Cardiff Lane, Dublin 2

www.instituteofchemistry.org

Originated 1922
Incorporated 1950

The Professional Body for Chemists in Ireland

Contents

A Message from the President.

Dear Fellows, Members, Graduates and Associates,

Since the last edition of Irish Chemical News was published in the Spring, we have had a busy calendar of events. The first was our Annual Congress, which was hosted by UCD on April 30th. The Congress 2015 theme was 'Asymmetric Synthesis' and featured presentations from distinguished researchers working in this field on this island. They included four contributions from the host University (Professor Declan Gilheaney, Professor Pat Guiry, Dr. Paul Evans and Dr. Francesca Paradisi), as well as presentations from Professor Karl Hale (QUB), Dr. Gerard McGlacken (UCC), Dr. Fintan Kelleher (ITT), Dr. John Stephens (NUIM) and Professor Mauro Adamo (RSCI). There were also a number of poster presentations. This was the 40th Annual Congress of our Institute and we thank Dr. Eoghan McGarrigle and his committee for organizing this very successful event. We also thank our sponsors: Labplan, Sigma-Aldrich, Mason Technology, Fisher Scientific, Lennox, Waters and Agilent Technologies.

On May 1st, The Institute of Chemistry of Ireland participated in a joint Awards Symposium with the Royal Society of Chemistry, at Queen's University, Belfast. The recipient of the 2014 Annual Award for Chemistry, Thorri Gunnlaugsson of TCD, gave the third of his Eva Philbin Award lectures during this symposium, after which I had the pleasure of presenting him with his award. The titles of his lecture was "Self-assembly supramolecular structures and material made from novel acyclic ligands". Thorri had already delivered his award lecture at two venues last year.

The Irish Universities Research Colloquium took place in NUI Maynooth on June 24th & 25th. This is always an interesting event, as it showcases the huge variety of research being conducted in our 3rd level institutions.

A packed programme of oral presentations, as well as poster sessions was given over the two days, showing that Irish Chemistry is alive and well and the future looks bright.

The Institute of Chemistry of Ireland is affiliated to EuCheMS, The European Association for Chemical and Molecular Sciences. As your representative, I attended the 2015 General Assembly of EuCheMS, which was held in Vienna on September 28th & 29th. This gave me a good insight into the activities of EuCheMS and its divisions and working parties. I also had the opportunity to make the acquaintance of the Presidents of other European chemical societies and the chairs of some of the divisions. There is a brief report on the General Assembly on the EuCheMS website and you can download some of the presentations here: http://www.euchems.eu/about/general-assembly/2015-vienna-austria.html

The Institute, as you may be aware, makes a number of awards in chemistry at various levels. At present, the two main awards for established chemists are the Eva Philbin Annual Lecture series and the Boyle-Higgins Award. The former is given to a distinguished chemist, of international repute, who may be based in Ireland or abroad. The recipient gives a public lecture in Dublin and at two provincial locations. Former winners of this award have included Sir Martyn Poliakoff, Baroness Mary Archer and Professor Peter Atkins.

The Boyle-Higgins Award is given to a distinguished chemist working in Ireland and who is a member of The Institute of Chemistry of Ireland, or to an Irish chemist working overseas. It is usually given for a lifetime contribution to chemistry, when the recipient is close to retirement. Previous winners have included Professor Thorburn Burns (QUB), The late Professor D.A. Brown (UCD) and Professor Dervilla Donnelly (UCD and DIAS)

This year, the Institute is introducing a new award, to be made to an Irish chemist who has made a significant contribution to Industrial Chemistry. Henkel is sponsoring the inaugural Industrial Chemist of the Year 2015 award and the name of the winner was announced at this year's Congress. The recipient is Donal Coveney, of TopChem. He will give a lecture at IT Sligo on November 11th, during Science week and he will also give his lecture at a joint awards seminar to be hosted by UCD on November 26th. The seminar will also feature the winner of the 2015 Eva Philbin Award for chemistry, which this year goes to Professor Michael Zaworotko, who holds the Bernal Chair of Crystal Engineering at The University of Limerick. Details of both of these awards and the programme for the awards night will be circulated shortly to all members and we hope that it will be well supported. The event is free of charge and is open to anyone who is interested.

To keep up to date with the institute and our activities, you are invited to visit the Institute website regularly at www.institute.org or www.chemistry.org and to engage with us on social media. You can find links to the Institute on Facebook, twitter and LinkedIn on the main website. If you have a suggestion as to how we might better serve our members, or if you would like to become more actively involved with our work, or serve on one of our committees,

please contact us. You may send an e-mail to the Institute at info@instituteofchemistry.org , or to my personal e-mail: mfranklin@eircom.net. If you prefer to write to us, the postal address is: Institute of Chemistry of Ireland, PO Box 9322, Cardiff Lane, Dublin 2.

I look forward to hearing from you.

Margaret Franklin, FICI, President. October 2015.

The Institute & Science Week Ireland 8 – 15 November 015

http://www.science.ie

The institute of Chemistry of Ireland has chosen 'Photochemistry' as the title for this year's Schools Newsletter competition, in order to highlight "The international Year of Light". (Crystallography was the theme last year, for the international Year of Crystallography)

Donal Coveney has been selected to receive the inaugural ICI Industrial Chemist of the Year award 2015 and will give one of his award lectures at Sligo IT during Science Week.

The Institute is also sponsoring the Schools science quiz during Science Week.

Again we thank our Congress Sponsors:-

Excellence is our Passion

Editorial

This is the second edition of Irish Chemical News (ICN) since I became editor. To me publication of our Journal is a critical and important activity of the Institute. We have managed to have 2 editions per year in the last 2 years but I really want this to become a quarterly publication over the next 2 years and then a bimonthly journal. For 2015 I aim to have 3 editions and I expect to have the third in December this year.

This is a challenge and in particular getting a bank of academic papers. Academics tend to focus on preparation of papers for publications in high prestige peer reviewed journals. I hope to accumulate a bank of academic papers so that I can publish ICN on a more regular and predictable basis.

Not to repeat myself too often I really want to encourage academics and especially post docs to make an effort to provide papers for ICN publications. This is an opportunity to inform a mainly Irish chemical community of the wide range and important chemistry research work being undertaken in Irish Universities, Institutes of Technology, and research institutions. After all a lot of Irish and European tax payers money goes into funding the research work.

The story is similar with our pharmaceutical and chemical industry. Given the successes of IDA, Enterprise Ireland and SFI Ireland has an enviable success story to tell. Again I call on industrial chemists, and hopefully CEOs will encourage and support my call, to seriously consider telling us of some of the great successes you have. We are trying to encourage industry chemists to become more visibly involved and enhance the profile of chemists in Ireland. We have our inaugural winner Donal Coveney founder of TopChem based in Sligo who will deliver a lecture in Sligo IT on November 11th and UCD later on the 26th. He will also provide a paper for ICN. This award is generously sponsored by Henkel Ireland. As this is the first time we have made this award The Institute very much welcomes feedback from industry as to what format it should take and whether it should be individuals or groups. We would welcome more companies to come in and support awards for chemists which may lead to more than one award.

The lead paper in this issue is Part 1 of a two part paper on how chemistry can aid Justice in the Criminal Justice System. It's a paper by Dr **Seán Ó Muircheartaigh** titled **"Chemistry and Law - complementary sciences".** Seán O'Muircheartaigh advised the Birmingham Six defence on the legal and scientific shortcomings of Dr. Skuse's evidence. He further indicated that there was no other substantive evidence produced. This resulted in the prosecution withdrawing this critical evidence and contributed to their release.

I have started sourcing articles from other journal sources and companies offering services/products. We have an article in statistical modeling, a profile of an Irish company Innopharmalabs, and a general interest article on Pyrex which was 100 years old this year.

As China emerges as a major player on the world stage, there is increasing cooperation between China and Ireland. I have a paper on The International Strategic Collaboration Programme- China (ISCP China) originating with Maynooth University. This enabled a half day Workshop at Maynooth and a two day Symposium hosted between TCD and the RSCI with some 42 speakers delivering a range of lectures on diverse topics.

While President early last year the Institute was approached by representatives of a Yunnan Province Government delegation to see if we would facilitate them to discuss the safety, storage and transport of hazardous chemicals. With my experience in China and after some consideration by Council and with vital support from Henkel Ireland we agreed to facilitate the delegation. The meeting took place in Henkel R&D Tallaght on Friday 16th of October 2015. A short report is included on the event.

Patrick Hobbs MSc, FIFI, CChem, CSci, MRSC.

Editor ICN,

Immediate Past President.

Donal Coveney:TopChem
Henkel Industrial Chemistry
Award 2015

"Jumping through hoops and chasing our tails – challenges in securing market approval of pharmaceutical products".

TopChem Pharmaceuticals develops generic pharmaceutical products mainly for the US market. While these products are known chemical entities, we develop our own synthetic processes, delivering high quality pharmaceutical grade active ingredients. In this we face many challenges. Even though most of these products have been on the market for many years, as a new entrant we are quite rightly judged by the highest standards. This leads us to into a labyrinth of analytical investigations in an effort to track and trace potential impurities. This lecture will focus on some case studies, which touch on synthetic and analytical challenges encountered in our product development.

Michael Zaworotko
Bernal Chair of Crystal Engineering, UL.
ICI Eva Philbin Award 2015

"Crystal Engineering of Task-Specific Materials: Addressing Pharmaceutical Materials"

That composition and structure profoundly impact the properties of crystalline solids has provided impetus for exponential growth in the field of *crystal engineering* over the past 20 years. This lecture will address how crystal engineering has evolved from structure design (form) to control over bulk properties (function). Strategies for the generation of ***multicomponent pharmaceutical materials, MPMs***, which can serve as drug substances, will be highlighted by three case studies, including one that addresses brain bioavailability of lithium.

The Institute of Chemistry of Ireland

Awards Seminar

Thursday 26 November 2015

O'Brien Science Centre, UCD

Henkel Excellence is our Passion

The Awards

The Eva Philbin award

The Institute of Chemistry of Ireland Annual Award for Chemistry was inaugurated in 2005. It recognises the major contribution to chemistry of individuals who also have an excellent reputation for communication. The recipient presents a keynote lecture in several locations in Ireland. Since 2007, the lectures are termed the Eva Philbin Lecture Series.

The Industrial Chemistry Award

This is a new award, which in 2015

is being sponsored by Henkel.

It recognizes the major contribution to industrial chemistry made by a chemist working in Ireland.

Institute of Chemistry of Ireland Awards Seminar.
UCD Belfield Campus, November 26th 2015.

Location: **UCD O'Brien Centre for Science, Intel Lecture theatre H1.26**

PROGRAMME

Henkel Excellence is our Passion

5.30 Welcome & Coffee/Tea

6.00 ICI Industry Award Lecture Sponsored by Henkel: Dr Donal Coveney
Title : **Jumping through hoops and chasing our tails – challenges in securing market approval of pharmaceutical products".**

7.00 ICI Eva Philbin Award Lecture: Prof Michael Zaworotko
Title: "Crystal Engineering of Task-Specific Materials – Pharmaceutical Materials".

8.00 Wine Reception

For more information visit www.waters.com/upc2

or contact

0208 238 6100 and ask to speak to a Waters Specialist

UCD School of Chemistry Seminar Programme 2015-2016

*_**Seminars will take place in room <u>S3.56</u> unless otherwise indicated**_

Pre-seminar coffee and tea will be served 15 minutes before the seminar behind the glass wall on the third floor (A3)

Wed 23rd Sept 2015 4.00 pm	**Professor Bill Baker, University of Florida** Title: *'Marine biodiscovery - New Chemistry for Old Diseases'*
Thurs 1st Oct 2015 4.00 pm	**Professor Robin Bedford, University of Bristol, UK** Title*: 'Casting Iron in New Catalytic Roles'*
Wed 14th Oct 2015 4.00 pm	**Professor Mike Towrie, Rutherford Appleton Laboratory, SFTC, UK** Title: *'Lasers in Chemistry, Making Molecules React*'
Fri 23rd Oct 2015 4.00 pm	**Professor Adam Lee, Aston University, UK** *Title:'Nanostructured Catalysts for Sustainable Chemical Transformations'*
Fri 30th Oct 2015 4.00 pm	**Professor Kimberly Hamad-Schifferli, MIT, USA** Title: '*Engineering the Nano-Bio Interface for Biomedical Applications'*
Mon 2nd Nov 2015 4.00 pm	**Professor Samir Zard, École Polytechnique, Université Paris-Saclay, France** Title: TBA
Wed 4th Nov 2015 4.00 pm	***Professor Charlotte K. Willans, University of Leeds, UK*** Title: *'N-Heterocyclic Carbenes: Synthesis, Activity and Reactivity'*
Fri 6th Nov 2015 4.00 pm	**Professor Eva Rentschler, Johannes Gutenberg Univ Mainz, Germany** Title: '*3d/4f Metallacrown Complexes as Molecular Magnets'*

Early November Date TBA	**Professor Don Craig, Imperial College London, UK**
Mon 16th Nov 2015 4.00 pm	**Professor Michael Grätzel, École Polytechnique Fédérale de Lausanne, Switzerland** *Title: 'Mesoscopic photosystems for the generation of electricity and fuels from sunlight'*
Wed 18th Nov 2015 4.00 pm	**Professor Stephen Daly, UCD School of Geology** Title : *'Geochemistry and Mineralogy of Uranium'*
Wed 26th Nov 2015 5.30 pm	ICI Eva Philbin Award Lecture, **Professor Mike Zaworotko** (UL) ICI Industry Award Lecture, **Dr Donal Coveney** (TopChem)
Early December Date TBA	**Professor Lopez-Ortiz, University of Almería, Spain** Title: TBA
Fri 11th December 2015 - Full Day	CSCB Symposium Details TBA see below

RCSI

The Centre for Synthesis & Chemical Biology (CSCB) will be holding its 14th annual symposium,

'Recent Advances in Synthesis and Chemical Biology XIV',

Friday 11th December 2015 in the Royal College of Surgeons in Ireland.

Plenary lectures will be delivered by five international experts:-

Professor Jane Clarke,

Professor Nils Metzler-Nolte,

Professor Norio Shibata,

Professor Stephen Clarke,

Professor Miquel Pericas.

Further details will be available on the RCSI website in due course.

Portable benchtop NMR spectrometer from GPE for Fluorine, Proton or Dual NMR

The spectrometer offers spectroscopic resolution at a fraction of the size and maintenance of current NMR instrumentation. The design brings analytical performance and point-of-need utility to the benchtop, fume hood or glovebox due to the compact size of the machine.

The NMReady was the first 60 MHz spectrometer available on the benchtop NMR market. Given its small footprint (Dimensions: 9.5 x 11x 17 inches) and light weight nature (only 45 lbs), the spectrometer is ideal for incorporation directly into the laboratory. The NMReady is compatible with all standard consumable 5mm NMR tubes, also available from GPE Scientific, so sample preparation is simple and fast.

The machine offers good sensitivity and the high resolution allows spectra to be measured quickly. The data can be processed directly (even while wearing safety gloves) through the built-in resistive touchscreen without connecting an external computer.

Contact Information:

GPE Scientific Ltd, Unit 5, Greaves Way Industrial Estate, Stanbridge Road, Leighton Buzzard, Bedfordshire, LU7 4UB. UK.

Phone: +44(0)1525 382277

E-mail: info@gpescientific.co.uk

Website: http://www.gpescientific.co.uk/products/chemistry/nanalysis-nmready-benchtop-spectrometer

Company Information:

GPE Scientific Ltd was established in 1962 and is a leading distributor and manufacturer of laboratory equipment, glass blowing products and specialised glass components for the industrial, laboratory and research markets. There are many reasons to choose GPE Scientific above our competitors; we pride ourselves in stocking thousands of products from leading suppliers providing you with the best selection of laboratory equipment on the market. This includes being the exclusive distributors for Chemglass Life Sciences and Chemical Reactors, Norell NMR Tubes and Accessories and the portable Nanalysis NMReady Benchtop Spectrometer.

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

School of Chemistry Faculty of Engineering, Mathematics and Science

SEMINARS 2015-16: First semester Date	Speaker	Title
1-10-15	Prof. Donal O'Shea Dept. of Pharmaceutical & Medicinal Chemistry RCSI	Real-Time Near Infrared Fluorescence Imaging: research tools with the potential for clinical use
8-10-15	Prof. Michael E.G. Lyons School of Chemistry TCD	Adventures in electrochemical water splitting
15-10-15	Prof. John P. Lowry Dept. of Chemistry NUI-Maynooth	Psychoanalytical Chemistry: Sensors and Behaviour
22-10-15	Prof. Catherine S. J. Cazin School of Chemistry, University of St. Andrews, UK	*N*-Heterocyclic carbene transition metal complexes: User-friendly catalysts for the synthetic organic chemist
29-10-15	Prof. Siddhartha Sen School of Mathematics TCD	Emergence of Spontaneous Coherent Mesoscopic Structures
5-11-15	Prof. Eva Rentschler Institute of Inorganic and Analytical Chemistry Johannes Gutenberg Universität Mainz, Germany	3d/4f Metallacrown Complexes as Molecular Magnets
12-11-15	Prof. Peter Robertson School of Chemistry and Chemical Engineering Queen's University Belfast, UK	The Photocatalytic Destruction of Cyanotoxins in Water
19-11-15	Prof. Christian Brueckner Department of Chemistry University of Connecticut, USA	The Breaking and Mending of Porphyrins: Synthesis of Porphyrin Analogues Containing Non-Pyrrolic Building Blocks
26-11-15	Prof. Mari-Luz López Rodríguez Depto. Química Orgánica I, Universidad Complutense de Madrid, Spain	Expanding the potential of druggable GPCRs
3-12-15	Prof. Leigh Jones School of Chemistry Bangor University, UK	Which is more fun? Synthetic Control vs. Serendipity in Molecular Magnetism
10-12-15	Prof. Paul H. Voorheis School of Biochemistry & Immunology TCD	Protein Folding Mechanisms: The Role of Surface Structures

Global Experiment Day Science Week Ireland

The RSC has a big event planned for Science Week in Ireland, and you can get involved. In partnership with Pharmachemical Ireland, we are putting Ireland on the RSC Global Experiment map for 2015!

The simple experiment on hydrogels engages people of all ages with science and chemistry, so, on Tuesday 10th November 2015, Global Experiment Day we want as many people as possible carrying out the experiment and uploading their results to the world map

What can you do? Options include:

- Approach a local school or community group, volunteer your services as a chemistry advocate and go along on the day to help them with the activity.
- Spread the word in person and online, using the hashtag #GlobalExpDay.
- Carry out the experiment with family members and upload your results to the official website.

Everything you need to find out about the global experiment is on the website including how-to videos lots of detail and extension ideas. Our regional Education Coordinators John and Stephanie are also on hand to support so feel free to email John.odonoghue@tcd.ie or s.nelson@qub.ac.uk to discuss your plans or ask any questions that you might have. They are both also on Twitter - @johndhodonoghue and @sosciencecsteph.

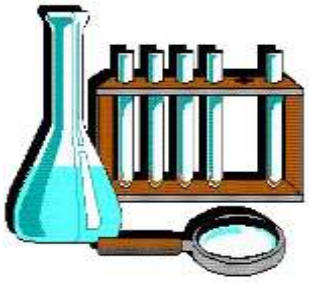
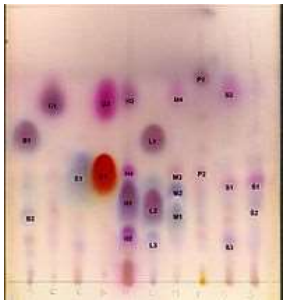
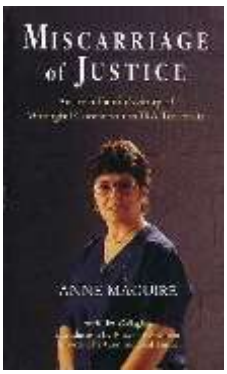
Face to face training and discussion sessions in Dublin and Cork have been set up, to help you get the most out of the day. You'll have a chance to practice the experiment, get tips on the questions to ask to get people thinking, and discuss strategies for varying or extending the exercise. You'll also get to socialise a bit with other members over tea/coffee and biscuits.

Session Type	Venue	Date	Time
Training and questions	University College Cork, Room G20, Kane Building	Wednesday 28th October 2015	12-1pm
Training and questions	Carrigaline Court Hotel, Cork	Wednesday 28th October 2015.	4.30-7.30pm
Training and questions	Trinity College Dublin SSR Room Main Chemistry Building	Thursday 29th October 2015	1-2pm and 6-7pm

Session Type	Venue	Date	Time
GE day main event	Limerick Institute of Technology Sports Hall	Tuesday 10th November	9am - 3pm (2 sessions)
GE day event	University College Cork, Primary Schools Quiz	Tuesday 10th November	6pm-8pm

Please register for a place at any of the participation or training events, by emailing Angela (mckeowna@rsc.org). Sadly, places are limited, so please register as soon as you can.

"Chemistry and Law - complementary sciences". Part 1

Seán Ó Muircheartaigh, B.Sc. PhD., MBA, LLB, F.I.C.I. Hugh Ryan gold medalist 1965 (UCD). Retired lecturer RTC Galway / GMIT; (1973-2009); ex Pfizer research and development chemist (1969-1974).

Chemistry and Law - complementary sciences.

This paper investigates how seven persons of Irish origin were convicted of terrorist offences and spent long terms of in British jails for crimes they did - in the opinion of many – not commit. The Maguire legal case was overshadowed by that of the Birmingham Six, as the Maguires had served their sentences and (with the exception of Giuseppi Conlon who died in prison) had been released whereas the Birmingham group were sentenced to spend the rest of their lives in prison.

The Maguire case continued in the courts from 1974 to 1992. A judge and jury convicted them initially and it took three Law Lords to partially exonerate them in 1992. At least seven of the top forensic / analytical scientists in the world assisted the courts in their deliberations.

Preliminary:

This legal case is one of the most important forensic case of all time. Subsequent to the release of the Maguire Seven, an Inquiry was set up by the British Government under Sir John May to review the issues involved. This took about four years to complete at a cost of £2.14 million pounds sterling to the British taxpayer. Sir John appointed a subcommittee to thrash out the science of the case under Professor T S West. The deliberations of this Inquiry were referred to in the Judgement of the Court of Appeal in 1992.

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The Facts:

[COA (unrevised = draft) judgement: Much of the details given in this paper were obtained from a draft unrevised judgement of the Court of Appeal. This differs significantly from the final judgement and this fact is to be acknowledged. This may well have been a preliminary document circulated to all parties before final judgement was delivered. All relevant documentation was supplied on request to the author as honorary forensic adviser to the Birmingham Six.]

"On 4 March 1976, in the Central Criminal Court, Anne Rita Maguire, Patrick Joseph Maguire, Patrick Joseph Conlon, William John Smyth, Vincent John Patrick Maguire, Patrick Joseph Paul Maguire and Patrick Joseph O'Neill were each convicted of a separate count charging an offence contrary to S4(1) of the Explosive Substances Act 1883. The particulars of each count alleged that on a day between 1 and 4 December 1974 the defendant knowingly had in his or her possession or under his or her control an explosive substance, namely

nitroglycerine, under such circumstances as to give rise to a reasonable suspicion that he or she did not have it in his or her possession or control for a lawful object.

The sentences were as follows: Mrs. Maguire 14 years, Patrick Maguire 14 years, Conlon 12 years, Smyth 12 years, O'Neill 12 years, Vincent Maguire 5 years and Patrick Maguire junior 4 years' detention.

All the defendants sought leave to appeal against conviction and sentence. On 30 July 1977 this court dismissed all the applications for leave to appeal against conviction. Leave to appeal against sentence was granted to O'Neill and his sentence was reduced to eight years. Otherwise the applications for leave to appeal against sentence were refused.

On the 23rd January 1980 Mr. Conlon died while serving his sentence."

The Crown's case at the trial:

"The Crown sought to establish that each of the male applicants had nitroglycerine (NG) on their hands. For this purpose they relied upon the factual evidence of the TLC tests given by Mr. Elliott and the opinion of Mr. Elliott, Mr. Higgs and Dr. Hayes that these results showed that the substance was NG. ….

... that the results could not be confused with a non explosive substance which might mimic the results on the TLC……..

… that NG could not have got there innocently ..that the presence under the nails of traces of NG was only consistent .. (could only have got there) ..by handling or kneading of explosive…."

…"the case against Mrs. Maguire was based on the positive tests on the gloves…."

Discussion:

****

The first step in examining this verdict is to state that the evidence which convicted Mrs. Maguire was, in the author's opinion totally absurd. There was no close causal connection between the gloves and Mrs. Maguire. If the gloves had NG on them, there is no basis to say that Mrs. Maguire was responsible. Apart from this, the test was carried out by a seventeen year old apprentice technician who - it would appear - had no formal qualifications in chemistry.

****

"There were two distinct factual issues at the trial and appeal:

Firstly - was the substance on the male appellants hands and Mrs. Maguire's gloves nitroglycerine (NG)?

Secondly, if so, could there be an innocent explanation for the presence of the NG? It is implicit in the Jury's verdict that they answered both issues against the appellants.

……. the case really depended on the scientific evidence and as the judge told the Jury (i.e. in the original trial), they could not convict unless they accepted it".

[A description of the original trial is to be had online, as are the John May Inquiry reports (interim, second and final). The final judgement is also on the internet.] There was considerable disquiet about the verdicts, and eventually the case was referred back to the Court of Appeal by the British Secretary of State. The Court of Appeal indicated that it had the task of deciding whether or not the original judgement was safe and

satisfactory. The Court emphasized that it was neither appropriate nor possible to carry out a retrial, especially as a key witness – Mr. Elliott - had died. Nevertheless the court indicated it would allow the defence to argue any grounds of appeal they wished.

The Court of Appeal therefore considered *inter alia* whether the spots found on the TLC plates were NG; whether it was possible that there was another non-explosive substance which mimicked NG; whether there was material irregularity because of non disclosure of evidence in the trial; the relevance that PETN (another explosive) was indistinguishable from NG using the TLC test and that this was known by prosecution but not disclosed to the defence at the trial; the issue of accidental contamination of the hands of the accused and

Whether contamination occurred before testing took place or in the laboratory during analysis.

Although the court of appeal had said it was allowing the appellants to argue all new points, it overruled nearly all of them on the basis that no new substantial evidence had been produced. Therefore, the issues being discussed had already been decided by a court and / or jury, and the matter was therefore "res judicata" – i.e. - the matter had been decided.

Firstly: was the substance on the male appellants hands and Mrs. Maguire's gloves nitroglycerine (NG)?

"….are we satisfied that the results showed that the substance was NG?

Extensive experiments were done by both the RARDE scientists and My Yallop (defence expert and former retired head of laboratory at RARDE) with a view to seeing if any other substance could be confused with NG in the TLC test. Those tests have continued after the trial. Nothing has been found. Professor Thorburn Burns said the search had been "not undiligent" He put it this was in his report:

'Any compound having a false positive reaction must have the following characteristics:

- persist on hands
- be ether extractable
- chromatograph with an R_f close to NG
- Hydrolise to nitrite ion under the same of similar conditions than does NG
- Despite extensive laboratory based laboratory searches prior to trial at RARDE and by Yallop and since, no such compound has been reported other than PETN and EGDN. I discount EGDN which appears always with NG.'

This evidence is unchallenged.

[P4 COA unrevised]

> ……..
>
> Moreover, as we have said, in spite of diligent search, substance X has not been discovered. In our judgement ….. based on all the evidence in the case, the substance was NG (nitroglycerine)."
>
> [P31 COA unrevised]

Secondly, if so, could there be an innocent explanation for the presence of the NG

[West Committee conclusions: (May, 2nd report p9)]:

"Conclusions on accidental contamination of Maguire samples in 1974.

… We have attempted to summarise briefly the reasons for and against thinking that contamination might have arisen from various sources. Opinion varied in the committee largely because of the absence of incontrovertible data against which to test the various hypotheses we advanced and perhaps because of the different weights given by members to what was available.

The committee counsels extreme caution over any attempt to translate this speculative review into actual probabilities of contamination thus to explain the original results. Whilst in respect of a number of possible contamination sources opinion was divided between those committee members who felt that contamination was likely or highly likely and those who felt it was neither, those that took the latter view accept the view that the possibility of contamination cannot be absolutely excluded"

Confirmation that nitroglycerine could be transferred innocently from a contaminated towel to the hands of innocent users: (from court of appeal final judgement):

[His Lordship then referred to the evidence of Mr. Elliott and Mr. Higgs and continued:] In the course of the May inquiry Professor Thorburn Burns carried out a number of experiments with the assistance and co-operation of the scientific advisers of the Crown and the appellants. It is necessary to describe some of these experiments.

"The professor took a new cartridge of Gelamex which contained about 30% nitroglycerine, he unwrapped it, handled it and squeezed it in his hands and returned it to storage. He then washed his hands fairly briefly with soap and dried them on a well used but freshly laundered hand towel. After handling some mugs and glasses he rifled his hands through a box containing plastic gloves. Four subjects C, D, E and F then washed their hands and dried them on the towel. The results, shown in nanograms (ng) of nitroglycerine were as follows:

	Right Hand	Nails	Left Hand
C	24,900	717	17,300
D	13,900	68	5,500
E	5,500	388	4,399
F	6,200	93	11,200

These results came from swabs taken immediately after contamination. They do not therefore allow for the effects of delay. It is clear however that substantial quantities can be transferred to the hand of those subjects from the towel "

The scientific witnesses who gave evidence at the trials, appeal and May Inquiry / West Committee: (ref COA)

Mr. Elliott: (trial only: died some years before Appeal)

Senior Scientific Officer. Presumably well qualified and probably FRSC. "His honesty was never questioned at the trial, his opinions were. He is described by those who knew and worked with him as meticulous and a fast experienced worker who took great care in the work.

Mr. Wyndham He joined the forensic laboratory of that establishment in 1974 a few months before the tests were carried out in connection with this case. He was 17 at the time. (He carried out the analysis on Mrs. Maguire's gloves). He would not appear to have any qualification in chemistry – even A level. He was possibly a part time student at the time. There appears to be no evidence he carried out test wrongly but he was clearly grossly inexperienced and unsuitable for such a critical analysis.

Mrs Brooker (Kemp): "Mrs. Kemp was a scientific officer. She joined the forensic laboratory in 1973 and left in 1977. She had an 'A' level in chemistry and is obviously a responsible person who was competent to carry out TLC tests. She judged the results herself and was competent to do so."

"Mr. Higgs was a Fellow of the Royal Society of Chemistry and a chartered chemist. He began work with RARDE at the age of 16 working on explosives at Fort Halstead. He went to Woolich in 1973 and took over from Mr. Yallop as head of the forensic laboratory there. … He was a very knowledgeable about explosives, particularly those used by terrorists**. He himself had not done TLC tests, but was well aware of the theory and practice of them.**"

Dr. Hayes was a careful and impressive witness He joined the forensic laboratory at RARDE in July 1974. He held the degrees of B.Sc. in chemistry, Master of Science, and Ph.D. in forensic science. He was also a chartered chemist and a member of the Royal Society of Chemistry.

Professor Thorburn Burns He would appear to be a forensic adviser to the Court of Appeal. He was also a key scientific adviser to the May Commission and West committee. He could be considered a neutral "honest broker" type of expert to give impartial evidence. He was awarded a multitude of awards including the Boyle Higgins gold medal of the Institute of Chemistry of Ireland in 1990. He was professor of analytical chemistry in Queens University Belfast.

Professor T.S. West CBE, FRS: Professor of Analytical Chemistry in the Imperial College in London. He set up a world famous research team that pioneered atomic absorption and atomic fluorescence spectrophotometry. He chaired the scientific committee that examined the science of this case for the May commission. Unquestionably one of the great British scientists of the 20th century. Decorated (CBE) for his contribution to Science.

Dr / Professor Brian Caddy Lecturer and subsequently professor of forensic science in Stathclyde University, the UK's top academic institution of forensic science. Consultant to appellants i.e. Maguire 7.

Dr J B F Lloyd Ph.D DSc. OBE – decorated (OBE) for his contribution to forensic science; retired from the Home Office Forensic Science Service and private consultant to appellants.

Dr Marshall Head of Forensic Explosives Laboratory at RARDE (FSS)

Dr A Scapelhorn Home Office Forensic Science Service.

Mr Yallop retired head of RARDE (Forensic Science Service Lab UK)

Mr Clancy retired head of RARDE (Forensic Science Service Lab UK)

The West Committee set up to thrash out the science of the case consisted of Professor T S West (chairman), Professor Thorburn Burns, Dr. Lloyd, Dr. Caddy, Dr. Scapelhorn, Dr. Marshall and Mr. Higgs. This is probably the most experienced and decorated forensic / analytical science committee ever assembled, certainly in the UK, containing s it does several world class scientists with vast experience.

Evidence given in trial with regard to TLC plates:

"The evidence was to the effect that the pink spots had a similarity of intensity of colour across the plates. It was suggested that it would be remarkable if each tested area of the hands and the nails the same quantity of NG. This matter was not explored at the trial when more accurate recollections would have been available. But as we have explained the test is not a quantitative one; similarity of colour to the standard means a quantity of 200 to 1000 ng. After that the spot becomes diffuse and possibly will have a yellow centre. It is not possible to conclude that precisely the same quantity was found at each source. Both Mr. Higgs and Dr. Hayes, and no doubt Mr. Elliott too) was surprised at so many positives, but this is because on field tests, as opposed to experiments with HTK's (hand test kits) were rare. We do not think this point casts any doubt on the integrity of the tests."

They defence lawyers made the following points:

(a) There might be another non explosive chemical in ordinary everyday use that might mimic NG substance "X"
(b) No certainty the substance on the TLC plates was NG in absence of confirmatory tests.
(c) There might have been some accidental contamination of the samples before they were tested. Possible contamination of samples before they reached RARDE was investigated at trial. Possible contamination in laboratory could have occurred in particular by contamination of the ether used.
(d) Contamination of hands and gloves could have been by contact with object that was itself contaminated such as a towel.
(e) Contrary to evidence given at trial, NG under fingernails was not proof positive of handling or kneading explosives.

Apparent Conclusions of Maguire trials:

(1) Nitroglycerine (NG) was proven to be on the hands and gloves of the Maguire seven.
(2) There was no acceptable evidence to suggest that another non explosive substance was responsible for the spots found on the TLC plates.
(3) Even though there were some technical shortcomings in the evidence these were not deemed by the jury or courts to be significant.
(4) The suggestion that the evidence was fabricated by prosecution scientists or that contamination of the samples occurred during collection storage or analysis was not accepted.
(5) There was a possibility that the towel in the Maguire bathroom was contaminated with NG and that all the Maguire Seven had the explosive transferred to their hands by this route. "We are satisfied on the evidence of Professor Thorburn Burns that it is not safe to try and extrapolate back from the results to reach any conclusion as to the primary source of contamination. In other words it is impossible to identify one or more of the appellants as the primary source of contamination …… On the grounds that the possibility of innocent contamination cannot be excluded and on this ground alone, we think that the convictions of all the appellants are unsafe and unsatisfactory and the appeals are allowed and the convictions quashed."

Further interesting point:

The test samples from the Maguire Seven which were used in 1974 had been kept stored since the trial. Re-examination with modern more sophisticated techniques showed the presence of NG not only in the samples that were positive in 1974, but also in those that were then negative!

Some detailed background information on Griess TLC:

Thin Layer Chromatography: (ref = COA appeal unrevised)

[This excellent review, clearly written by a scientist, can be skipped by persons not interested in the scientific details].

The following is a description taken from court of appeal judgement (unrevised):

"Since the integrity of these results and the interpretation put upon them by the experts lay at the heart of the trial and also this appeal, it is necessary to give a brief outline of TLC. The system was used both for analyzing samples from HTK's (hand test kits) and other samples. The first stage is the extraction of the suspect substance from the swab or other item to be tested. This is done by washing in ether, which is placed in a beaker and the ether allowed to evaporate. The residue is then spotted onto a glass plate treated with silica gel on which standards or controls of known explosives were also applied. Normally these explosives were NG, RDX, TNT and Nitrobenzene (NB). All the spots were placed on a line known as the origin. The plate was then placed in a tank containing a quantity of liquid known as an eluent, usually toluene, in order to draw the known standard and the suspect substance up the plate by capillary action. The eluent front can be seen to rise on the plate. When it reaches a point 10 cm above the origin the plate is removed from the tank. Different substances rise up the plate at different rates, which can be measured after being made visible. This rate of rise is not expressed as an absolute measurement, but as a proportion of the total distance travelled by the eluent. The ration is called the R_f value. When the plate is removed from the eluent tank both the standard spots and the suspect spot will have risen up the plate, but will not be visible at this stage either in ordinary or ultraviolet light, and the plate has to be subjected to two further chemical processes before they become so. NG is an organo nitro compound of the nitrate ester grouping, and the plate must first be sprayed with sodium hydroxide (caustic soda) to liberate the nitrite ion from the nitrate compound; at this stage the plate will appear white from the spray. The plate is then heated in an oven to 110 degrees C and is then sprayed with what is known as Griess reagent which reacts with the nitrite present to form a pink spot. It is at this stage known as visualisation, that the distance travelled up the plate by the standard and suspect spots can be seen. If the suspect reached the same level as the standard a positive was recorded. If the two did not exactly coincide, a positive would still be recorded provided the difference was small, not more than 3 mm either side of the standard; this was known as the parameter. Professor Thorburn Burns was of the opinion that 0.03 was an acceptable parameter for recording a positive.

The test is a qualitative and not a quantitative one. That is to say it can give a positive for the substance but cannot give the amount. However, the practice at RARDE was to put a standard of 200ng (a nanogram is a millionth of a gram). If the pink colour spot of the suspect sample was equal to or exceeded the intensity of that standard, a positive was recorded; this would mean a minimum of 200 ng was detected. Otherwise the test was negative, although sometimes, usually in trials or experiments rather than in field tests, it might be recorded that there was a faint positive.

The test is a highly discriminating one: the substance must rise the same level as the standard; it must be soluble in ether; it must not show up on exposure to ultraviolet light, or after heating or spraying with sodium hydroxide; and it must produce a pink spot when sprayed with the Griess reagent…..

…..The mechanical part of the Griess testing – that it up to the final stage when the Griess reagent is applied and the plate is visualised, was often done at RARDE by relatively junior employees, in particular at the material time by Mr Wyndham, Mrs Brooker, and Mrs Cashen; but the visualisation was done, except sometimes in the case of Mrs Brooker who was the most senior and experienced of the three, by more senior

officers namely Mr. Elliott, Dr. Hayes, Mr. Berryman and occasionally Mr. Higgs. But in fact the test on the appellants HTK's were done by Mr. Elliott, who was the most experienced person at RARDE in the practice of TLC and they may also have been visualised by Dr. Hayes."

Chemical structure of azo dye in Griess test (1974):

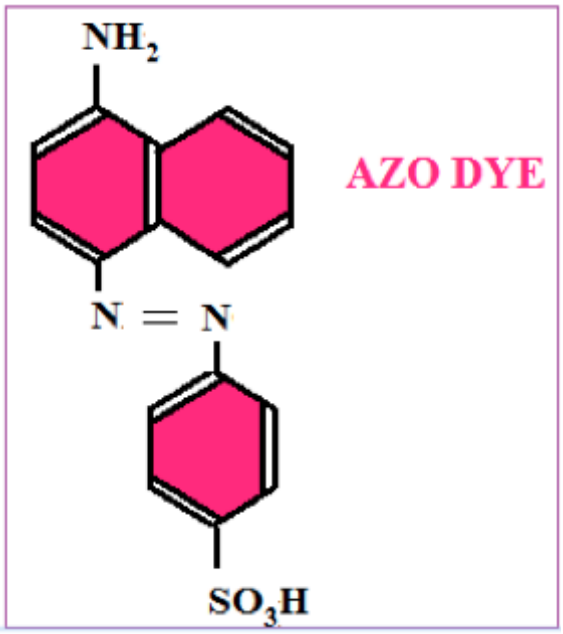
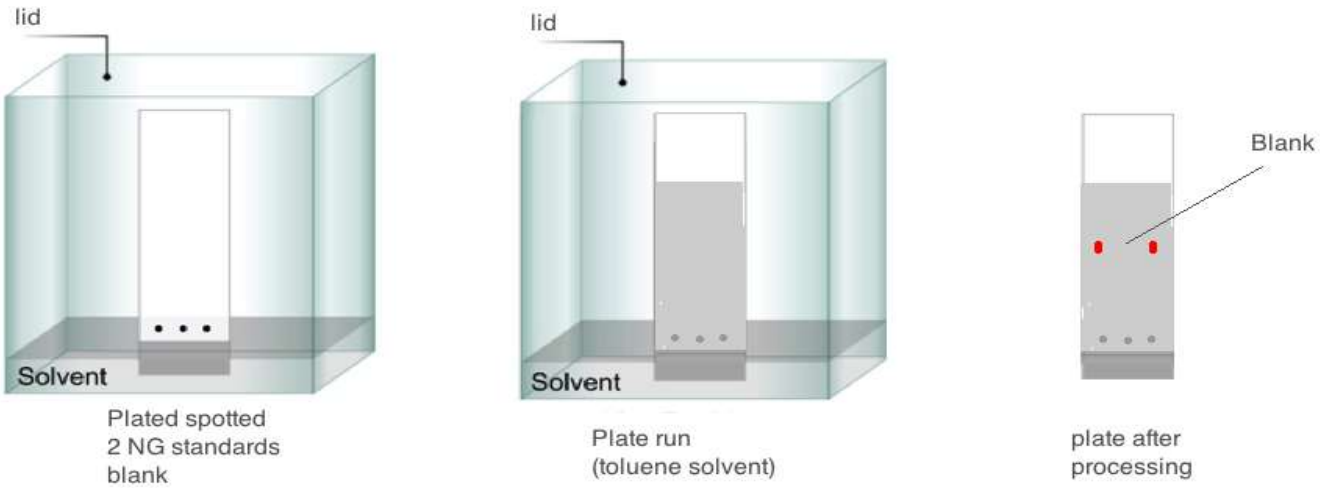


Diagram of Thin Layer Chromatography (Griess) for Nitroglycerine

(Excellent description of TLC on Wikipedia):
http://www.chemguide.co.uk/analysis/chromatography/thinlayer.html

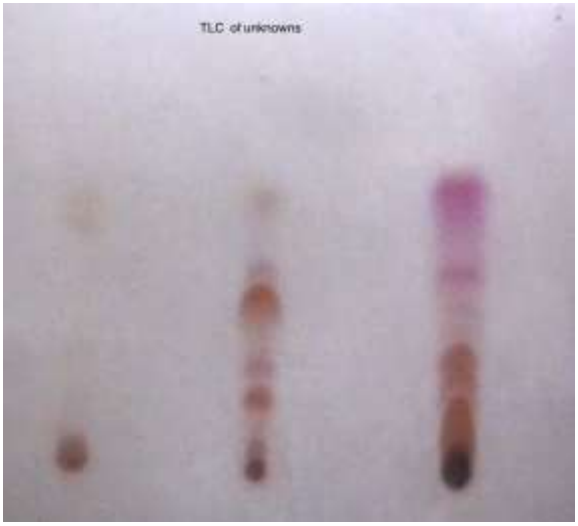


The observation of the substantial pink coloured spots on the TLC plates in Maguire case indicated a considerable amount of nitroglycerine was present.

The TLC (Thin Layer Chromatography) Griess test:

This is a thin layer plate showing pink spots of standards of nitrite with Griess reagent:

Below is a thin layer plate of a very impure sample with multiple spots, some possibly NG: this shows that TLC is not a very selective analytical technique.



Final Comments

There are four conclusions in the investigations / judgements that might not be to the liking of the Maguires and their co-defendants:

- That nitroglycerine was found on their hands / gloves,
- That it was impossible to say whether this was caused by contamination before or during analysis, but that this was unlikely.

- That the original samples stored securely since 1974 were found years later to still contain NG. This applied to the samples that contained the NG in 1974 and also to others which were negative at that time.
- The Court of appeal only accepted the proposal that the NG on the hands of the Maguire Seven came from contamination from a towel in the Maguire household.

Conclusion Part 1:

It is clear that it was the opinion of the court that nitroglycerine was found on the hands / gloves of the Maguires. Professor Thorburn Burns showed that it was possible that this explosive presence could have been caused by innocent contact with a contaminated towel. The level of such contamination was very substantial as confirmed by Professor Thorburn Burn's experiments. The forensic evidence was very complex with experts of equal status holding opposing views. Given the conflicting evidence, the lay jurors cannot be blamed for their conclusions.

The author is convinced of the innocence of the Maguires. Part 2 will suggest what, in the author's opinion went wrong.

Part 2 will revisit the judgement on the basis of legal and scientific first principles. As can be seen above, the evidence provided by the prosecution was substantial enough to convince four judges (including three Law Lords – (the cream of British judiciary) and a jury. A super inquiry assisted by one of the most expert analytical / forensic committees ever assembled, chaired by a Court of Appeal judge, were unable to come to any definitive conclusion? The author saw a neighbour of Mrs. Maguire on television who said that she did not believe that such a good and religious hard working woman was involved in a terrorist campaign. She was totally convincing.

Part 2 to follow in a later issue.

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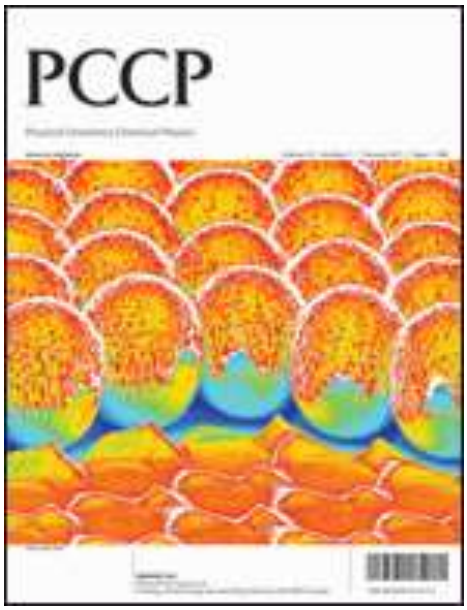

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International guest speakers include:

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Peter Dobson, University of Oxford. Founder of Oxonica and Oxford Biosensors Ltd., Director of Begbroke Science Park and Strategic Advisor on Nanotechnology to UK Research Councils.

Marty Burke, University of Illinois. Leading the new field of "molecular prosthetics" with several patents licensed to Sigma-Aldrich.

Jos Put, former global CTO of DSM Company, Netherlands & member of governing Board of Mesa+ Institute with 30 years experience of turning materials into profitable products.

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European Chemistry and Chemical Engineering Education Network

Report on EC2E2N Meeting, Ljubljana, Slovenia 27-29 April 2015

www.**ec2e2n**.net/

I attended this meeting and also the ECTNA AGM as a representative of the University of Limerick and the Institute of Chemistry of Ireland.
This was the 19th annual meeting of the European Chemistry Thematic network, which started in 1996 and has had 6 successive rounds of EU funding. It is the most successful and productive subject network in Europe. It involves a network of over 100 institutions, mainly universities but also including professional bodies. The last round of funding runs out in September.

The conference involved reports and working sessions of the 8 working parties in this round. These will mostly complete their work by the end of the network. However, it was agreed that the network would continue under the auspices of ECTNA, although there would be no more EU funding. A meeting has been scheduled for 2017 but it is possible that in future years the ECTNA meetings might be attached to EuCheMS meetings. Funding will no longer be available for attendance at meetings.

A memorandum of agreement was signed at the meeting between ECTNA and EuCheMS, to promote future cooperation and in particular with the Division of Chemical Education of EuCheMS. There is, and has been, overlap between the membership and activities of EuCheMS divisions and ECTN and this agreement should increase the collaboration, wit joint projects.

A new President of ECTNA was elected unanimously for a 3 year term: Professor Pavel Drasar from the Czech Republic. New members of the ECTNA council were also elected. It is intended that several working groups will be run under the new structure, but largely through on-line communication. These new working groups are:

- Project Proposals, leader Evangelia Varella
- Using the EChemTest, leader Peter Gaertner
- Teaching Qualifications and Innovative Teaching, leader Paul Yates (p.yates@chester.ac.uk)
- The Transparency Database, leader Anne-Marie Billet
- Links with Other Organisations, leader Franco de Angelis.

The one on Teaching Qualifications and Innovative Teaching is new and should be of interest. The aim is to produce an on-line course for postgraduates and new chemistry lecturers on basic principles of innovative teaching.

The current working groups are (see http://www.ec2e2n.net/2/index to access the reports and membership of these groups):

1. **Towards Excellence in School and University Teaching**
   Iwona Maciejowska, Jagiellonian University of Krakow, Poland; maciejow@chemia.uj.edu.pl.

2. **Enhancing Professional Abilities**
   Eugenio Caponetti, University of Palermo, Italy; caponett@unipa.it.

3. **Entrepreneurship**
   Antonio Lagana, University of Perugia, Italy; lagana05@gmail.com.

4. **Impact of Chemistry in Everyday Life**
   Antonio Floriano, University of Palermo, Italy; michele.floriano@unipa.it.

5. **The Virtual Educational Community**
   Ioannis Kozaris, Aristotle University of Thessaloniki, Greece; ikozaris@chem.auth.gr.
6. **Broadening Student Horizons**
   Gabriella Borzone, University of Genova, Italy; gabriella.borzone@unige.it.

7. **Re-tuning for Chemistry/Chemical Engineering in Europe in 2020**
   Evangelia Varella, Aristotle University of Thessaloniki, Greece; varella@chem.auth.gr.

8. to 11. **Project Management; Dissemination; Exploitation of project outcomes; Quality Assurance**
   Anthony Smith, Coordinator, CPE Lyon, France; coordinator@ec2e2n2.net.

I have been involved in WP1: Towards Excellence in School and University Teaching, together with Odilla Finlayson (DCU) and Claire McDonnell (DIT). This WP has been involved in three projects:

1. *School Chemistry Teacher Training Guidebook* : this will provide a free electronic resource for chemistry teacher educators.
2. An e-chemtest for student chemistry teachers to test their pedagogical content knowledge (PCK).
3. A database of teaching methods and pedagogical issues relevant to teaching chemistry at third level and a register of expertise. http://starfish.innovatievooronderwijs.nl/information/395/

The final reports and materials produced by the working groups and publications of the network will be available on the website.

ECTN has been a very valuable and productive thematic network and it is hoped that this will continue in future, due to the strong links built between individual chemists and chemistry departments across Europe.

Peter E. Childs
Emeritus Senior Lecturer,
Dept. Of Chemical and Environmental Sciences, University of Limerick.
peter.childs@ul.ie

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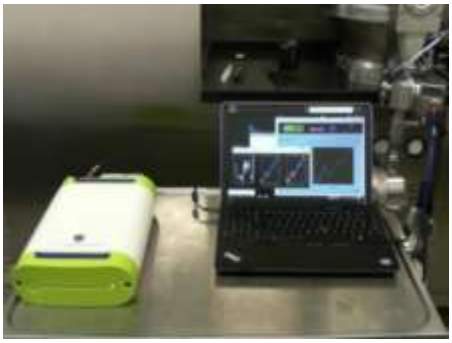

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Colin Quigley, Level 6 Certificate, Pharmaceutical and Medical Device Operations.

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Kristina Vushkarniik, Level 7 BA, Pharmaceutical Business Operations

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Report on The 2015 EuCheMS General Assembly

The 2015 EuCheMS General Assembly was held in Vienna, on Monday & Tuesday, September 28th & 29th. It was attended by over 40 delegates, representing affiliated chemical societies. The Institute of Chemistry of Ireland was represented by Margaret Franklin, President of the Institute.

The meeting took place at the WKO (Chamber of Commerce) building, where the delegates were welcomed, on day one, by Herbert Ipser of the Austrian Chemical Society, who gave a presentation on the activities of his society. This was followed by a presentation by David Cole-Hamilton, President of EuCheMS, who gave an update on the activities of the organisation. In his address, David called for EuCheMS to become the independent voice for chemistry in Europe. It has 41 member societies, based in 32 countries, representing about 160,000 chemists. He outlined the Mission of EuCheMS, placing chemistry at the heart of policy & planning in Europe. We must present chemistry as a provider of solutions to global challenges. But we need to speak with a single voice. Professor Cole-Hamilton outlined the activities of EuCheMS, which include advising the European Institutions, lobbying the parliament & Commission (e.g. through the MEP-Scientist Link Scheme); running parliamentary workshops (on Energy Storage, CO2 utilisation, Employability, Protecting Endangered Elements). EuCheMS organises short subject specific meetings, which in 2015 included the following: Food, Water & Energy (Rome); Zero-Carbon Energy (Edinburgh) and Feeding the World (Food & Energy EXPO, Milan). As well as this, EuCheMS holds a major chemistry conference every two years. David referred to the press release 'Chemists Against Chemical Weapons' which was issued on 26th April, 2015, to commemorate the centenary of the first large-scale use of chemical weapons in Ypres, Belgium, during World War 1. EuCheMS has a Young Chemists' Division, The European Young Chemists Network (EYCN) as well as 12 Divisions and 5 working parties, dealing with various branches of Chemistry. About 500 scientists and researchers are members of EuCheMS divisions. EuCheMS has four strategic planning task groups, makes various awards and issues a number of publications.

Following this presentation, the meeting was brought up to date on EuCheMS policy activities by Nineta Majcen and Bruno Vilela. Eckart Ruhl gave a report on the Divisions and Working Parties and Fernando Gomollon-Bel gave an account of the activities of the European Young Chemists' Network.

There were presentations from four nominated candidates seeking election to the Executive Board. Two of the candidates were present in the room, but the other two gave their presentations via Skype. There were also presentations from three organisations seeking to become supporting members of EuCheMS: , Fraunhofer Institute for Interfacial Engineering and Biotechnology IGB, FECCIA, and ERIC. They were all accepted, bringing the number of affilliated members ot 46.

There was also an invited talk by Prof. Reiner Salzer on the outcomes and future of the *European Employability Survey for Chemists and Chemical Engineers* as well as a talk from Dr. Robert Parker, RSC Chief Executive, on *Public Attitudes Towards Chemistry*, which was published by the RSC earlier this year and showed a more positive attitude, on the part of the general public, towards chemists than chemists themselves believed.

Day I of the General Assembly ended with a pleasant social event; a dinner hosted by the Austrian Chemical Society Gesellschaft Osterreicher Chemiker.

The second day of the G.A. dealt with various business matters: One member society was excluded for non-payment of membership fees, despite repeated reminders. Two new members were elected to the Executive Board. The Treasurer presented the accounts for approval and the budget for 2016.

There was a lengthy discussion on a proposal from the American Chemical Society to hold a joint chemistry conference in Mexico in 2018. Eventually, it was decided to take part, on a trial basis, but with some modification to the original proposals.

Four presentations were given, showing the results of the four strategic task groups:

1: Vision & Staffing, 2: EuCheMS Income & Funding 3: Interactions between Divisions & Secretariat; 4. Survey of Member Societies

At the conclusion of the meeting, The President of EuCheMS, David Cole-Hamilton gave a final summing up of the outcomes of the General Assembly and thanked the General Assembly host, the Gesellschaft Osterreichischer Chemiker.

Next year the General Assembly will go south, taking place in Seville, Spain, right before the 6th EuCheMS Chemistry Congress, in September 2016.

Some of the presentations given at the General Assembly can be downloaded from the EuCheMS Website:

http://www.euchems.eu/about/general-assembly/2015-vienna-austria.html

A group photograph of all of the participants can be downloaded here:

http://www.euchems.eu/fileadmin/user_upload/events/EuCheMS_Events/150928_GA/Group_Final.JPG

Report by

Margaret Franklin, FICI,

President,

The Institute of Chemistry of Ireland

7/10/2015

China-Ireland Research Partnership

International Strategic Collaboration Programme (I S C P)

Background

The International Strategic Collaboration Programme- China (ISCP China) began as a Science Foundation Ireland funded initiative to build research capacity between Irish and Chinese universities with knowledge intense industries in areas of national priority. The main objectives of ISCP China to date have been to strengthen and extend the existing research relationships; develop new China-Ireland collaborations focused on research excellence and to utilise the experience of research collaboration with China to help Irish companies compete in the world's second largest economy. The programme is led by Maynooth University in collaboration with Dublin City University (DCU), the Royal College of Surgeons in Ireland (RCSI), Dublin Institute of Technology (DIT) and Trinity College Dublin (TCD).

The programme has focused on collaboration in three thematic research areas: biomedical science, information and communication technology, and nanotechnology. In addition to new partnerships, impressive joint publications, conference papers and exchange of staff and students, the programme has led to important benefits for Irish industry. Industry leaders have led some of the joint workshops held in Ireland and used the academic network to explore new opportunities for hi-tech exports. Conversely access to Chinese industries has allowed the Irish partner universities to showcase Ireland as a destination for foreign direct investment.

Scientific Workshops:

In terms of scientific outputs, two of the most relevant workshops in 2015 were themed on "Catalysis & Sensing for our Environment Symposium 2015 (CASE 2015)" and "Supramolecular Chemistry Ireland (SCI)".

The **CASE Symposium** was held in TCD and RCSI from 9-10 July 2015 supported by ISCP China, RCSI and various local businesses. This symposium is an important event in the scientific calendar and previous symposia have been held in: The University of Bath (UK, 2008); East China University of Science and Technology (China, 2009); The University of Birmingham (UK, 2011); Shanghai Institute of Organic Chemistry (SIOC) (China, 2012); University of Texas at Austin (USA, 2013) and Xiamen University (China, 2014). The workshop also built on a successful ISCP-China Ireland-China Symposium on Nanotechnology, held in TCD on the 12-14 May 2014.

Symposium website: https://2015case.wordpress.com

Prof John Boland (TCD)
& Prof Xuhong Qian (ECUST).

The **Supramolecular Chemistry Ireland Symposium** is the largest meeting of its kind in Ireland and brings together supramolecular chemists with interests in organic, inorganic, physical and biological chemistry. This year it was held in the historic Renehan hall of Maynooth University on Wednesday 8 July 2015. The symposium has been held annually since 2000 in the School of Chemistry, Trinity College Dublin, so this was the first time it had been located outside of TCD. SCI 2015 brought together a host of world renowned participants ranging from invited speakers, to a poster session covering a broad range of supramolecular topics. Supramolecular chemistry studies the interactions between molecules: how they recognise each other, assemble and function on a molecular scale. It provides a bottom up approach to nanoscale systems with applications ranging from medical devices to materials science. Coinciding with CASE 2015 in Dublin, SCI 2015 combined the best of supramolecular chemistry research from China to Ireland and beyond in an intense and productive meeting. The symposium also contributed to building a network of scientific collaboration worldwide but especially with excellent scientists and key state laboratories in China.

Conclusion:

During the two-year programme, SFI funding to ISCP China has strengthened existing relationships in China and built new scientific and industrial collaborations. The project will conclude its SFI funded activities in November 2015, however, this will not be the end of this important and beneficial partnership. The ISCP consortium partners will continue to build on the strategic research alliances with Chinese partners, using funding from Chinese sources and industry (Ireland and China). This continued collaboration will not only assist the research in the partner Universities, but will help Irish industry maximize the value of this effective research network.

For further information please contact: iscp@nuim.ie

Sponsors:

ISCP China, The Royal Society of Chemistry, Maynooth University.

The Institute & Henkel Host Yunnan Delegation from Yunnan Provincial Department of Production Safety Supervision & Administration

Henkel Excellence is our Passion

Culture Based Safety | Check Before Starting | Come Back Safely

The Institute in cooperation and hosting by Henkel Ireland facilitated a meeting with the Yunnan delegation to talk about safety in handling and the storage of hazardous chemicals. Their Department has responsibility for the safety of chemicals and wanted to see what regulations the industry worked under, systems the chemical companies had in place to manage the chemicals and how these systems were implemented in practice.

Representing the Institute were:

Dr. Patricia Cullen (facilitator), Margaret Franklin (President), Dr Ray Leonard (Council member) and Patrick Hobbs (Editor ICN).

The delegation consisted of 6 members: 1. Mr. Yang Yalin (leader) 2. Ms. Hu Liping 3. Mr. Wang Houjiang 4. Mr. Xue Jian 5. Mr. Cheng Zongwen 6. Mr. Zhang Jianzhong and Dublin based interpreter Li Xiang.

Henkel Tallaght: Dr Patricia Cullen, Fergal Gilhawley, John Cahill, Eddie Nolan, Laura Byrne

Henkel Ballyfermot: Sharon Mulvey, Richard Teehan.

The meeting opened with Patricia defining the objectives for the day and expected outcomes.

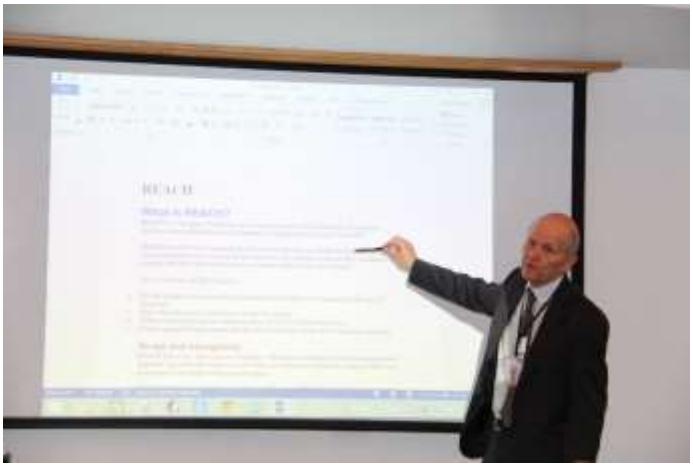
Patrick Hobbs then talked about the PSM systems at the former Arch Chemicals/Lonza site.

Topics outlines included: Responsible Care, REACH, Arch's SETCO, Management of Change, Safe Start, Operational Excellence, Sustainability Programme, Quality Management Systems: ISO 9001,ISO 14001, OHSAS 18001, PHA, HAZOP, Risk Analysis, Annual Quality Plans, Safety Meetings, Safety Tours, Safe Act Tours, Audits Internal & External.

This was followed by a presentation from Fergal Gilhawley Site SHE Manager covering hazardous chemical storage, ADR, IATA, Sustainability and Responsibility Care. Compliance standards and regulations and how people were treated by inclusiveness, and a non-blame culture. It was explained that these systems required investment both monetary and in training. In practice there is some level of resistance but by working with staff at all levels cooperation and involvement was achieved. Henkel did not operate in blame and punish environment. The delegation did explain that the culture was different in China where there was a blame and punish culture. Many companies in China do not have the resources of Western multinationals and the systems we used in Ireland would need adaptation to Chinese conditions.

This was followed by a plant tour of the facility conducted by John Cahill and Eddie Nolan. This showed the high standard of housekeeping in the filling operations areas, clearly marked walkways, signage, high visibility PPE, marked routes for forklifts. On return to the conference room we had a presentation from

Laura Byrne on Behavioral Based Safety and the training requires. At Henkel this programme has resulted in a dramatic reduction in lost time accidents and near misses.



After a working lunch the group adjourned to the Ballyfermot site where chemical synthesis is carried out. We were shown how the chemical storage is organized and the segregation of the hazardous materials and the controlled access to toxic chemicals. Next we given a tour of the synthesis and distillation plant where the pressure relief and venting systems on plant vessels were pointed out.

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086 389 8647
andreina.moran@sial.com

Barbara O'Leary, Chair Eurachem Ireland Committee 2 October 2015

Eurachem Ireland Recent Activities

Eurachem Ireland is an organisation for people working in chemistry in Ireland, with a focus on analytical chemistry. Chemistry students are welcome too. Eurachem Ireland promotes the objectives of Eurachem (www.eurachem.org) in Ireland including good quality practices. To be informed of the activities of Eurachem Ireland (www.statelab.ie/eurachem.html) you are invited to:

1) Join the mailing list by emailing eurachem@statelab.ie.

2) Join the Linkedin group 'Eurachem Ireland'.

TrainMiC® Metrology in Chemistry Workshop

Over thirty people attended the Eurachem Ireland workshop, TrainMiC® Metrology in Chemistry Part I, held on World Accreditation Day, 9 June. The event was hosted by the State Laboratory and attendees were from a range of public sector and private sector organisations. Topics covered included Traceability of Measurement Results; Validation of Measurement Procedures; and Uncertainty of Measurement. The presenters, Joseph Fitzsimons and Sean Earley, are accredited TrainMiC® trainers.

TrainMiC® is a European programme about how to interpret the metrological requirements of ISO 17025 for chemical and bio-analytical measurements. The vision of TrainMiC® is to improve the quality of analytical results by promoting and providing a European-wide, harmonised training in Metrology in Chemistry.

Eurachem Working Groups

Eurachem is a network of organisations in Europe, having the objective of establishing a system for the international traceability of chemical measurements and the promotion of good quality practices. Eurachem's technical activity is carried out by its various Working Groups. The Eurachem Ireland Committee issued a call for new members for the Working Groups. Thanks to an enthusiastic response, there are now Irish representative on all of the Working Groups:

- Education and Training
- Measurement Uncertainty and Traceability
- Method validation
- Proficiency Testing
- Qualitative Analysis

Eurachem Analytical Measurement Competition

Unfortunately the popular Eurachem Analytical Measurement Competition (EAMC) did not take place in 2015 due to unforeseen circumstances. The competition will return in Spring 2016 when Athlone Institute of Technology will be the hosts.

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Improving Processes With Statistical Models

By Malcolm Moore, Robert Anderson, and Phil Kay, SAS

Introduction

Do you face scientific, engineering or business challenges that can't be solved by an appeal to expert judgment, simple spreadsheet analysis, or by varying only one thing at a time?

Do you seem to have more problems than time available to solve them?

Are you forced to regularly make decisions from incomplete data or information, limiting your understanding of the real drivers of robust, effective and efficient processes?

Does the need to fix problems with existing processes limit the time you can spend on innovating and developing new processes and products?

JMP® statistical discovery software from SAS helps you gain insights to fix such issues quickly and permanently, giving your organization a competitive edge now and freeing up resources to innovate for future growth.

Finding workable solutions – whether in research, development, manufacturing, sales or marketing – from prior data is sometimes difficult due to the complex, noisy relationships between many variables that are difficult or impossible to easily spot. Learn how JMP users are solving more scientific, engineering and business problems correctly the first time – and in less time – by extracting powerful insights from existing data using proven, simple statistical modeling methods.

The real-world case studies that follow will help you discover best practices to interactively explore the patterns in your data, build useful statistical models of the important patterns of variation, and visually interact with these models to communicate and drive key improvement opportunities.

How can statistical modeling help my business?

Let's see how one manufacturer is using JMP to add value. The organization was unable to consistently meet demand for one of its products. Often it was able to manufacture without issues, yet at other times the organization had significant yield and quality issues. The primary incoming material was a natural product with considerable variation in key properties, so the manufacturer had to make routine adjustments in the process. Operators made these adjustments based on experience, yet overall the company was unable to get the process running at more than 75 percent of its theoretical capacity.

Significant volumes of process data existed, but engineers were unable to make sense of it with existing software. This meant the critical variables to adjust for incoming material variation were not well defined. Demand for the product was increasing, and to facilitate this growth, the company was faced with building a new production facility at significant capital cost to meet market needs.

Using the integrated statistical modeling, profiling and simulation capabilities of JMP, the engineers created a powerful new understanding of the process. They created statistical models involving all the measured inputs, from which they identified the critical ones for consistent operations. This allowed them to define operating envelopes (control tolerances) for the critical inputs to ensure consistent product quality and throughput. With a robust operating envelope, they could reduce the number of process adjustments for incoming material variability. And when an adjustment was necessary to correct for a major change in the input material, they used the statistical model to define which other inputs to adjust and by how much. This yielded a process with predictable product quality and increased throughput.

The resulting increase in capacity saved hundreds of millions of dollars by avoiding the need to build a new production line, and enabled millions in additional revenue via the resulting predictable increase in capacity. Improving the current process enabled enhanced profitability, increased market share and faster business

growth, freeing up capital for other projects. The organization is now adopting statistical modeling upstream to reduce variation in input material and further improve production predictability, capacity and quality.

When should you consider statistical modeling?

Many companies are applying statistical modeling routinely to help predictably, efficiently and effectively drive technical and business decisions. As the above example illustrates, the value to your business and personal satisfaction of solving what appear to be insurmountable problems is huge.

When do you know if statistical modeling might help you? Here are some tell-tale signs:

- You spend a lot of time dealing with unanticipated problems.
- Your problem-solving efforts yield unpredictable returns – and the same problem or a related one reoccurs.
- You feel you don't have the complete picture and have to make decisions based on incomplete information.
- You transfer products and processes with limited understanding of how they work.
- You feel stuck in a vicious circle where managing existing problems or processes limits your time for optimization, innovation and new development.

Learning is incremental

Learning is often incremental. Figure 1 illustrates how we typically start with data or a theory, which is analyzed to help assess our situation or theory, which typically leads to more questions that require collection of new data to provide answers. We may iterate many times through this cycle of learning before building a good enough picture of our situation to make a reliable decision. When under time pressure we may omit one or more cycles of learning, with the impact that we may not have closed the gap between the real world and what we think is happening based on our learning to date.

JMP statistical discovery software from SAS helps you extract more knowledge from each cycle of learning, determine the set of inputs, and understand how they work or interact together to create your problem. By extracting more information from each cycle of learning, JMP reduces the number of cycles of learning required to deliver the information you need to make the correct decision, and increases the predictability of getting to those decisions with a limited budget and time.

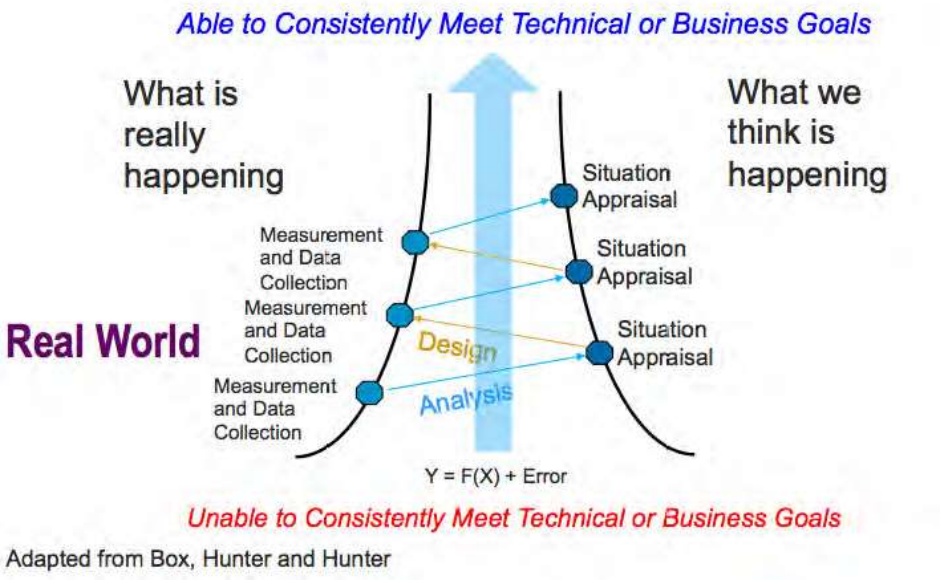


Figure 1: Learning is incremental

Why apply statistical modeling?

Statistical modeling results in many personal and business gains. You can:

- Reduce number of learning cycles. Statistical modeling helps extract more information from complex problems where many factors together are responsible for your opportunity, problem or issue.
- Reduce total problem-solving time. By increasing the knowledge gained from a cycle of learning, statistical modeling helps reduce the total number of learning cycles needed to create the knowledge required to make reliable decisions.
- Increase predictability of improvement and problem-solving activities by extracting more information from your data and reducing the number of learning cycles needed for key decisions. Statistical modeling makes answering your research, development, production, marketing and sales questions more predictable and effective.
- Increase useful understanding. Rather than creating incomplete knowledge from your data – which may result in false solutions – statistical modeling helps extract key relationships from many input variables that may be related to or even interacting with each other, increasing clarity and diminishing confusion.
- Make sustainable decisions within the required time frame, instead of using non-statistical approaches resulting in poor decisions based on incomplete understanding, which cause problems that must be solved again and again.
- Transfer more complete process knowledge to upstream colleagues.
- Increase time available for new projects to grow future opportunities because it is less likely the same problem comes back to be solved again (and again).

Where to apply statistical modeling

You can apply statistical modeling anytime you have data that can be organized into rows and columns, and tabular or graphical summaries alone are unable to provide the understanding needed for a reliable decision. This is likely to be when:

- No single input is exclusively responsible for output variation, the problem, or the improvement opportunity.
- You need to understand relationships between two or more inputs and one or more outputs.
- Inputs usually vary together, so are correlated and it is difficult to determine which inputs may be responsible for output variation.
- There are holes or gaps in your data table that reduce the amount of data that can be used with non-statistical approaches.

In product design situations, statistical modeling can improve the understanding of the relationship between attributes and product performance, generating needed product concept and product improvement insight. These are complex multivariate problems where commonly used visualization and modeling methods are often ineffective in extracting nonlinear and higher dimensional effects, leading to increased time to market and reduced product performance.

In development of high-tech products, we need to learn how to make high-margin, complex product designs. Technically it is difficult to realize a product that meets all technical requirements and tolerances, and competitive time pressures result in rushed development. This leads to problems in manufacturing and subsequent redevelopment, which are costly and time consuming. This in turn diverts the resources that should be aligned with product development for new cycles, creating a vicious circle.

In high-tech manufacturing, we are faced with a continual pipeline of new products that need to be made. New technologies may be introduced that require us to develop, qualify and introduce a new process on a regular basis to keep pace with the product design changes that are needed to sustain our competitiveness. The next cycle often starts before yields are optimized with the current cycle. Each new process or technology presents previously unseen problems and challenges, and we are faced with more problems than

resources to address them. Engineers struggle to keep their heads above water. And the volumes of data just keep growing.

Sales and marketing must continually attract new customers, help existing customers get more value from products and services, and help customers find new problems or improvement opportunities. There is often an abundance of data, but since not all customer segments behave the same, it is difficult to extract knowledge that can help increase the efficiency and effectiveness of sales and marketing activities.

What is a statistical model?

To benefit from statistical modeling, you obviously require data. It will need to be organized with observations (measured units) in rows and variables (measured values of different attributes) in columns. Some variables may be numeric; others may be character data. Your input variables are referred to as Xs and the other variables are referred to as Ys or outputs.

Given this framework, a statistical model is an empirical model that relates your set of inputs (Xs) to one or more outcomes (Ys).We think of a statistical model as being derived from the relationships in our data to separate the output variation into signal and noise:

$Y = f(X) + E$

Where

- Y is one or more continuous or categorical responses.
- X is one or more continuous or categorical predictors.
- $f(X)$ describes predictable variation in Y (signal).
- E describes unpredictable variation in Y (noise).

Extracting a useful model – particularly when your Xs are correlated and there are nonlinear and interactive effects of the Xs on our Ys – is getting easier with technology such as JMP.

Case Study 1: Improving an existing process using data exploration and data mining

Three levels of modeling are used:

1. Visual modeling via dynamically linked graphs with zoom and filter to identify major effects.
2. Explanatory modeling using decision trees to isolate joint or interaction effects.
3. Predictive modeling using multiple regression to identify and exploit the way in which many Xs operate together to create variation in our Y.

Example 1

A mature manufacturing process occasionally produces out-of-specification products. Each time this occurs, it requires engineers to troubleshoot and attempt to find the root cause. Key process stages get checked to confirm operation within validated ranges, and no obvious assignable cause emerges. While this effort continues, the process returns to normal without making any changes. Engineers breathe a deep sigh of relief and go back to normal duties – until the next time.

Over the years, many theories as to the cause have been proposed, but none confirmed. Yet continuation of this situation represents significant wasted cost and opportunity:

- Manufacturing and disposal cost of rejected batches costs money.
- Each rejected batch must be reported in an annual product review, and products with a high reject rate are likely to come to the attention of a regulatory agency (or customer).
- In some cases the regulatory agency might remove the license to manufacture due to lack of process understanding.

- In other industries, customers might switch to an alternative supplier able to meet their quality and supply needs.
- Declining market share and reputation.
- Lower profitability affects dividends returned to investors and the availability of capital to reinvest.

Data on the process is abundantly available, and prior approaches to extract meaning from this data include engineering judgment, tabular and graphical summaries, basic statistical comparisons and simple regression. The solutions proposed have not prevented problem reoccurrence. After the last exception, an engineer fresh from a statistical modeling workshop suggested the problem might be due to many factors working together, and that a statistical modeling approach might be helpful. The manager was dubious at first; an engineer himself, he thought his engineers should be able to solve the problem using their engineering knowledge alone. The engineer from the workshop pointed out the obvious: If the problem was easily solved using engineering knowledge alone, why was the problem still unsolved? After some persuasion her manager agreed to allow the engineering group to give statistical modeling a try.

Figure 2 represents a process map of the production process. It is a secondary drug process that involves milling an active pharmaceutical ingredient (API) into a powder of uniform particle size. The milled material is then blended with other ingredients to bulk up and evenly distribute the API. This blended material is then compressed into tablets, which are finally coated to aid shelf life, taste and other properties. At the end of the process, a dissolution test is performed, and if the average dissolution value of several tablets is less than 70 percent dissolved at 120 minutes, the entire batch of tablets is rejected, incurring disposal cost.

The first step was to identify the data that was routinely measured, which is identified in bold type on the process map (Figure 2).The engineer also wanted the variables in gray, but these measurements were not routinely made, so she decided to progress and see what headway she could make with the data that was available to her. Getting her data into a spreadsheet view with rows representing observations and columns representing variables (Figure 3) was straightforward, and she was soon ready to explore and statistically model her data.

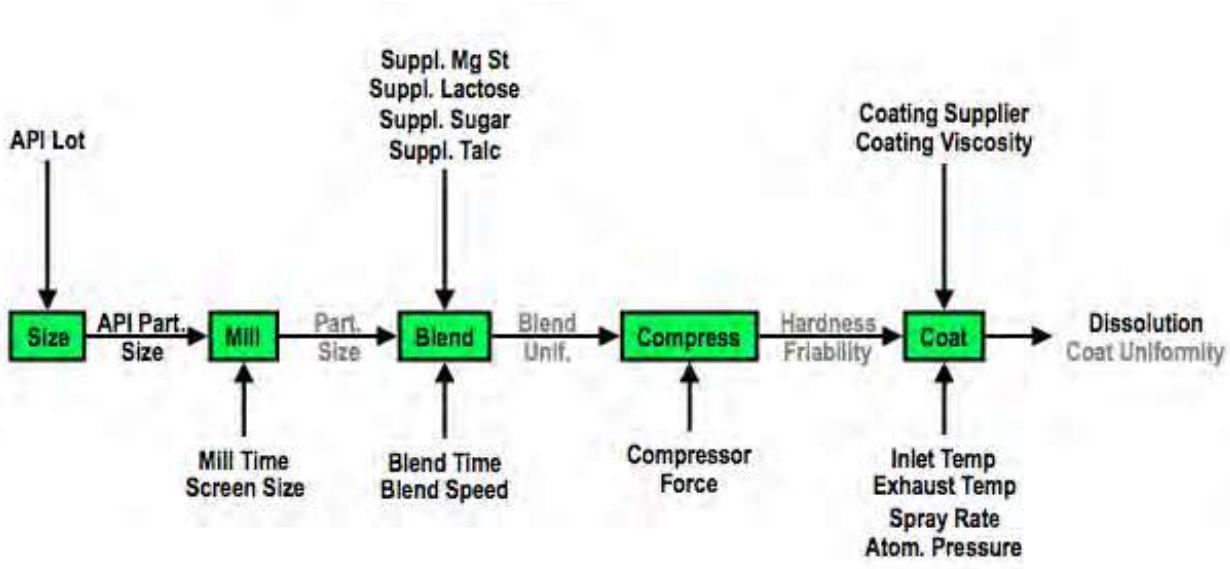
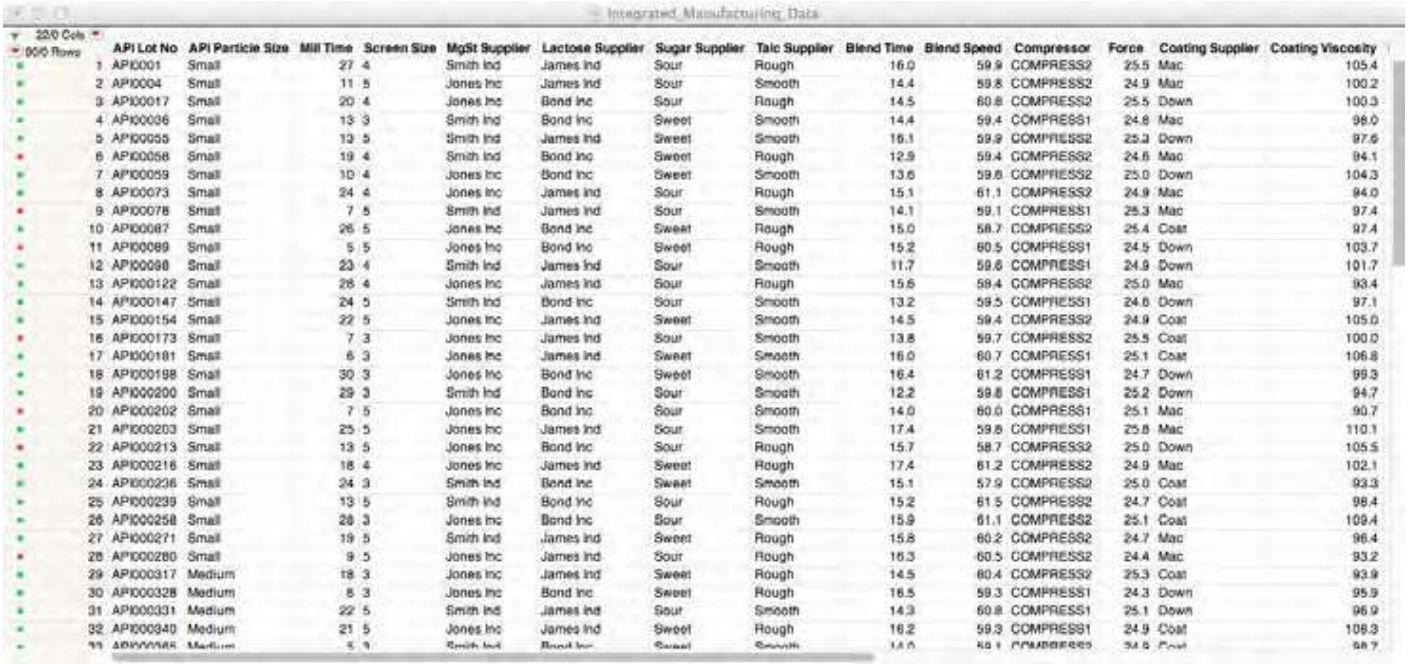


Figure 2: Manufacturing process



Integrated_Manufacturing_Data

22/0 Cols
90/0 Rows

	API Lot No	API Particle Size	Mill Time	Screen Size	MgSt Supplier	Lactose Supplier	Sugar Supplier	Talc Supplier	Blend Time	Blend Speed	Compressor	Force	Coating Supplier	Coating Viscosity
1	API0001	Small	27	4	Smith Ind	James Ind	Sour	Rough	16.0	59.9	COMPRESS2	25.5	Mac	105.4
2	API0004	Small	11	5	Jones Inc	James Ind	Sour	Smooth	14.4	59.8	COMPRESS2	24.9	Mac	100.2
3	API00017	Small	20	4	Jones Inc	Bond Inc	Sour	Rough	14.5	60.8	COMPRESS2	25.5	Down	100.3
4	API00036	Small	13	3	Smith Ind	Bond Inc	Sweet	Smooth	14.4	59.4	COMPRESS1	24.8	Mac	98.0
5	API00055	Small	13	5	Smith Ind	James Ind	Sweet	Smooth	16.1	59.9	COMPRESS2	25.3	Down	97.6
6	API00056	Small	19	4	Smith Ind	Bond Inc	Sweet	Rough	12.9	59.4	COMPRESS2	24.6	Mac	94.1
7	API00059	Small	10	4	Jones Inc	Bond Inc	Sweet	Smooth	13.6	59.8	COMPRESS2	25.0	Down	104.3
8	API00073	Small	24	4	Jones Inc	James Ind	Sour	Rough	15.1	61.1	COMPRESS2	24.9	Mac	94.0
9	API00078	Small	7	5	Smith Ind	James Ind	Sour	Smooth	14.1	59.1	COMPRESS1	25.3	Mac	97.4
10	API00087	Small	26	5	Jones Inc	Bond Inc	Sweet	Rough	15.0	58.7	COMPRESS2	25.4	Coat	97.4
11	API00089	Small	5	5	Jones Inc	Bond Inc	Sweet	Rough	15.2	60.5	COMPRESS1	24.5	Down	103.7
12	API00098	Small	23	4	Smith Ind	James Ind	Sour	Smooth	11.7	59.6	COMPRESS1	24.9	Down	101.7
13	API000122	Small	28	4	Jones Inc	James Ind	Sour	Rough	15.6	59.4	COMPRESS2	25.0	Mac	93.4
14	API000147	Small	24	5	Smith Ind	Bond Inc	Sour	Smooth	13.2	59.5	COMPRESS1	24.6	Down	97.1
15	API000154	Small	22	5	Jones Inc	James Ind	Sweet	Smooth	14.5	59.4	COMPRESS2	24.9	Coat	105.0
16	API000173	Small	7	3	Jones Inc	James Ind	Sour	Smooth	13.8	59.7	COMPRESS2	25.5	Coat	100.0
17	API000181	Small	6	3	Jones Inc	James Ind	Sweet	Smooth	16.0	60.7	COMPRESS1	25.1	Coat	106.8
18	API000198	Small	30	3	Jones Inc	Bond Inc	Sweet	Smooth	16.4	61.2	COMPRESS1	24.7	Down	99.3
19	API000200	Small	29	3	Smith Ind	Bond Inc	Sour	Smooth	12.2	59.8	COMPRESS1	25.2	Down	94.7
20	API000202	Small	7	5	Jones Inc	Bond Inc	Sour	Smooth	14.0	60.0	COMPRESS1	25.1	Mac	90.7
21	API000203	Small	25	5	Jones Inc	James Ind	Sour	Smooth	17.4	59.8	COMPRESS1	25.8	Mac	110.1
22	API000213	Small	13	5	Jones Inc	Bond Inc	Sour	Rough	15.7	58.7	COMPRESS2	25.0	Down	105.5
23	API000216	Small	18	4	Jones Inc	James Ind	Sweet	Rough	17.4	61.2	COMPRESS2	24.9	Mac	102.1
24	API000236	Small	24	3	Smith Ind	Bond Inc	Sweet	Smooth	15.1	57.9	COMPRESS2	25.0	Coat	93.3
25	API000239	Small	13	5	Smith Ind	Bond Inc	Sour	Rough	15.2	61.5	COMPRESS2	24.7	Coat	98.4
26	API000258	Small	28	3	Jones Inc	Bond Inc	Sour	Smooth	15.9	61.1	COMPRESS2	25.1	Coat	109.4
27	API000271	Small	19	5	Smith Ind	James Ind	Sweet	Rough	15.8	60.2	COMPRESS2	24.7	Mac	98.4
28	API000280	Small	9	5	Jones Inc	James Ind	Sour	Rough	15.3	60.5	COMPRESS2	24.4	Mac	93.2
29	API000317	Medium	18	3	Jones Inc	James Ind	Sweet	Rough	14.5	60.4	COMPRESS2	25.3	Coat	93.9
30	API000328	Medium	8	3	Jones Inc	Bond Inc	Sweet	Rough	16.5	59.3	COMPRESS1	24.3	Down	95.9
31	API000331	Medium	22	5	Smith Ind	James Ind	Sour	Smooth	14.3	60.8	COMPRESS1	25.1	Down	96.9
32	API000340	Medium	21	5	Jones Inc	James Ind	Sweet	Rough	16.2	59.3	COMPRESS1	24.9	Coat	108.3

Figure 3: Analysis-ready data

One visual modeling approach illustrated in Figure 4 involved plotting the Y (dissolution) against the Xs using side-by-side histograms and dynamic linking to select the failing batches – those with a dissolution below 70 percent dissolved at 120 minutes – and seeing whether the failing batches were clustering at one end of the data range of one or more Xs. Some obvious clustering of defects seems to occur at low values of mill time, high values of screen size and higher values of spray rate.

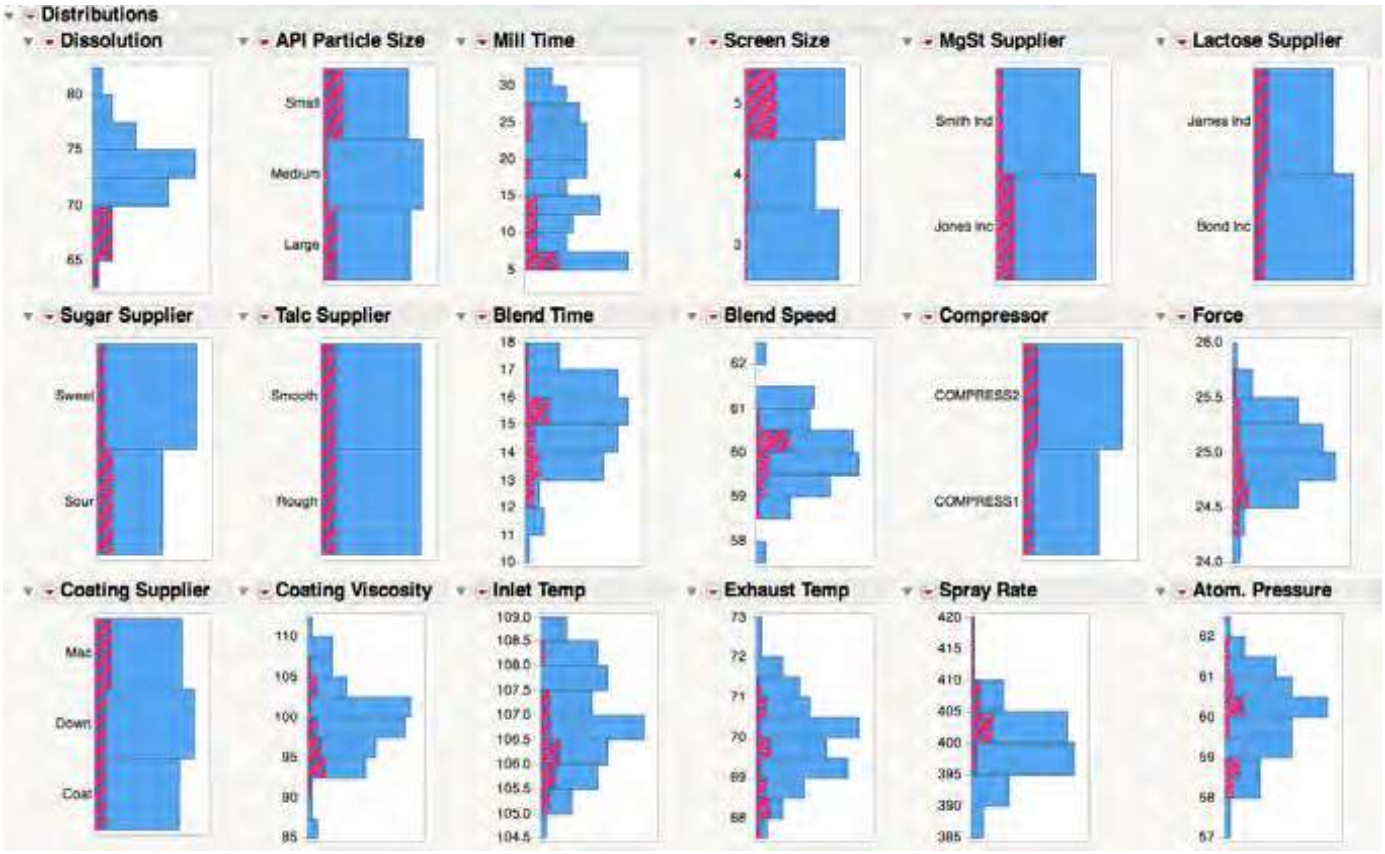


Figure 4: Visual insight

Many of the Xs appear to be related to the dissolution failures, and the engineer wanted to explore how some of the factors may be interacting. A decision tree was constructed using recursive partitioning to identify the top Xs. This can be thought of as an organizational chart of some of your Xs that might be responsible for the variation in a Y. In our particular case, it shows that at the top of the tree we have an overall reject rate of 15.6 percent. With the subset defined by a screen size of 3 or 4 and a spray rate of less than 404.1 (the right-hand branch of the tree), we have a reject rate of 0 percent. Contrast this with a high reject rate of 80 percent in the left-hand branch, which is defined by screen size of 5 and mill time of less than 11 minutes. A decision tree is an organizational chart of the conditional way in which some of our Xs sort the Y from good to bad.

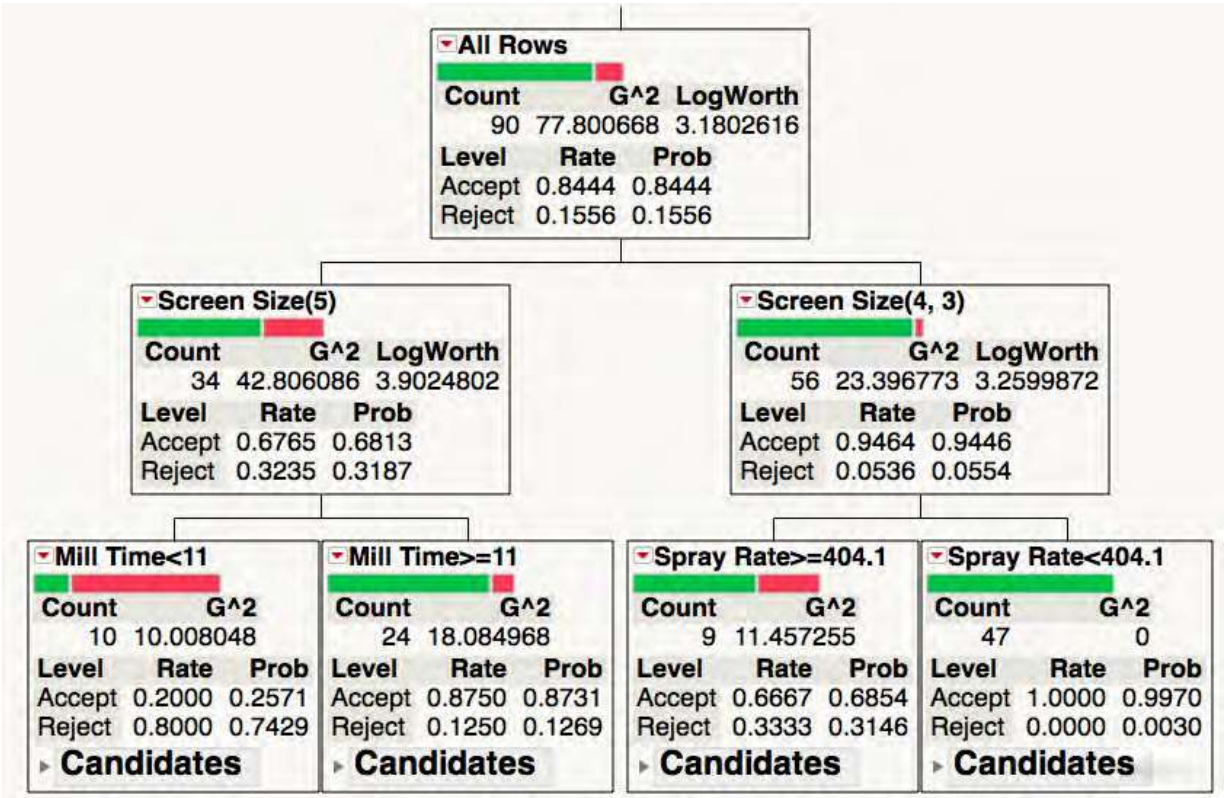


Figure 5: Explanatory insight

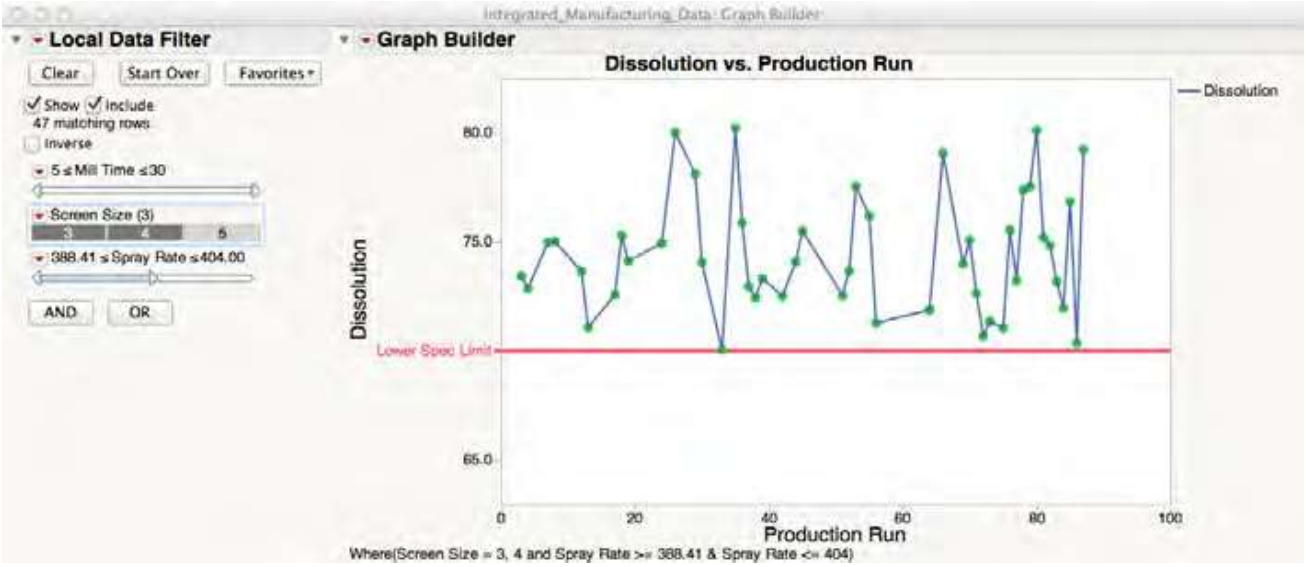


Figure 6: "Best" subset identified by decision tree

While the solution proposed by the decision tree is an improvement, Figure 6 shows the trend of dissolution for this subset and indicates the process is sometimes likely to operate close to the threshold of failure. It is necessary to shift the mean dissolution to a higher value and preferably shrink the variability around the

mean to ensure all future batches stay above the lower specification limit of 70 percent dissolved by 120 minutes.

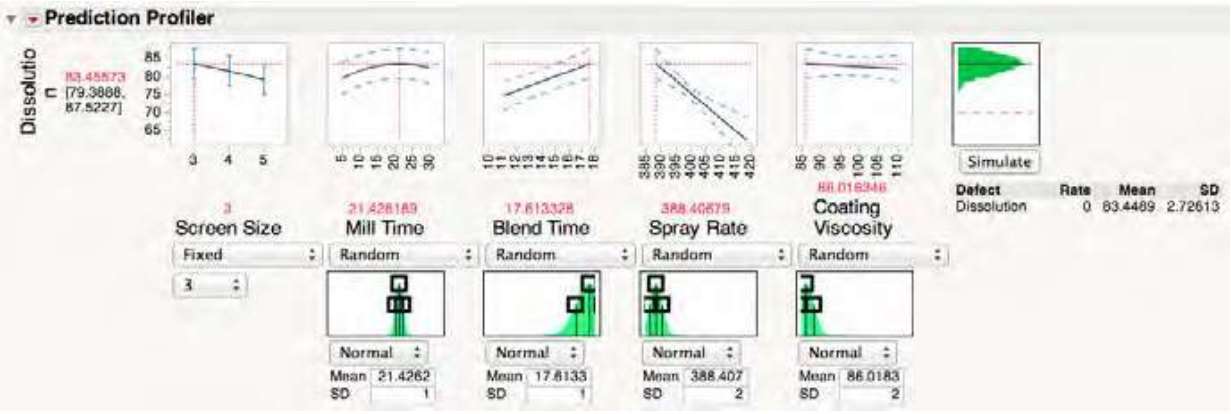


Figure 7: Predictive insight

To gain the level of improvement needed, the engineer used a multiple regression model. Figure 7 shows the critical Xs determined by this method, which are Screen Size, Mill Time, Blend Time, Spray Rate and Coating Viscosity. Further, it shows the nature of the relationship between each X and average dissolution. To get the biggest gain in average dissolution, we need low screen size, a middle-to-high mill time, a high blend time, a low spray rate and low coating viscosity. At the values indicated of 3, 21.4, 17.6, 388 and 86, respectively, the model indicates we can expect an average dissolution of 83.5.

The model can also be queried using Monte Carlo simulation to determine how much variation in the Xs can be tolerated before transmitting undesirable batch-to-batch variation into dissolution. f Mill Time, Blend Time, Spray Rate and Coating Viscosity were unable to be controlled exactly in large-scale manufacturing, and if, for example, the uncontrolled variation is defined by normal distributions with standard deviations of 5, 1, 3 and 5 around the respective means, then Monte Carlo simulation of 5,000 production runs from these input distributions indicate we can expect an output distribution for dissolution with a mean of 83 percent and a standard deviation of 2.7 percent. Further, none of the batches would have a dissolution value below 70 percent dissolved at 120 minutes.

Changing the settings of the five critical inputs to those indicated in Figure 7 resulted in a robust and adequately controlled process, as indicated by the next 20 production batches in Figure 8.

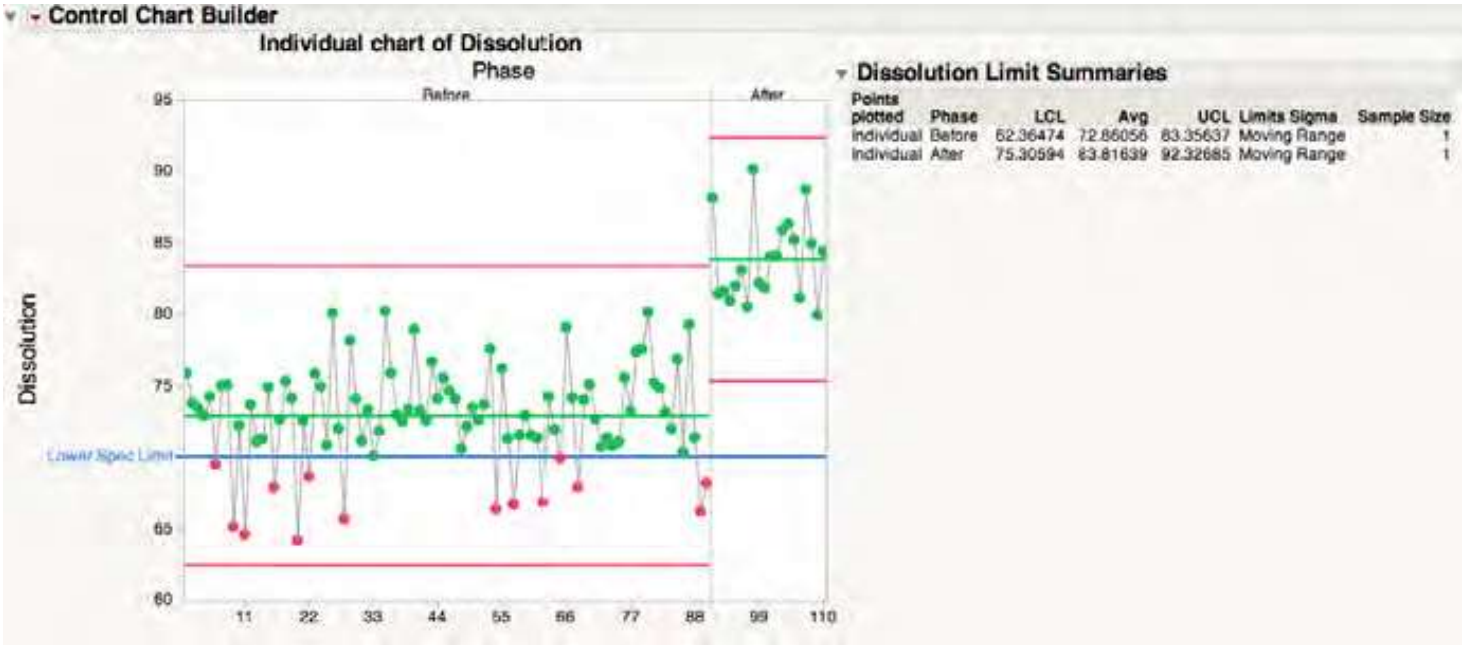


Figure 8: Before vs after comparison of dissolution

Summary

Visual and explanatory modeling provided clues as to some of the Xs responsible for the excessive variation in dissolution. Predictive modeling identified the complete set of Xs affecting dissolution and helped the engineers understand the way in which these Xs operated together to drive undesired variation in dissolution. Profiling and simulation capabilities around the model provided the necessary insight to understand what was causing batch-to-batch variation in dissolution and provided the insight needed to fix the problem for good. The solution created significant savings by eliminating the cost of dealing with rejected batches and reduced regulatory risk.

Case Study 2: Accelerating R&D using data exploration and data mining

This case study will introduce additional modeling methods that are helpful when our Xs are strongly related to one another, e.g., X1 and X2 would be described as strongly related if X2 increases (or decreases) when X1 increases. Special modeling methods such as ridge or lasso regression, partial least squares and neural networks may be beneficial in such situations.

Example 2

A drug discovery company typically has several million chemical compounds in its library and wishes to improve efficiency and effectiveness of drug candidate identification and improvement using data from the company's chemical and biological databases. In particular the company is keen to improve the knowledge created to answer questions such as:

- Which compounds are more likely to be active for a particular disease?
- Which parts of a molecule should be targeted to improve activity or safety, and how?

The chemical database contains various chemical descriptors, e.g., length, shape, charge and molecular weight. The biological database contains activity and safety indicators for various target diseases. To improve the knowledge gained from these databases, we need to devise better models of the relationship between chemical descriptors and biological activity/safety.

Chemists frequently used 2-dimensional and 3-dimensional visual insight methods, multivariate modeling methods that assume linear relationships between chemical descriptors and activity/safety were also used. The relationships between activity and chemical descriptors are complex and it is the way in which many descriptors operate together that influences activity. Two-dimensional and three-dimensional visual insight methods do not scale to providing insight from how a few descriptors influence activity to how many descriptors work together to influence activity. Current multivariate statistical technology was too complex for many researchers and did not cope particularly well when the relationships are interactive and/or nonlinear in nature.

Many researchers were not performing multivariate statistical analysis or were not able to extract nonlinear and interactive effects with multivariate statistical analysis. Therefore the company was not realizing the potential value of multivariate statistical analysis. Decisions were based on partial understanding from visualization methods or less-effective multivariate modeling methods, resulting in a larger number of learning cycles, which affected the speed and predictability of R&D.

Getting his data into a spreadsheet view with rows representing observations and columns representing variables (Figure 9) was straightforward, and the chemist was soon ready to statistically model his data.

21/0 Cols
40/0

	Activity	Chemical Structure	Charge	Andrews Binding E	Bioav. Score	MW	Smiles Length	CMR	ClogP	logD(ph4.6)	logD(ph6.4)	logD(7.4)	re
1	Inactive		1	15.6	0.55	355.48	41	10.247	1.654	-3.39	-1.59	-0.62	
2	Inactive		1	12.5	0.55	281.43	36	8.809	3.979	1.52	2.05	2.91	
3	Inactive		1	13.8	0.55	344.5	39	9.881	4.153	-0.3	0.75	1.72	
4	Inactive		1	12.5	0.55	260.32	28	7.195	1.381	-3.3	-1.57	-0.58	
5	Inactive		1	12.5	0.55	245.31	27	6.947	0.777	-3.34	-1.55	-0.56	
6	Inactive		1	16.9	0.55	403.59	46	11.893	2.261	-2.58	-0.79	0.15	
7	Inactive		1	14.5	0.55	399.55	43	10.963	4.43	1.7	2.52	3.44	
8	Inactive		1	18.9	0.55	384.51	42	10.513	2.54	-0.36	1.43	2.42	
9	Inactive		1	16.5	0.55	375.99	40	10.664	3.737	0.34	2.11	2.93	
10	Inactive		1	13.7	0.55	275.38	33	7.595	2.735	-0.95	-0.42	0.36	
11	Inactive		1	15.6	0.55	412.58	48	12.401	3.67	0.72	2.5	3.31	
12	Inactive		1	17	0.55	379.9	40	9.736	0.094	-0.78	0.99	1.8	
13	Inactive		1	17	0.55	356.89	41	9.978	1.775	-1.23	0.57	1.54	
14	Inactive		0	10.3	0.55	256.34	30	7.359	4.123	2.59	4.11	4.92	
15	Inactive		1	16.8	0.55	410.52	47	11.292	0.091	-1.85	-0.07	0.84	
16	Active		-1	11.9	0.56	420.46	61	10.77	2.734	-1.53	-1.46	-1.54	
17	Active		0	1.1	0.55	272.38	37	7.949	3.154	3.65	3.61	3.39	
18	Active		-1	5.4	0.85	260.38	34	7.465	2.158	2.35	1.01	0.03	
19	Active		-1	9.3	0.56	397.51	41	11	2.22	1.38	0.94	0	
20	Active		0	7.1	0.55	413.45	48	9.87	2.636	2.17	2.26	2.24	
21	Active		0	8.7	0.55	468.36	54	11.942	4.553	1.86	1.86	1.86	
22	Active		0	3.2	0.55	319.44	36	9.477	2.868	2.81	3.41	3.43	
23	Active		-1	10.4	0.85	444.69	53	12.506	4.605	5.17	5.17	5.17	
24	Active		-2	11.9	0.56	346.43	43	9.14	3.278	2.2	0.43	-0.5	
25	Active		0	24	0.55	384.45	51	10.121	0.013	-2.22	-0.91	-0.94	
26	Active		-1	8	0.56	358.52	42	10.141	2.944	3.21	1.59	0.63	
27	Active		2	31.3	0.55	410.58	49	11.476	2.948	-1.62	0.01	1	
28	Active		-2	10.7	0.56	481.36	52	10.936	2.114	3.43	2.38	1.41	
29	Active		-2	14	0.56	467	57	11.98	0.024	1.92	0.6	-0.38	
30	Active		-1	12.3	0.56	430.6	50	11.537	3.573	5.01	3.68	2.7	

Figure 9: Analysis-ready data

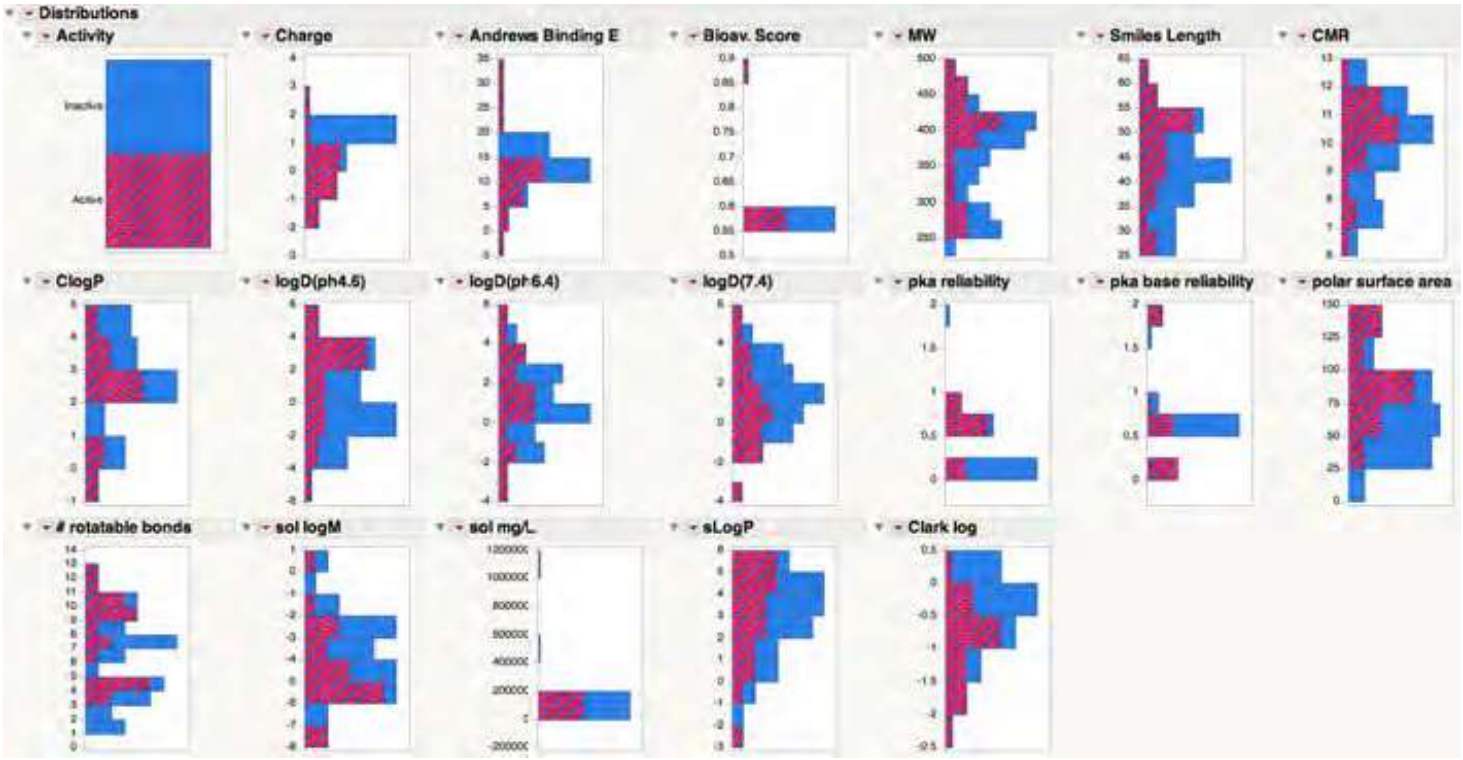


Figure 10: Visual insight

By plotting activity alongside the Xs using side-by-side histograms, as illustrated in Figure 10, and using dynamic linking to select the active chemicals, it was possible to see if the active chemicals clustered at one end of one or more Xs. Some obvious clustering of active chemicals seems to occur at low values of charge, high values of smiles length (bigger molecules), higher log dissolution at pH 4.6, larger polar surface area and lower Clark log.

Regular two-dimensional graphs as depicted in Figure 11 enable drill-down to view molecular structure or other images.

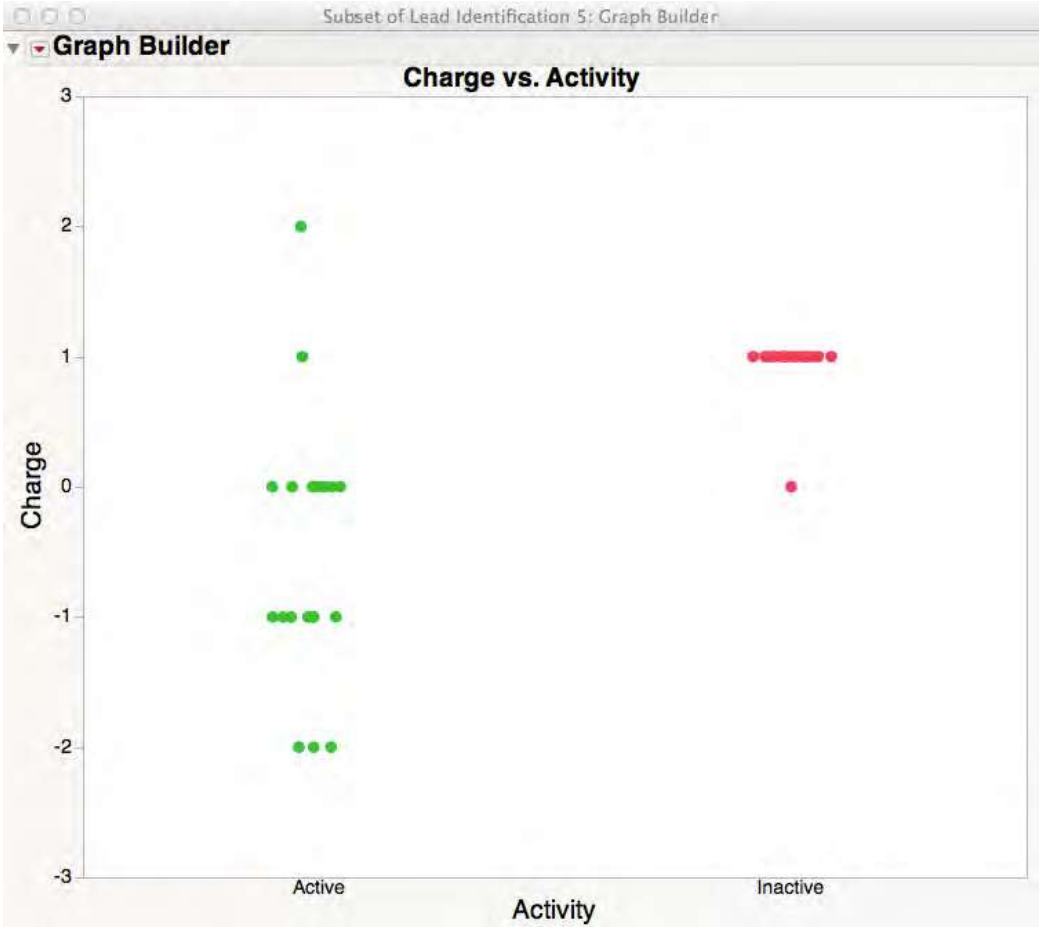


Figure 11: Hover over any data point to generate a pop-up graph showing detailed molecular structure

Various statistical modeling methods were investigated and compared, including lasso regression, logistic regression, partial least squares and neural networks. A neural network was determined as the best model since it was able to predict the activity of other compounds not used in model building more accurately than any of the other methods. Based on examination of the Profiler resulting from the neural network model in Figure 12, it appears that the neural network model was able to identify nonlinear relationships between the Xs and activity.

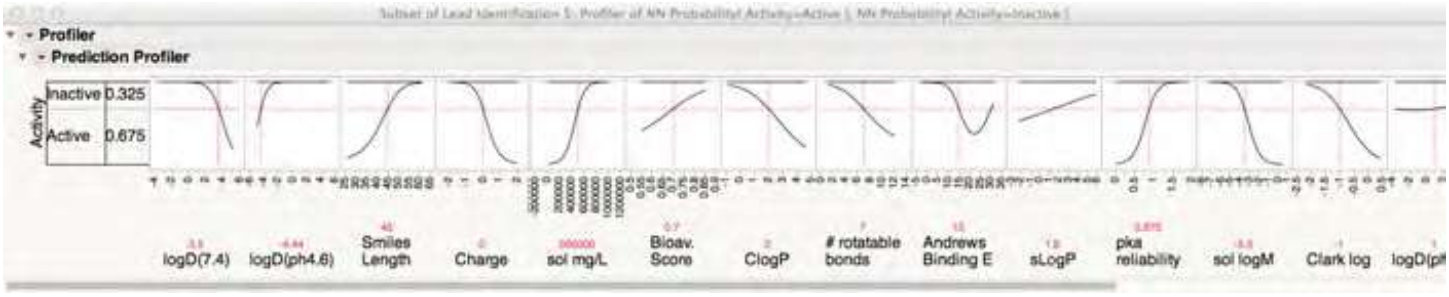


Figure 12: Profiler of neural network model

The neural network model was used to score the chemicals database to predict the probability of each chemical within the database being active for the target disease. The top 5 percent of chemicals – the top 5 percent with the highest prediction probability – were selected for further study. From a chemical understanding perspective, the Profiler suggests that chemicals with a low log dissolution at pH 7.4, a high

log dissolution at pH 4.6, a long smiles length (larger molecules), a lower charge and so on are more likely to be active chemicals.

Summary

Visual modeling is effective for low-dimensional problems; however, predictive modeling better provides the insight necessary to solve high-dimensional problems. Predictive modeling delivered a scoring formula to rank or sort the database from most likely to be active to least likely to be active, and the top 5 percent of chemicals were selected for further study.

Statistical modeling drives deeper understanding better, faster and easier, with the resulting benefit of fewer cycles of learning and shorter R&D cycles and a more predictable outcome. Because of the easy-to-use interface of JMP statistical discovery software, more researchers are able to gain a better understanding of their data with statistical modeling.

Conclusion

To keep it brief, just two examples were presented. With access to data on the process or system you wish to investigate, you could similarly create a spreadsheet view of your data and start to model the dependence of your Ys on your Xs.

This paper has attempted to explain:

- What is a statistical model.
- Types of problem that benefit from statistical modeling.
- Simple and effective ways to build statistical models.
- How to extract understanding from statistical models.
- How to present and communicate statistical models and resultant understanding to other stakeholders.
- How to make better decisions, faster.

Statistical modeling might help you or your company to:

- Accelerate innovation.
- Deliver robust products and process that work every time.
- Speed time to market.
- Deliver a competitive edge.
- Improve customer loyalty.
- Increase growth and return.
- Reduce costs.
- Enhance your brand and claim more market share.

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Pyrex At 100

Corning's century-old glass innovation has had a revolutionary impact on cooking and chemistry

By **Stephen K. Ritter**

C&EN Chemical & Engineering News Volume 93, Issue 20, pp. 35-36, May 18, 2015.

Department: **Science & Technology**
Keywords: **Pyrex**, **Corning**, **CorningWare**, **glass**

http://cen.acs.org/articles/93/i20/Pyrex-100.html

Before heading out the door after a day of research at **Corning Glass Works** in 1913, physicist Jesse T. Littleton grabbed the sawed-off bottom of a round borosilicate glass battery jar. He did so at the behest of his wife, Bessie, who had broken her ceramic baking dish. Bessie used the ersatz dish to cook up a sponge cake, one that turned out uniformly shaped and so light and perfectly browned that Littleton knew he had something special on his hands.

Corning took the baking discovery and turned it into Pyrex, a much-loved brand of glass baking dishes, measuring cups, and storage containers for the kitchen. The same qualities that made Pyrex ideal for cookware—transparency, temperature resistance, and chemical inertness—were also ideal qualities for laboratory and industrial glassware. So Corning also introduced Pyrex beakers, Erlenmeyer flasks, and graduated cylinders for the lab, as well as pipelines and reactor liners for manufacturing plants.

MAKING HISTORY
An assembly of Corning's iconic Pyrex lab glassware.
Check out historic Pyrex photos at **http://cenm.ag/pyrex100**.
Credit: Courtesy of Corning

Corning is spending this year **celebrating the 100th anniversary** of the commercial launch of Pyrex, arguably one of the most important technological developments in the history of materials science.

"What an invention!" says Columbia University chemistry professor **Ronald Breslow**, a past-president of the American Chemical Society. It's hard to believe that a single material, Pyrex, has dominated laboratory chemistry for 100 years, Breslow adds.

Turns out there is a bit more to the Pyrex development story than just a good sponge cake, says Jeff Sauer, business director of laboratory glass at Corning Life Sciences. Corning had started out 60 years earlier as a company specializing in industrial glass and ceramics, Sauer explains. The company's forte was glass lenses for signaling lamps used by railroads.

When the first commercial lightbulbs came along in the 1880s, Corning was there to produce teardrop-shaped glass globes to protect the filament. And the company's glass tube technology later helped bring radio and then television to the masses. Pyrex was an extension of those developments.

THE GLASSBLOWER
In this company archive photo, a Corning glassblower puts the finishing touches on a "distillation cow" for isolating multiple samples.
Credit: Courtesy of Corning

The borosilicate glass from which Pyrex was born was first made by German chemist and glassmaker Otto Schott in 1893. Borosilicate **glass is typically made** by fusing sand (silica) and borax (sodium borate) in a hot furnace followed by shaping the molten material by hand or machine. Schott's company began selling the glassware under the name Duran. Before Schott, firms used soda (sodium carbonate) and lime (calcium oxide) to make glass, but incorporating boron oxide from borax reduces the material's coefficient of thermal expansion, meaning it can better withstand dramatic changes in temperature.

In 1908, Eugene C. Sullivan, Corning's first director of research, developed Nonex glass—short for nonexpansion—a variation on borosilicate glass designed especially for railroad lamps. "What made Nonex suitable for railroad lenses is that the glass can withstand the intense heat from the light source on the inside and the sometimes extreme cold and wet weather on the outside," Sauer says.

Nonexpansion was a great property, Sauer notes, but it made the product too durable. The glass lasted for a long time, which reduced the number of reorders and affected sales. "Corning scientists had to come up with **other applications for the resilient glass** to help the company stay in business."

That's where the Littletons figure in. The glass that Bessie used to bake her sponge cake contained too much lead, making it unsuitable for kitchenware. But once the Corning team got the lead out, a star was born.

"By 1915, people were cooking in glass," Sauer says. "At the time, that was unheard of."

Lab glassware was a different story. Before 1915, lab glass was primarily made in Germany and Austria, Sauer adds. But the outbreak of World War I cut off American scientists from their supply. "The war created a sudden, great market need for laboratory glass," Sauer says. Corning met that need by selling Pyrex labware.

By the end of the war in 1918, made-in-America glass cookware and labware were firmly established, and Corning was the leading supplier. Pyrex wasn't just replacement glassware for American scientists, it turned out to be superior: In 1918, the U.S. Bureau of Standards gave Pyrex a higher rating than any other brand of lab glassware.

After its launch, Pyrex became part of a string of laboratory successes, Sauer says. One famous Pyrex user was Charles A. Lindbergh, known for his daring 1927 solo airplane flight from New York to Paris aboard the *Spirit of St. Louis*. Lindbergh had studied engineering before dropping out of college to be a flyboy. After crossing the Atlantic, he worked in the lab of Nobel Prize-winner **Alexis Carrel** at Rockefeller Institute, in New York City.

Lindbergh created glass devices that could be heat-sterilized and used to culture cells or to pump fluids through organs to keep them functioning before transplants. Lindbergh's glass perfusion pump, a forerunner of machines used in operating rooms today, is credited with helping make heart surgery and organ transplants possible.

FROM THE C&EN ARCHIVES

Read a 1943 C&EN report on the development of Pyrex, as well as other past C&EN stories about glassware

March 10, 1943 Action On The American Chemical Front: Development of Pyrex glassware based on information furnished by Corning Glass Works
(http://pubs.acs.org/doi/abs/10.1021/cen-v021n005.p312)

April 25, 1943 Proper Care Will Prolong The Life Of Chemical Glassware
(http://pubs.acs.org/doi/abs/10.1021/cen-v021n008.p552)

Nov. 25, 1944 Glass Is An Important War Material
(http://pubs.acs.org/doi/abs/10.1021/cen-v022n022.p1999)

April 30, 1951 E. E. Kimble, Pioneer In American Glassware, Honored
(http://pubs.acs.org/doi/abs/10.1021/cen-v029n018.p1738)

June 19, 1961 Controlled Nucleation And Crystallization Lead To Versatile New Glass Ceramics
(http://pubs.acs.org/doi/abs/10.1021/ccen-v039n025.p116)

Jan. 15, 1962 Kimble Expands Hard Glass Line
(http://pubs.acs.org/doi/abs/10.1021/cen-v040n003.p038)

Nov. 16, 1964 Glass—A Special Report
(http://pubs.acs.org/doi/abs/10.1021/cen-v042n046.p080)

Dec. 1, 1975 Corning And Others Join Efforts To Restore Priestley Lab
(http://pubs.acs.org/doi/abs/10.1021/cen-v053n048.p0260)

Nov. 24, 2003 What's That Stuff—Glass
(http://pubs.acs.org/cen/whatstuff/stuff/8147glass.html)

Jan. 16, 2006 Glassblowing: An Essential Craft
(http://cen.acs.org/articles/84/i3/Essential-Craft.html)

Jan. 16, 2006 Glass: Tricks Of The Trade
(http://cen.acs.org/articles/84/i3/Tricks-Trade.html)

Oct. 27, 2008 Corning Invigorates R&D
(http://cen.acs.org/articles/86/i43/Invigorating-RD.html)

Dec. 5, 2014 Donald Stookey—The Guy Who Gave Us CorningWare— Dies At 99
(http://cen.acs.org/articles/92/web/2014/12/Donald-StookeyGuy-Gave-Us-Corning.html)

The famous glass figured into another notable development in the early 1940s, when scientists used Pyrex Fernbach flasks to grow mold to produce penicillin and Pyrex rubber-stoppered bottles to package the antibiotic during its initial mass commercialization. And in the 1950s, Jonas Salk grew the original cultures for his polio vaccine in Pyrex Fernbach flasks.

Because it remains stable in the face of thermal fluctuations, Pyrex is often the material of choice for reflective optics in astronomy, Sauer adds. In the mid-1930s, the Hale Telescope at the Palomar Observatory, in California, was built using a 200-inch, 20-ton Pyrex disk. At the time, it was the largest piece of glass in the world.

In addition to research successes, the first radio message from the South Pole was transmitted over antennas made with Pyrex glass insulators. And Pyrex glass windows flew aboard the Project Mercury spacecraft in the U.S.'s first human spaceflight program.

"Pyrex has been essential to cooking and chemistry," says Catherine T. (Katie) Hunt, a retired R&D director at Dow Chemical and an ACS past-president. "Whether cooking up my favorite chocolate sauce in a microwaveable Pyrex measuring cup or synthesizing a new material in a three-neck round-bottomed flask, whether scaling up a plant production run in a glass-lined vessel or scaling down to a lab-on-a-chip biomedical device for genomic testing and individualized medicine applications—thank you, Corning, for enriching our labs and our lives with Pyrex!"

Although Corning's Pyrex remains a venerable lab product, Pyrex cookware is no longer manufactured by Corning. The firm divested its consumer products division in 1998, licensing World Kitchen to make and sell Pyrex glass and **CorningWare** ceramic products for the home. Pyrex cookware sold today in North America has also changed—it's made of less expensive soda-lime glass now, rather than the original borosilicate glass.

A utilitarian invention like Pyrex will always remain important for day-to-day home cooking and chemical and biological lab work, Sauer believes. But he admits innovation has its limits after 100 years. "Lab glassware is a mature product line, so a beaker or flask from 100 years ago is virtually unchanged."

Corning has moved on to use its early achievements in glass to develop newer products, such as optical fiber for high-speed Internet and scratch- and fracture-resistant Gorilla Glass to protect smartphone screens. But Sauer says it's a rare day when he doesn't grab some Pyrex. "I was just drinking my coffee out of a 400-mL Pyrex beaker mug this morning," he says.