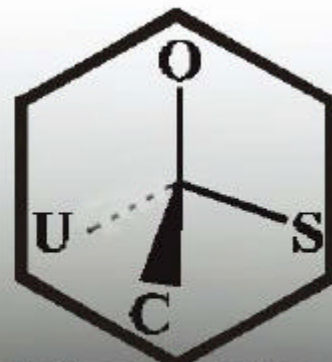


February 2004

Touch-Paper



The Newsletter of the Open University Chemistry Society

AGM elects a new Chair

The Society now has a new Chair, Carole Arnold, who was elected at the AGM held at The Great Barr Hotel, Birmingham on 1 November 2003.

Some twenty members were present for the business of the meeting, and for the Saturday lecture by member Kathie Yeowell on her work at Imperial College and the Daresbury HPCX and Sunday's Presidential Address by Lesley Smart on the work she is heading at The Open University into the development of fuel cells for various applications.

Reports were received from officers and committee members about the activities of the Society during the preceding twelve months, and ideas for events were discussed for the 2004 programme.

President's Report

News from the Chemistry Department

Simone Pitman is on maternity leave looking after Matthew, returning in January 2004, and Eleanor Crabb looking after Lucy, returning at Easter. Mike Bullivant returns in November 2003 after a year's leave spent travelling to the Far East, Australia and New Zealand. Yao Zhong-Xu and Sotiris Missailidis have been made full-time permanent lecturers, and three original members of the Chemistry Department will retire in 2004 - Keith Bolton, David Johnson and Charlie Harding.

Courses

The Faculty is seeking to cut 240 points of courses to make room for new innovations. The Department is considering having three third level courses of 20 points each, plus two residential school courses of 10 points - Chem 777 and S342. Alternatively, three third level



Carole Arnold - the new Chair of OUCS

courses of 15 points each, plus two residential school courses of 15 points - Chem 777 and S342. It is hoped to keep ST240 going, but this has not yet been finally agreed.

The Department has bid for a new course in analytical chemistry called 'Investigative Chemistry' to run as three 10 point courses, one at each level.

A new version of S343 Book 2 'Metal-Ligand Bonding' has just been written by Rob Janes and Elaine Moore, to be co-published with the RSC as part of the Molecular World series.

BBC

A new series of 'Rough Science' has just been filmed in California, starring the Department's Mike Bullivant again.

University

A memorial service was held at the OU in October for the founding Vice Chancellor, Walter Perry, and there is a web cast of this event on the OU website.

New Building

An artist, Simon Paterson, has been commissioned by the Chemistry Department and the Planetary and Space Sciences Research Institute to create a suitable artwork installation for the foyer area. The President is on the steering committee for this.



**Lesley Smart
OUCS President**

Chair's Report

In the absence of a formal Chair for the preceding year, Frank Hollis agreed to act as caretaker. Thanks were expressed to Frank for his taking on this role.

Treasurer's Report

Paul Everett reported that the bank balance at the end of October 2003 was £1229.51 and that the Society had turned round the deficit of 2001 into a small operating profit of £34.13 on a turnover of about £2000 in 2002.

This had been achieved due to making a small profit on the Revision Days, but most especially by implementing the cost-cutting measures agreed at the previous AGM, particularly by streamlining the administration of the Society. The Treasurer expressed thanks to all those who had worked to achieve these savings.

He reported that membership subscriptions were down for 2002, but marketing income had increased, despite having purchased the presentation OUCS bowls. A change in bank arrangements meant that interest is no longer received on the account, but instead the Society has unlimited transactions without charge.

Membership Secretary's Report

Carol Houghton reported that the Society had lost 195 members in 2002 taking the total to 341. Membership at November 2003 was 324, including 66 new members and 42 renewals of membership. 184 members are due to renew at the end of 2003, and urged members to renew their membership for the good of the Society and to enable its range and location of activities to be increased, thus making it attractive to potential members. It was agreed that members whose subscriptions were due would get a personal invitation to renew with the February *TouchPaper*. She urged all members to promote the Society at all possible opportunity.

Editors' Report

Sue Whitaker and Roger Beck reported that two editions of *TouchPaper* had been produced in 2002, but the aim was now to produce three editions a year of at least ten pages, and that this had been achieved for 2003. Some welcome unsolicited contributions had been received, and the Editors expressed thanks to those members who had sent them. They urged all members to be on the lookout for suitable material to include and encouraged any member who was thinking about writing a piece to contact them to discuss the details. They also aimed to use *TouchPaper* to strengthen the Society's links with the Chemistry Department by means of reporting more departmental news, and including more accounts of research and other activities by departmental members and research students. They were delighted to report the active support of Professor David Shuker, both in encouraging departmental members to contribute news and material and in arranging for the production of *TouchPaper* through central reprographics as part of departmental support. Issues about quality of some parts of the publication will be addressed directly with the person who does the

work. The Editors had updated the Introductory Edition that is sent in the first mailing of course materials to students on chemistry and related science courses, and Kevin Church had arranged for 7600 copies to be inserted for 2004 courses. Finally the Editors apologised for the delay in mailing the October 2003 edition - it became caught up in the postal strike that affected large parts of the country during that month.

Marketing Report

Carol Houghton reported that the Society held current stocks of T-shirts, sweat shirts, mugs and caps totalling £697.10. A new T-shirt design for Revision Weekends had been purchased based on the 'world tour' theme of the music industry. Polo shirts of various colours with the OUCS logo have been ordered, and new designs for T-shirts and mugs have been commissioned, especially for those attending Open Days.

It was agreed that OUCS goods will be promoted by means of a marketing leaflet for distribution and a permanent advert and order form in *TouchPaper* and on the website.

Carol reported that Janine Newburn had volunteered to take over the Marketing post, and she was welcomed to the post by the meeting. Thanks were also expressed to Carol for her hard work in producing and marketing the Society's goods.

Revision Events 2003

Pat Wilson reported that the Bristol Chemistry day had been well attended, and thanked Ruth Williams for her support and help with some of the arrangements.

Carole Arnold reported that Lorraine Durcan had taken over receipt of applications for the York weekend, Paul Everett had updated the database for courses and badges and she herself had organized the tutors and timetabling, liaised with York University and maintained the accounts. 22 staff and 186 students attended the weekend. Most sessions were very popular, but that for S204 will need more registrations to run, and those for S282 and S283 may have to be combined to be viable. 70% of the feedback forms distributed were returned, indicating satisfaction with the teaching and the venue. In order not to make a loss, the fee will have to be increased by £5 for the 2004 event.

Adverts for the Revision Events will be included in the second course mailings in 2004, in the June *TouchPaper* and on a Science Revision Website. Thanks were expressed to Pat, Carole, Lorraine, Paul and all those involved in organizing the revision events.

Future OUCS Events

Forest of Dean Weekend 20-21 March 2004

Alec Thomson is organizing an OUCS weekend in the Wye Valley and Forest of Dean, based at How Caple Grange Hotel. There are several attractions in the vicinity for members, and a committee meeting will be held on the Saturday morning. (Post-meeting note - this event has had to be postponed, details later.)

Carole Arnold announced that the AGM and Lecture Weekend was booked at The Great Barr Hotel, Birmingham, for 30-31 October, and that she was already in touch with prospective speakers.

Officers 2004-2005

Some posts will be up for election in 2004. If any member is interested in discussing what is involved in carrying out the duties, please contact Carole Arnold or any other

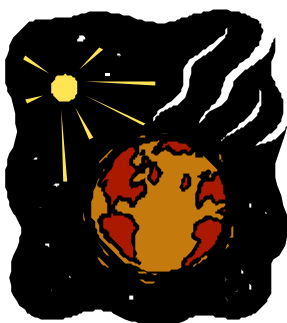
committee member.

There are vacancies for regional representatives in R01, R02, R03, R09, R12 and R13.

If you have a little time to spare and feel that there are events or places in your area that you think would be of interest to OUCS members to visit, please contact Carole or any member of the committee. We shall be delighted to hear from you, and can help you with publicity and organization if required.

Paradoxical Ozone

Climate models continue to throw up numerous paradoxes and anomalies in the predicted concentrations of ozone and thus the impact of its depletion on the environment and life on earth. Now, a Portuguese team has analysed the state of play and reckons our views of the photochemistry of this gas are at odds with what actually happens at different levels in the atmosphere. Stretched oxygen and odd hydrogen species are suggested that offer a clue to explain the so-called 'ozone deficit problem' and the 'HO_x dilemma' in the upper stratosphere and mesosphere.



Chemist António Varandas of the University of Coimbra in Portugal points out that the words 'ozone' and 'hole' have all but melded themselves to each other because of the mass media interest in the so-called hole in the ozone layer. Ozone is densest at an altitude of between 25 and 30 km, but the ozone layer that envelops our planet and protects us from ultraviolet radiation actually extends well into the mesosphere up to 85 km. At this altitude, the chemistry of ozone attains, what Varandas refers to, as its 'greatest simplicity'.

Not everything is as simple as it seems

But, simple in appearance does not necessarily mean simple to understand. Paradoxically, it is in the mesosphere that there remain several important mysteries about the chemistry of ozone that are yet to be unravelled. The clues that studies of this seemingly simple ozone chemistry might yield about its behaviour could lead to a clearer vision as to how to deal with that ozone hole.

Ozone is generally considered to form in the same straightforward photochemical way throughout the atmosphere - dioxygen is split by light and the two 'O' moieties combine with other dioxygen molecules to form the familiar O₃ system. In contrast, when it comes to ozone (odd-oxygen) destruction, it is location that is all important. Its degradation is most complex over the poles where winds, ice clouds, and low temperatures promote its reaction with halogen and nitrogen species. As Varandas goes on to explain, in the upper stratosphere and mesosphere, ozone chemistry seems mostly to be controlled by catalytic reactions involving odd hydrogen HO_x species - x = 0, hydrogen; 1, hydroxyl; 2, hydroperoxyl. The HO_x species being derived from the photochemical oxidation of water.

This chemical simplicity appeared to fit the early atmospheric models but, despite this simplicity, the models of the

1980s severely under-predicted the amount of O₃ to be observed at these high altitudes. The 50-60% shortcoming soon became known as the 'ozone deficit problem'. Advances in experimental methods during the mid-1990s, ironically, led to additional conflicts between theory and results, with some teams consistently reporting an ozone deficiency while others came up with novel ozone sources to explain their finding higher than anticipated levels. As if to complicate matters further, the so-called 'HO_x dilemma' would soon emerge from between the clouds.

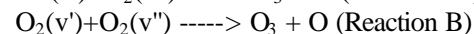
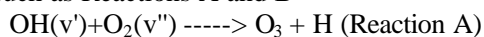
Holes in theories

Conventional models were failing atmospheric scientists experimenting in the mesosphere too, leading to holes in their theories of how HO_x photochemistry proceeds in the middle atmosphere. Hydroxyl measurements at 50 to 80 km were showing a 25-30% lower than predicted concentrations. All kinds of fudge factors were included in the kinetic analysis of the myriad species involved, with little resolution of either the ozone deficit or the HO_x dilemma.

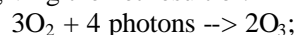
Varandas and his colleagues have now come up with a radical new theory that could reconcile both the deficit and the dilemma by demonstrating their interrelatedness. Their proposal suggests a mechanism for the formation of ozone that is based on stretched odd hydrogen and oxygen molecules under the hypothesis of non-local thermodynamic equilibrium, or as he calls it local thermodynamic disequilibrium (LTD). This being the occupation of quantum states at odds with the Boltzmann statistics appropriate at conditions of thermal equilibrium.

Local thermodynamic disequilibrium

The crucial premise in Varandas' proposal is therefore the abundance of high vibrationally-excited species in the middle atmosphere in accordance with the LTD hypothesis. Reactions such as Reactions A and B

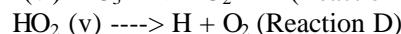
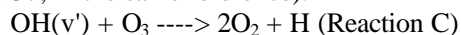


where v' and v'' represent the vibrationally-excited states of the reactant species, could then be embedded in an eight-stage reaction mechanism (Reactions 7 to 14 in Varandas' paper, in press) giving the net result of:



ozone is produced from dioxygen.

Two other reactions are key in his proposal - reactions C and D (31 and 37, in the same reference).



where v is a collective variable of three indices. (cont. over)

Chemistry/PSSRI Building on Campus - Progress Report



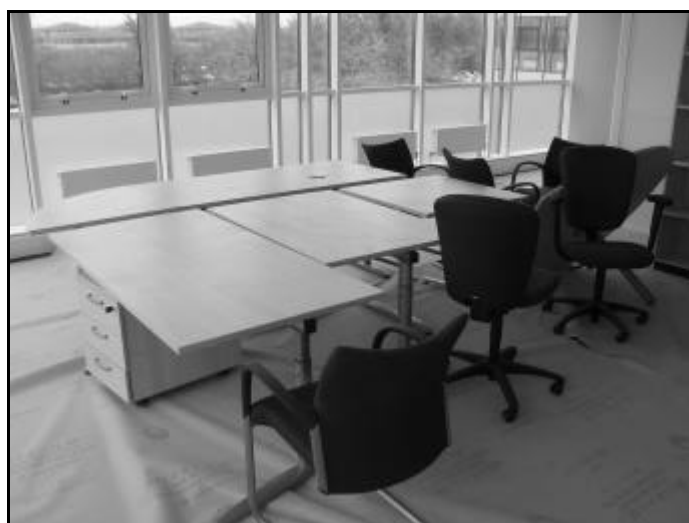
View from the East Car Park, 19 January 2004



The fume chambers are in!
November 2003



The interior, November 2003



TouchPaper editorial office in future...



When included in a mechanism involving nine elementary reactions (Reactions 16 to 24 in Varandas' paper) they lead to clues to explain the observed peak in the OH concentration at about 40 km as well as to larger concentrations of HO₂ at higher altitudes, in agreement with observation.

A hypothetical dilemma

The Coimbra team concedes that much of the paper is hypothetical, but emphasise that the concepts do find support in at least a dozen consistent theoretical studies of the elementary chemical reactions involved. They also point out that the reactions C and D, if they do indeed occur in the atmosphere, could have an effect on the profile of atomic hydrogen at different altitudes. This could be confirmed eventually by comparing actual observations with standard model simulations to see whether the theoretical H deficit is valid. There is no evidence yet even of the existence of such a deficit, but given the emergent complexity of atmospheric chemistry, almost anything might be possible given the right

observations. They also emphasise that the standard atmospheric models often incorporate hundreds of chemical reactions, a multitude of measurements on long-lived species, and many assumptions about solar light. His analysis may have the merit of simplicity, which could be a breath of fresh air for atmospheric chemists.

Reference

A J C Varandas. Are vibrationally-excited molecules a clue for the 'O₃ deficit problem' and 'HO_x dilemma' in the middle atmosphere? *J Phys Chem A*, in press. DOI:10.1021/jp036321p.

David Bradley

'The Alchemist' January 2004

Source: ChemWeb.com, <http://alchemist.chemweb.com>

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Editorial

Welcome to the February edition of *TouchPaper* for 2004. If you are a new member of OUCS we hope that you will enjoy your membership and meeting fellow members through attending events organized by the Society nationally or in your region. If you have an idea for a place to visit that you think would be of interest to the wider membership, please contact the Carole Arnold (Chair) or any other committee member.



You will read elsewhere in this edition that the new building on campus, known prosaically as 'Building 10', that will house the Department of Chemistry (and the Planetary and Space Sciences Research Institute) is due to be completed in April. This is an exciting time for the Department because of this, and we hope to bring you details and pictures of the building and its facilities that will enable the teaching and research work of the Department to be expanded after it is opened.

The AGM and Lecture Weekend last November is reported at the beginning of this *TouchPaper*, and it was good to see those members who were able to attend. It was agreed that the meeting was successful, and those present heard two highly interesting lectures from member Kathie Yeowell and our President Lesley Smart. Plans are well advanced for speakers at the next AGM and Lecture Weekend at the end of October. Put the date in your diary now, full details will be available later. If you have heard, or heard about, a chemistry or chemistry-related lecture that you thought was brilliant, tell the Society Events Organizer, Carole Arnold, about it so that she can try and lure them to the Lecture Weekend.

If you are currently studying a chemistry or related science course, you will find the dates for revision events in the autumn in the ChemSoc Diary. These events are highly valued by those who have attended them previously - comments like 'being worth at least a grade higher in the course result' have been heard! Full details and booking forms will be sent in the next *TouchPaper*, and will be posted on the FirstClass conference and the OUCS website.

We would like to say that we have been inundated with material for *TouchPaper* but we haven't!! It's hard to believe that no one has been anywhere, seen anything or heard anything that would be of interest to fellow OUCS members, but we have to assume from the evidence that this is the case. So we shall continue to use our judgement in producing material for inclusion from our own sources, and take silence as assent to its content, unless your letter box acts as a revolving door to the recycling bin!

Best wishes for your studies, tutoring or research in 2004 - or whatever you are just about to write about!

Roger Beck and Sue Whitaker
Joint Editors

Course reviews - the inside story

Have you done a current OU chemistry or related course? Would you be prepared to write a course review for *TouchPaper*? If so, please contact the Editors who will commission you to write a piece of up to 500 words about the course, warts and all, that you think would be helpful to others contemplating taking that course. The committee has agreed that a fee of £10 will be paid to those who write a commissioned course review that is published.



I thought I took the red pill.....

ChemSoc Diary

20-21 March 2004

Committee Meeting

18 September 2004

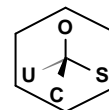
Bristol Revision Day for S205, ST240, S343 and S344 (details from Pat Wilson and in June 2004 *TouchPaper*) Your course not included????? Contact Pat!

1-3 October 2004

York Science Revision Weekend for ST240, S204, S205, S207, S216, S269, S282, S283, S343, S344, SD329, S381, S357, SMT356 (details from Lorraine Durcan and in June 2004 *TouchPaper*)

30-31 October 2004

AGM and Lecture Weekend at The Great Barr Hotel, Birmingham (details in June 2004 *TouchPaper*)



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?	A Problem for Chemists.....																?		
?	?	?	?	?	?	?	?	?	?	?	?	?	?	?	?	?	?	?	?

What was created in 1843, has covered over a million miles, yet if something is not done within the next four years will suffer irretrievable loss to its fabric?

Answer - Isambard Kingdom Brunel's revolutionary ship, the ss Great Britain.

The past

The ss Great Britain was built in 1843 in the specially constructed Great Western Dockyard in Bristol for the Great Western Steamship Company by Brunel, along with Thomas Guppy, Christopher Claxton and William Patterson. Today she is recognized as one of the technological fore-runners of much modern shipping, and exemplifies the industry and inventiveness of the Victorian era and the birth of international passenger travel. She is over 320 feet long, 50 feet wide and originally weighed 1930 tons. She has 165 wrought iron frames, arranged in 20 overlapping 'strakes' with each strake fabricated from butt-jointed wrought iron plates around 180 cm x 60 cm. Originally conceived as a paddle steamer, her constructors quickly saw the advantages that the new technology of screw propulsion could give the vessel, and converted her and her engines to power a sixteen foot iron propeller. At the time of her launch in 1843 she was by far the largest ship in the world, over 100 feet longer than her rivals, and the first screw-propelled, ocean-going, wrought iron ship.

1839-1846 Luxury Passenger Liner

She was designed initially for the Trans-Atlantic luxury passenger trade to carry 252 first and second class passengers and 130 crew. Her first few voyages successfully demonstrated her potential, but were not great financial successes, with far fewer passengers than anticipated. Her career in this trade was short-lived, as she ran aground on the sands of Dundrum Bay in Northern Ireland in 1846. Although her hull was not badly damaged, her engines were ruined, and the expense of re-floating her did great damage to the financial resources of her owners. She was the first screw propeller-driven iron ship to cross the Atlantic, and the first ship to have a six-masted schooner rig and clipper bows. She also pioneered waterproof bulkheads, iron wire rigging, a balanced rudder, iron lifeboats and a 'patent log' to establish the distance travelled.

1852-1876 Emigrant Clipper

Under Gibbs Bright and Co, the ship prospered, and the new owners took advantage of the upsurge in emigration that the Australian gold rush encouraged, and re-built the ship, to use her as a fast and luxurious emigrant carrier, taking people to Australia. A 300 foot long deck house was added to the ship's upper deck, a new 500 hp, Penn



The ss Great Britain beached in the Falkland Islands

engine was fitted, and her internal accommodation was rebuilt to allow her to transport 750 passengers in three classes. She now had a radically different external appearance, being lower in the water, with more massive superstructure and twin funnels. For her initial voyage, she carried four masts – two 'fore and aft' and two square sails. After this voyage she was re-masted, to carry three masts, all square sails. Over the next 24 years and 32 voyages she was a frequent sight in Australian waters, as well as making stops in Cape Town, St Helena, and the odd trip to New York. The ship averaged 60 days out and 60 days home - a very fast time for the nineteenth century, and carried over 15 000 emigrants.

1854-1870's Troops, horses and cricket teams

Between 1854 and 1855 and she was chartered by the Government to carry troops to and from the Crimean War. At one stage she carried 1650 French troops, as well as 30 horses. Over the course of the conflict, the vessel carried over 44 000 troops. Following this episode she was again rebuilt, with her hurricane deck expanded breadthways to her bulwarks. This deck was henceforth known as the 'Spar' deck. Her masts were re-positioned, and a new, wider funnel replaced the earlier twin funnels. In this configuration she was again chartered by the Government for a further trooping voyage, carrying the 17th Lancers and 8th Hussars to the Indian Mutiny. In 1861 she carried the first ever English cricket team to tour Australia - they won 6, drew 4 and lost 2! She took the second team in 1863, which included E M Grace, brother of Dr W G Grace, later the Captain of the English side.

1882-1886 Windjammer

By the late 1870's the ship was showing her age, and her owners were not able to maintain their full registration as a passenger vessel. However, the ship was still serviceable, and her sleek hull profile allowed her easy conversion into a fast three-masted sailing ship. Her engines were removed, as was her upper 'Spar' deck, and her hull was clad with pitch pine sheathing. In this guise, barely recognizable as the same vessel launched in 1843, she took Welsh coal to San Francisco around Cape Horn. On her third trip, however, she ran into trouble around the Cape, and was forced to run for shelter in Port Stanley, in the Falkland Islands. Her owners were not willing to have her repaired, and she was sold as a coal and wool storage hulk in Port Stanley.

1886-1970 Coal Hulk

Here she remained through the First World War, with coal from her hold helping to replenish the battle cruisers *Inflexible* and *Invincible* before the decisive battle of the Falkland Islands on 7 December 1914, in which the armoured cruisers *Gneisenau* and *Scharnhorst*, and light cruisers *Nurnberg* and *Leipzig* were sunk. By 1937 the ss Great Britain's hull was no longer watertight, and after being towed a short distance from Port Stanley, she was beached, holes were driven in her sides, and she was abandoned to the elements.

Even there her historic significance was recognised, as witnessed by attempts to rescue her in the late 1930's and 1960's, and by the raffle of souvenirs from her during the Second World War to raise funds for the purchase of Spitfires. Finally, in 1970, an epic salvage effort re-floated the ship, and she was towed back home across the Atlantic to Bristol. Her new life began, and she works today as an educational resource and international monument for current and future generations.

The future

The ss Great Britain Trust has decided to preserve all the original material from the ship's 127 year career. In January 2003 Eura Conservation, a company of specialist iron conservators, began work on areas of the hull above the waterline. The lower part of the hull will be enclosed in a dehumidified chamber beneath a glass plate, covered in water, built around the ship at her waterline. However, the topsides will still be exposed to the elements, and careful conservation treatment is needed to protect them from the risk of further chloride-accelerated corrosion. In areas where the iron is particularly fragile, the surface is being cleaned with blasting apparatus, which uses ground garnet to abrade the paint and rust. The bare metal surface, which is a dull grey colour after this cleaning process, is then given a coat of special protective paint to prevent further corrosion from taking place. After the first coat of paint has been applied, holes will be re-patched with new epoxy-based fibreglass.

In other areas, where the iron has not suffered severe corrosion, a different cleaning method - hydro-blasting - can be used to remove rust and paint. Once the whole surface has been cleaned and patched, a top-coat of protective paint will be applied. This should be effective in preventing corrosion for the next twenty years. Meanwhile, steel plates are being fixed over the ship's gunwales and welded to the steel deck. Once the deck and the gunwales have been made watertight it will be much easier to protect the original iron of the ss Great Britain from further



corrosion. The Eura team are also creating ducts for the circulation of dehumidified air within the ship's interior, since dehumidification has been identified as the best way of preventing further corrosion. The dehumidification plan aims to construct a flat glass plate roof at the level of the ship's waterline with a moisture-tight seal between the ship and the dry dock. Machinery will be used to dehumidify the interior and lower exterior of the ship to a relative humidity of around 20% (the level at which iron will stop rusting). The ship will appear to be afloat in the dry-dock, with visitors able to descend beneath the 'water' to view the ship's submerged hull.

In addition, the ship's structure will be supported where it has been weakened by corrosion and other damage.

Repairs to the dry dock and the caisson are necessary in order to maintain a safe and stable dehumidified environment for the ship.

Visiting

The ss Great Britain was visited in December 2003 by Pat Wilson, Sue Whitaker and Roger Beck. A really fascinating visit to see this wonderful ship and the essential but careful conservation work that is taking place.

The ss Great Britain is open daily except Christmas Eve and Christmas Day from 10 am to 5.30 pm (April - October) and 10 am to 4.30 pm (November - March).

Adults £6.25, Seniors £5.25, Children £3.75. Student concessions are available.

Tel: 0117 922 5737

With acknowledgements to the ss Great Britain Trust for the material adapted for this article.



The launch of the ss Great Britain in 1843



Isambard Kingdom Brunel



The balanced rudder and 16 foot propeller

What about combining a visit with the Bristol Revision Day on 18 September?

System Failure!!!!

My friend is having trouble with her system.

Last year she upgraded to Boyfriend 1.0 from GirlPower 4.2 which she'd used for years without trouble.

However, apparently there are conflicts between the two systems, and the only solution was to try and run Boyfriend 1.0 with the sound turned off. But to make matters worse, Boyfriend 1.0 is incompatible with several other applications, such as GirliesNightOut 3.1, Hunk 2.0 and Shopaholic 6.0.

Successive versions of Boyfriend proved no better; Boyfriend 3.0 has many bugs and left a virus in her system, forcing her to shut down completely for several weeks. Eventually she tried installing Boyfriend 2.1 as well as Boyfriend 1.0 only to discover when these two systems detected each other they caused severe damage to all her hardware.

Sensing a way out, she upgraded to Fiancé 1.0 only to discover to her dismay that this system requires rapid upgrading to Husband 1.0. However, whilst Husband 1.0 does come bundled with FreeSexPlus, it uses up all available resources, and is always crashing after infection with the smallest virus. It also installs TrashHouse 2000 which cannot be deleted from her system.

She also discovered that Husband 1.0 can be unstable



and costly to maintain. Any mistakes she makes are automatically stored in Husband 1.0 hard drive, cannot be deleted, and then resurface months later. Husband 1.0 also has an encrypted InterDiary Explorer, e-mail Porn-Search and is incompatible with any versions of Garden-QuickTime. Husband 1.0 also automatically runs PHOTOStrop, WINGZip and BlokePowerPoint, and no option on the Help Menu seems to work, leaving her to try and guess the fault herself.

The system footprint needs updating regularly requiring GadgetShop Browser Pro for new attachments, and LagerXpress needs to be re-installed every week. Husband 1.0 also comes with automatic downloads of new games and attachments, like MountainBiker 4.0 and SoccerSeasonTicket 2.0, that are recognized as illegal operations by her system. When Husband 1.0 attaches itself to HerCar 286 it often crashes or empties the system resources. Husband 1.0 also has a rather annoying pop-up called Mother-in-Law, which can't be turned off.

Recently she's been tempted to try Lover XP add-on, but there could be problems. If Husband 1.0 detects the presence of Lover XP, it will delete all MS Money files before un-installing itself.

Adapted from an original courtesy of
Peter Wood, Chief of Operations
First Base Technologies

How to Determine the Origins of Whiskey



Some of the earliest applications of chemometrics in the 1970s and 1980s were in the brewing industry, where it is important to check the quality of alcoholic beverages.

There are many reasons - one being to see whether an expensive brand name has been watered down or adulterated, another to check the quality of a product before it reaches the market.

A classic example relates to whiskey, more details being available in a well known paper published in 1978 and used as an example in Brian Rock's Website 'Introduction to Chemometrics'.

Origins of whiskey

How can we determine the origin of a whiskey? A problem is to check the authenticity of expensive brand-names. How can we be sure that a whiskey selling at £20 is really the true thing? Of course taste is an important factor, but it could be argued is not conclusive. What happens if someone opens up a bottle of expensive whiskey, tastes it, believes it is a little strange and then reports this, or someone orders a drink in a bar and feels that the whiskey is not quite the usual quality? This is unlikely to be used as conclusive evidence, maybe the customer has already had several drinks or maybe has opened a bottle and wants another one free. And how do customs officers test imported whiskey? Clearly it would be impracticable for them to spend all day drinking samples of every type of whiskey bottle that passes through their hands. So some analytical technique needs to be used.

Gas chromatography

Gas chromatography is ideal since whiskey can be injected straight onto a column, and the volatiles are then separated. Also GCs are portable and it is not necessary to bring the samples into specialised laboratories. One important aspect of pattern recognition methods is that it is not necessary to identify and assign every peak to a chemical constituent before coming to a conclusion. We are not really interested in the identities of the chemicals, mainly what the origin is of the whiskey.

There is some complexity in the analysis because whiskey can change in nature once a bottle is opened. So we are not only interested in brand new bottles, but ones that have been opened first. An experienced whiskey taster has first to open the bottle before he can check its flavour. Sometimes a bottle may have been open for a few days, for example in a bar, before the adulteration is suspected. A first step is to perform GC on a series of whiskeys. In the case reported, the aim was to distinguish an expensive whiskey called Chivas from other less expensive brands. Three groups were examined, 34 non-Chivas (NC) samples coming from a variety of cheaper sources, 24 Chivas (C) samples from bottles that were opened first for analysis, and 9 used bottles of Chivas (U). The aim is to be able to distinguish NC from C and U groups.

Principal Components Analysis

How can this be done? GC identifies 17 peaks common to all 67 samples. Using some data pre-processing it is possible to perform Principal Components Analysis (see Principal Components Analysis: Basic Ideas), and separation between the two groups NC and C and U. However, the line separating the two classes using a PC plot

(continued over)

is arbitrary and although promising, we want a somewhat more reliable approach.

Discriminant analysis

The next step is to discriminate between the groups. There are numerous approaches, but one method is to first determine which of the 17 peaks are going to be good at separating the groups. For each peak, a Fisher weight can be calculated, that indicates how well a feature separates two groups. It is quite simple and involves calculating the ratio between the square of the difference of the means of two groups to the sum of their variances. So for example, if the mean value of feature 1 for group A is 17, and for group B is 23, then the Fisher weight is 36 ($= [23-17]^2$) divided by the sum of the variances. The reason why the squared difference between the means is not used alone is that variables may be on different scales and so this technique enables the identification of small but diagnostic features that may not be obvious at first but are good at discriminating.

In this particular study we would like to find features that have high weights for separating both NC from C, and NC from U, but low weights separating U from C. In the published work, 6 main features were identified.

The final step is to perform discriminant analysis for these features, using approaches such as SIMCA (see Classification by Soft Modelling) and K Nearest Neighbours (see Nearest Neighbour Method for Classification). More modern methods such as support vector machines and neural networks may also be employed. As is usual the models can be validated in the normal way, and an automated approach used to determine whether a GC of a whiskey indicates it is authentic or not. Naturally these approaches have been continually refined over the years and are used in the brewing industry. Pattern recognition techniques are still not yet admissible as conclusive evidence in court, but they can very effectively identify adulteration, allowing a comprehensive and more expensive investiga-

tion of a small number of products suspected to be adulterated. Chemometrics combined with chromatography is very effective in narrowing down the number of suspect samples.

Reference

B E H Saxberg, D L Duewer, J L Booker and B R Kowalski. *Anal Chim Acta* 1978, **103**: 201–212.

Richard Breton

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OUCS visits the Dinosaur Coast - March 2003



Will Watts telling members about the geology and fauna - can you spot the dinosaur!

16 members and friends visited Scarborough for a weekend of activities in the town or to pamper themselves in the spa facilities. The committee met on

the Saturday morning. The highlight of the weekend was a guided walk and presentation by Will Watts, The dinosaur Coast Projects Officer, on the large reptilian fauna and geology of the Middle Jurassic fossiliferous rocks for which the area is famous. More details at www.yorkshirecoast.co.uk/scarb/index.htm

These are alleged to be error messages, that cause us to reach for the large hammer.....

A crash reduces
Your expensive computer
To a simple stone

Having been erased
The document you're seeking
Must now be re-typed

Yesterday it worked.
Today it is not working.
Windows is like that.

Chaos reigns within.
Reflect, repent and reboot.
Order shall return.

The Web site you seek
Cannot be located, but
countless more exist

Your file was so
big.
It might be very
useful.
But now it has
gone.

Windows NT crashed.
I am the Blue Screen of death.
No one hears your screams.

Program aborting.
Close all that you have worked on.
You ask far too much.

Three things are certain:
Death, taxes and lost data.
Guess which has occurred.

Serious error.
All shortcuts have disappeared.
Screen. Mind. Both are blank.

Stay the patient course.
Of little worth is your ire.
The network is down..



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There are vacancies for reps in Regions 01, 02, 03, 09, 12 and 13. If you have a little time to spare and feel that there are events or places in your area that you think would be of interest to OUCS members to visit, please contact Carole Arnold or any member of the committee. We shall be delighted to hear from you. Help is available with publicity and organization if required.

THANKS

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TouchPaper Schedule

It is planned to produce issues at the end of January, May and September each year. Please let the Editors have material for inclusion by the beginning of these months.



Presidents of OUCS

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1998-2000 Dr Ruth Williams

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2002-2004 Dr Lesley Smart