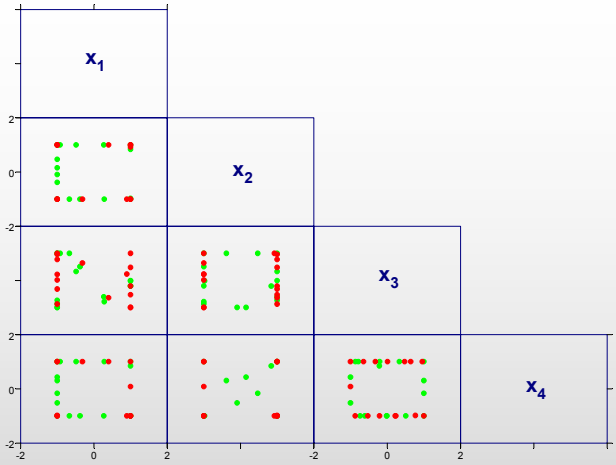
Design and Analysis of Experiments

Salt screening

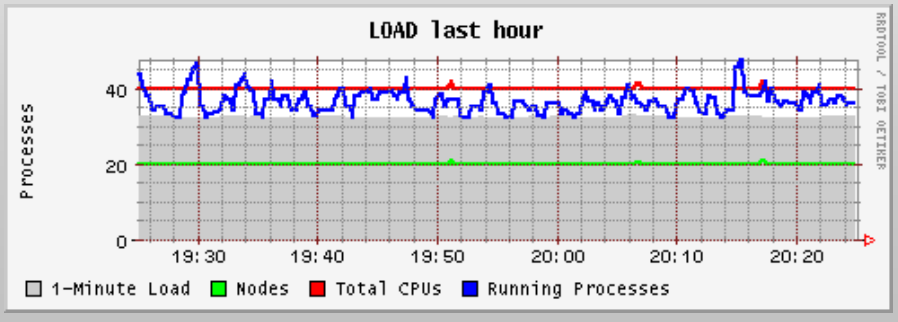
Combechem statisticians (David Woods, Susan Lewis) and crystallographers (Suzanna Ward and Mike Hursthouse) in Combechem are working on salt screening experiments for modelling the probability of new product formation in terms of several variables.

This led to research on designs for a class of nonlinear statistical models called generalised linear models and collaboration with John Eccleston (Queensland, Australia) and Ken Russell (Wollongong, Australia).

A new design criterion has been formulated which allows an efficient compromise to be made over a variety of models. Computer intensive algorithms for finding and assessing these *compromise* designs are run on a 20 node Beowulf cluster at Southampton Statistical Sciences Research Institute.



Projections for two compromise designs ● and ● under logistic regression



Design and Analysis of Experiments

Optimisation of a chiral catalyst Through designed experiments

Combechem (David Woods, Susan Lewis) has developed and run experiments using D- and V-optimal designs from computer search in collaboration with Mark Bradley and Katie McNamara of the Combinatorial Centre of Excellence. Optimisation of a chiral catalyst for enantiomeric excess (ee) is being achieved through screening and follow-up studies on 9 variables, including solvent descriptors and operating conditions. This approach allows clear interpretation of results and interrogation of fitted surfaces.

Further work

(Robert Stapleton and Susan Lewis) motivated by combinatorial chemistry experiments is the development of designs to discover which variables, from a large number of possibilities, have the greatest impact when experiments are run in arrays, such as wellplates, and when a linear model describes the observations.

solvent	base	equivalence of base	equivalence of reagent	additive
17	I	1	-1	yes
17	II	-1	1	no
30	I	1	1	no
30	II	-1	-1	yes
71	II	1	-1	no
71	I	-1	1	yes
89	II	1	1	yes
89	I	-1	-1	no
43	I	0	0	yes
58	II	0	0	no