



smarttea.org

# Smart Tea Project I A M

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## Replacing Lab Books

The lab book is a big block to publication@source, if it's not digital, it's difficult to share. Most experimental information is recorded in a lab book in a highly personal way. We have created a new analogy to fully understand the use of the lab book and successfully built and evaluated a working electronic replacement.

Observations and interviews ensured that we understood the chemistry lab environment. But we needed more than a general sense of what chemists did, how they did it or the role the lab book played.

A new user centred design technique was needed.

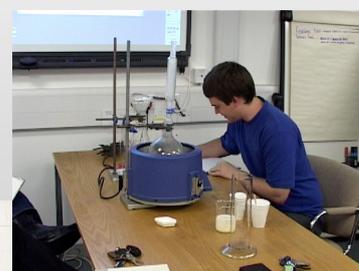


## Making Tea

Our resident chemist made tea as a chemistry experiment. A safe, repeatable procedure that we understood and could interrogate from the chemist's perspective. The analogy gave us a way to compress design time and had a language we (chemists and designers) could all understand.

Making tea gave us a way to ask questions that would not otherwise have been possible.

The process allowed us to learn what notes are taken and what information is omitted, "because it's obvious".



100ml Tea  
20 ml Milk  
3g Sugar  
Boil for 2 minutes

## The Software

A prototype electronic lab book has been built and evaluated. The system runs on a Tablet PC using the pen as the sole method of data entry. The chemist can take the tablet anywhere they go in the lab. The portable nature of the device is exploited by using Web services and wireless networking to remotely supply the tablet with all data. Chemists liked the idea of their data being instantly available, but 'safe'.



The system in use during evaluation trials. Chemistry experiments were performed solely using the system without the use of normal lab books. The various interface screens were designed to be run on a portable, Tablet PC or on separate fixed terminals. We intend to explore pervasive computing issues of the best ways to deploy the system.

Weigh-Station #1  
Sep 19, 2003 2:51:28 PM

mrg mrg/3828/4

Experiment Details

Name	Planned	Actual
Ethanolamine acetate	0.2500 g	0.2516 g
4chloro dipicolinic acid monoh...	0.5000 g	0.4950 g
Triethylamine	0.6 ml	0.6 ml
Methanol	100.0 ml	110.0 ml
Acetone	30.0 ml	0.0 ml

7 8 9  
4 5 6  
1 2 3  
0 .

Enter Del

All measurements completed.

120-1111-1000x | 202-2022-100x | 303-3033-500x | 444-4444-1000x | 999-1000-1000x

Escape

Out Weigh Liquid-Measure Bench Store

Interface for entering weights and measures showing ingredients and their planned amounts.

Bench-Station #1  
22-Sep-2003 16:01:39

dj djbj3403

Experiment Details

Stage	Instructions	Done
1	Decative 4-fluorinated biphenyl in butanone	<input type="checkbox"/>
2	Add K2CO3 powder	<input type="checkbox"/>
3	Heat at reflux for 1.5 hours	<input type="checkbox"/>
4	Cool and add Br110CB	<input type="checkbox"/>
5	Heat at reflux until completion	<input type="checkbox"/>
6	Cool and add water (20ml)	<input type="checkbox"/>
7	Extract with DCM (2x50ml)	<input type="checkbox"/>
8	Combine organics, dry over MgSO4 & filter	<input type="checkbox"/>
9	Remove solvent in vacuo	<input type="checkbox"/>

TIC

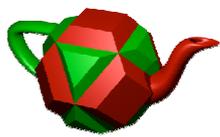
2 of 10 tasks completed.

Escape

Out Weigh Liquid-Measure Bench Store

The steps of the procedure with an area for freehand note taking. Each step has a separate area for taking observations.

We are now developing an OWL ontology for the plan and record of an experiment. An architecture of semantic services to support the tablet and other systems is also in development.



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## Interaction

To support the notion of publish@Source for the eScientist - End to end support of data capture and data access for scientists throughout the experimental process.

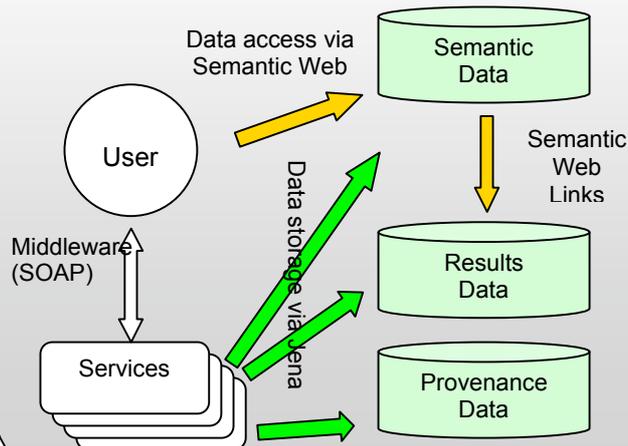
Making Tea gave us a new design elicitation method and a successful way to model the interaction. However the tablet was a prototype built without proper architecture or underlying storage model.



The Smart Tea project is now concentrating on developing process and record ontologies, addressing issues of provenance and designing the system architecture.

## Architecture

As services are used, the resulting data, the provenance of that data, and the semantic links between the data are recorded. The semantic links form the core of the publish@Source resource.



## Ontology development

Our ontology describes the plan and record of an experiment. It has been designed from a detailed understanding of real experiments in conjunction with chemists and knowledge representation experts. This diagram shows a fragment of the full diagram of a simple procedure. Once perfected it was used to design the OWL representation. A semantic storage system is in development.

An experiment plan consists of an Ingredients list plus a planned set of steps. The plan and record stages are distinct in the ontology.

The corresponding record showing processes and observations. Observations may be simple or the results of complex processes such as NMR spectra.

In-silico (software) chemistry processes can also be represented.

