Virtual Organisation design and application: A chemicals industry case study

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Abstract
This paper describes the application of technology developed by the EPSRC e-Science Pilot Project GOLD to a case study of a current chemicals R&D project. It illustrates the appropriateness of the Virtual Organisation model to highly complex and dynamic projects and the need and urgency to deploy VO technology in a knowledge economy.

1. Background

The UK fine chemical industries[1] have a $9 - $12 billion share of the $250 billion global markets. Manufacturers focus on new product development as a means of growth with time to market as the primary driver. Because of increasing competition it is now recognised that more structured mechanisms for managing the innovation process must emerge if companies are to extract maximum profitability.

An increasing trend to outsource services creates a supply network of specialist companies interacting with manufacturers. Different specialist companies may be involved at all stages in the R&D lifecycle, providing services ranging from basic research or safety testing, to commercial services. Many chemical companies use contract and toll manufacturers to increase capacity, retain flexibility and access specialist technology. Contract or custom manufacturers buy in raw materials and ship out finished product directly to the client customer. Toll manufacturers hire out plant and the client supplies all the raw materials.

Coalitions of this type are examples of Virtual Organisations (VOs). VOs are collections of organisations working together and sharing resources to achieve a set of common goals. Within this context, a chemicals R&D project is analogous to a VO, with a set of member organisations overlapping to various degrees with other projects. A large chemical company may operate hundreds of R&D projects, each with a VO of unique composition. Each project is a highly dynamic entity in which members, roles, relationships and even goals, directions, success criteria etc. may change frequently and rapidly in response to decisions made throughout the its lifecycle.

This paper describes a case study in chemical process development, conducted as part of the GOLD project. It explains the dynamic nature of such projects and how the VO concept is particularly conducive to their management. The paper then describes the GOLD VO software and explains how it was configured to represent the CPD (Chemical Process Development) project for proof of concept and demonstration purposes. Finally, it describes how the CPD project might have benefited from using the GOLD software.

[1] In the context of this document, 'chemical industries' means fine, pharmaceutical, agrochemical and other speciality chemical sectors.

2. Chemical Development Case Study

2.1 Overview

This case study is based on an actual chemical process development (CPD) project which has been in progress for just over 1 year and has currently reached Phase 3 of the plan described below. The project is being conducted in parallel with the GOLD software development phase and the two projects have close ties as one of the GOLD chemical engineering investigators provides professional services to the CPD project. The company initiating the CPD project[2] and providing high-level project management owns and operates existing batch processing plant that produces a widely-used chemical. The plant is approaching the end of its serviceable life and therefore needs either:

- A major refit to bring it up to date; or
- To be phased out/sold and a new plant built to replace it.

Eau de Chem chose the second option and at the same time decided to convert from batch to the more modern continuous operation. In making this decision it was recognised that new technology would have to be developed and that the outcome was far from certain: such a conversion can be highly complex and may turn out to be unfeasible or impractical. A VO approach for the project was adopted at the outset because the range of skills required is not available in either Eau de Chem or any single contractor. In addition the VO approach offers substantial cost savings, as will become clear.

In the following discussions, the role undertaken by the chemical engineer from the GOLD project team is that of the Reaction Engineering Consultant (RE),

[2] For confidentiality purposes, it will be known in this paper as Eau de Chem.

providing amongst other things a laboratory service analysing the details of the chemical reactions involved in the process; assessing the reaction kinetics; and reactor simulation and design. In addition to Eau de Chem and RE, there are a number of other project (VO) members providing a range of different specialist knowledge and skills when required. These participants include Pilot Plant Designers (PPD); Equipment Vendors (EV); Equipment Manufacturers (EM); and a Term Contractor providing engineering, procurement and construction services (TC). Figure 1 shows the VO configuration that had been established at the end of Phase 1, with solid arrows indicating relatively fixed relationships and dashed arrows representing more uncertain ones.

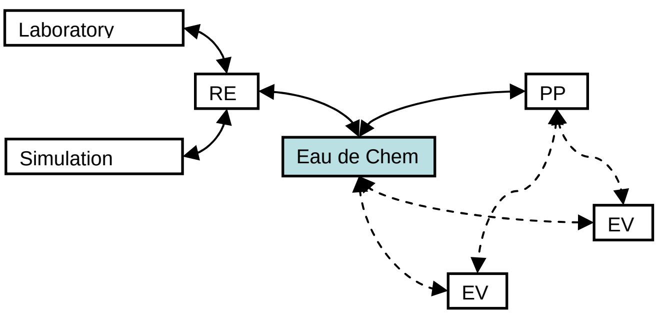

Figure 1: The structure of the Chemical Development Project at the end of Phase 1

2.2 Dynamic nature of CPD

The chemical R&D lifecycle is highly dynamic. Unanticipated changes in direction may occur at any time. The entire plan for developing a given product will not be known at the outset. It is not just that the details haven't been worked out yet: it is that even apparently unimportant details might have a significant effect on high-level project plans. For example, a need for different or additional outsourcing of specialist services may become apparent as project knowledge increases. Similarly, the operational, technical and legal basis of how a company accesses another's resources or the goals and criteria for the project's success may evolve as the result of environmental changes. Everything about a CPD project can change in unexpected directions at any time. It is crucial that the VO remain agile and flexible in order to respond to changes of this type and ensure that efficiency increases and time to market is minimised.

The initial project plan for the CPD project was based on 4 phases:

Phase 1 Preliminary laboratory / modelling investigations to determine whether the conversion from batch to continuous operation is feasible. Preliminary trials of downstream processing separation methods.

Phase 2 Design of a pilot plant using information collected in Phase 1.

Phase 3 Build and operation of the pilot plant to identify suitable modes of operation, potential problems with start-up/shut-down etc.

Phase 4 Design and build of the full production plant

Although this plan seems superficially straightforward, it is virtually certain that even small change in the project technology or the business environment may change even this high-level view, with further ramifications at every level of detail. Risk analysis revealed the following at the beginning of the project:

Conversion not feasible Conversion of the process to continuous operation may not be feasible for variety of reasons. For example, the chemical reactions may not be compatible with continuous operation. In which case upgrading existing batch plant may be the only option.

Downstream processing problems The new operating conditions might unexpectedly affect the downstream recovery of the catalyst and a new separation method must be found. This may require modification to the VO membership through the introduction of a new specialist partner.

2.3 Dynamic changes occurring during the course of Phase 1 and Phase 2 of the project

During Phase 1 the chemistry required for continuous operation was found to work well. However, downstream separation of the catalyst proved problematic using filtration technology. Trials using alternative continuous centrifuge technology were therefore initiated with a different equipment supplier.

Following the success of the chemistry a decision was made to move on to Phase 2 and the project transferred from an R&D budget to a capital budget and a new set of managers in a different country became involved. Phase 1 Centrifuge trials were now to be conducted during Phase 2.

Towards the end of Phase 2, a completely unexpected external event occurred: the supplier of the catalyst – a vital component of the reaction - ceased to operate without warning. It was therefore necessary to find a new supplier, but this was complicated by the fact that the catalyst is a naturally occurring substance and its properties vary considerably with the geographical region supplying it.

A new catalyst source joined the VO and Phase 1 Chemistry had to be restarted to ensure that its product was an adequate replacement. The catalyst worked well with the old batch plant but not in continuous operation laboratory trials. Many more catalysts had to be investigated and potential suppliers became temporary members of the VO. This also meant that the separation trials had also to be restarted.

The managers associated with the capital budget now required rapid communication of progress across all aspects the project including the now continuously changing pilot plant design and suppliers of catalysts. Project coordination and communication became increasingly important as the capital budget had been set and the decision to move to Phase 3 had to be made before the end of the financial year. This restriction had ramifications across the entire the project.

Another event also occurred at this point, Eau de Chem became involved in a company acquisition. This meant that an additional reporting structure for the VO needed to be put in to place quickly across other organisational boundaries. By the end of phase 2, the whole nature of the VO had changed, with many more companies and management groups being involved and the expectations of those companies differing from the expectations at the outset. In particular, the rate of expected progress of the project had been significantly increased due to the pressures of the financial year end.

Figure 2 indicates the implications of dynamic events in the CPD environment on the project, showing the more complex structure of the VO and the additional tasks required to complete the project during Phase 2.

3. The CPD as a virtual organisation

When unexpected events occurred, the CPD VO members collaborated to find a solution. This contrasts with a more conventional outsourcing model, where projects tend to be tree structured, with communication taking place more or less entirely up and down the branches.

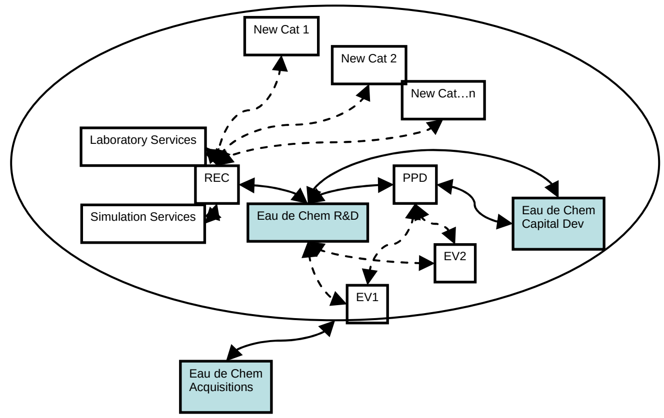

Figure 2: Complexity increases as unexpected events occur

VOs are more network-like in structure and therefore able to bring the full range of skills and resources belonging to their member organisations to bear on problems to solve them more efficiently. The CPD project was able to respond in an agile fashion, dynamically reconfiguring itself to address the new environment. Naturally, this agility is not without resource implications. In this case, the principle cost is the management effort required to coordinate the various partners and force effective communication. Urgency was also a factor, since the project was now operating on capital budget and so had to be completed by the financial year end. The potential cost of missed opportunity was therefore very great.

If this were the only project Eau De Chem participated in, the management costs might be tolerable. However, this is not the case: the same companies and the same managers are typically involved in several other development projects of similar complexity, but comprising different team membership and at different stages of lifecycle. The resources needed to maintain all CPD projects as agile as the above are simply not available. This is a difficulty that most chemical companies face.

To address this problem, software support for VOs is required. With appropriate middleware aimed at overcoming organisational boundaries, a group of separate organisations may function as a single organisation for the purposes of a project. This affords the opportunity for agile working with only linear management costs as project complexity and number of projects increases.

4. GOLD VOs

GOLD considers a virtual organisation to be *virtually an organisation*. In other words, it must exhibit some characteristic properties of a conventional organisation without actually being one [10, 11]. GOLD has developed service-based middleware, which helps to overcome organisational boundaries and facilitate this. The principle organisational properties considered in GOLD are:

4.1 Security

A conventional organisation typically has access to a variety of resources, such as services, physical resources, staff, information, knowledge etc. which it can bring to bear on problems in a more or less agile fashion. In VOs, these resources are distributed between the partners and access to them must be provided to other companies when required. An appropriate security infrastructure must be employed to provide access to resources across organisational boundaries [11, 12], without removing control of this access from the resource owner. To address this need, GOLD has developed a Role-Based Access Control scheme [1, 2], which uses XMACL policies to describe how a resource may be accessed and under what conditions. This is a very flexible approach, but may be difficult to manage since policies might contradict each other, leading to access control problems. This is particularly likely in a VO environment since the potentially large numbers of partners are unlikely to coordinate when defining their security policies. For this reason, GOLD has developed a tool [9] allowing policies to be verified mathematically against each other, assuring that no problems occur.

4.2 Trust

Trust plays an important role in conventional organisations, outsourcing relationships and supply chains. GOLD research indicates that trust between companies is based largely on familiarity, with reputation playing a lesser, but still important role.

However, in a VO environment, companies may indeed find themselves doing business with unfamiliar organisations, due to the necessity of dynamism. An example in the chemicals industry is REACH[3]: recent EU legislation regarding the central registration of chemical substances, which obligate companies to form consortia – potentially even with their competitors – to complete registration. The nature of trust in a dynamic environment may be quite different to trust in conventional organisations. GOLD provides mechanisms [3, 4, 5, 6] to protect the interest of companies in situations where conventional trust cannot necessarily be developed. These include: a non-repudiation service, which allows messages to be signed and counter-signed in a three-phase protocol, so that no involved party can subsequently claim that they did not receive the message; a secure audit trail for storing non-repudiable messages; and an electronic contracts system, whereby the rights and obligations of an organisation within some relationship can be specified. Together, these mechanisms can be used to generate evidence in the event of a dispute. Although these mechanisms are no substitute for trust through familiarity and experience, they provide a means of governance and monitoring of a VO's activities and a means of generating evidence in the event of a dispute. It allows relevant information about events occurring across organisational boundaries to be stored and shared when needed.

4.3 Coordination

Conventional organisations coordinate their internal activities in a variety of ways, including management hierarchy, procedures, staff directories and software support. In a VO, these methods are generally unavailable. For example, should a problem occur within a VO, it may be impossible to identify who should be informed. Additionally, since each partner may operate different processes and have different goals and priorities, it may not be clear who should make decisions should a crisis occur or who's decisions should take priority. Coordination across organisational boundaries is further complicated by the use of different software tools and control primitives. GOLD's solution has been to develop some very basic primitives, upon which more complex schemes such as workflow can be built. These primitives are based around an event model and implemented as a notification service. Services, applications and individuals can register to receive notifications when a particular type of event occurs within a VO (subject to access control) and act accordingly. To demonstrate that high-level coordination schemes can be used within this system, GOLD has integrated its notification service with the decentralised workflow engine DECS [7], also developed at Newcastle. This allows workflows in different organisations to be triggered by events occurring within the VO to provide a high-level coordination scheme operating across organisational boundaries. In principle, the notification service could be used to drive alternative workflow engines or other high-level coordination schemes.

4.4 Information management

Conventional organisations use databases, websites, intranets and wikis for dissemination of information, as well as procedures such as internal memos, meetings etc. and simple word of mouth. These methods are generally inapplicable across organisational boundaries, which can cause significant difficulties. VOs will tend to generate information of many types, including information about the VO itself (structure,

[3] Registration, Evaluation and Authorisation of CHemicals

configuration, security policies etc.) and information about the project(s) being carried out by the VO (documents, workflows, tasks to be carried out, the results of experiments etc.) This information may be distributed throughout an organisation and may be highly sensitive. Nevertheless, if the VO is to function, other organisations are likely to require access to some of that information. Moreover, services, applications and individuals may need to be informed if this information changes. For example, if an experiment is carried out a second time and the results change, this may be critical to the future direction of the project. If the end date of a task within one of the VO's projects changes, this may have implications to all parties. One of the most serious problems in large and complex collaborations is poor communication: often when information is not forwarded as appropriate. In many cases, the originators of that information will not know who needs to be informed of its existence or change. Sometimes, nobody within the VO will know in advance that some piece of information is important, even though it might turn out to be so at some future date. To address these problems, GOLD has developed a distributed information repository. This can securely store information about and generated by the VO in a distributed fashion. It can be linked with the GOLD notification service, so that interested parties can be informed of changes to information, subject to access control. This allows flexible exchange of information across organisational boundaries, yet ensure that it is subject to appropriate access control.

4.5 Visualisation

One of the major difficulties in VO construction is that every member organisation – and potentially every individual within that organisation – is likely to view the goals and purposes of the VO and the means of achieving them differently. For example, a toll manufacturer is unlikely to be concerned with the underlying reasons a company such as Eau de Chem might begin a project in the first place, since it is a contractor which will be paid regardless of whether the project is a success. Unfortunately, this conventional way of working is not conducive to virtual organisations. When problems occurred within the project, it was necessary for all parties to work together to solve them. This requires all parties to understand the problem in its full context. With complex problems, this can be very difficult, particularly when different cultures intersect. A classic problem in the chemicals industry is that as a result of training and environment, chemists and chemical engineers see things differently. For example, chemists may be concerned with developing an elegant and efficient reaction, whereas a chemical engineer might be more concerned with whether the reaction is practical within the extant constraints. Similarly, Eau de Chem, as the initiator of the project, may not possess the specialist skills to understand every process carried out by all parties throughout the course of a project. This makes it difficult to identify potential problems before they happen – or even after they have happened. A closely related problem is that some of the parties may believe they agree on some important point, when they are in fact at cross purposes. This can lead to major misunderstandings between VO members and the failure of projects.

Due to these difficulties, it is important to ensure that all parties understand each other's contribution to the project and the likely implications of their actions. To achieve this, a visualisation tool has been developed, which allows VO members to co-build different interacting views of the system. For example, figure 3 shows a *deployment view*, showing some of the components and structure of the CPD project and the VO-enabling GOLD services. It was created as part of an application developed to retrospectively recreate the CDP project elements using GOLD software as a proof of concept and for demonstration purposes.

Alternative views might include an *intentional view*, which describes the goals of the VO and its progression through the project, or a *physical view*, which might show the computers, networks and other physical resources involved in the project. Views are not static: they incorporate behaviour in the form of animations of the constituent objects. Behaviour in different views can share a trigger and therefore be linked. This can be used to show the consequence of some event on several views of the system. Finally, behaviour can be triggered by events generated by an external system. This allows the collection of views to reflect the changes occurring in a real system.

Because these views are co-built by all parties, they incorporate the knowledge and understanding of every stakeholder. During the co-building process, all parties will come to understand the roles and responsibilities of others. The views built will serve as a permanent record of the stakeholders' understanding of the VO. Because views can be used to reflect behaviour in real systems, the views can gradually become part of the instrumentation of the VO, allowing users to view the events of a project as they occur. Since the views act as a collective statement of each party's understanding of the VO, this is a very powerful mechanism for understanding the project and its current status, enabling problems to be identified early and solved collectively.

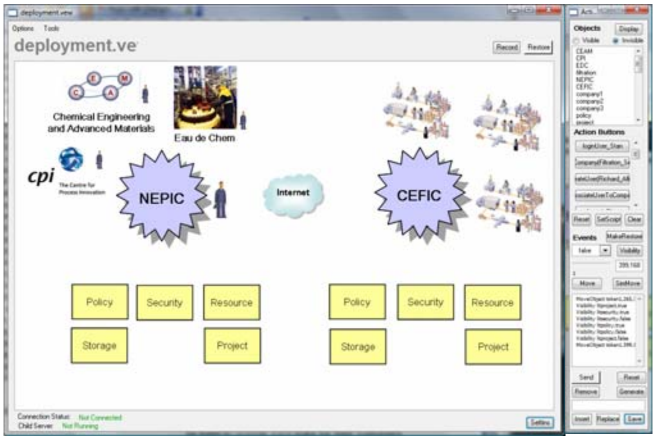

Figure 3: The GOLD demonstrator, showing the CPD VO

4.6 Architecture

The GOLD project interviewed many chemicals companies of varying size and function to determine requirements. The most significant findings are as follows [8, 11]:

1. Dynamism is of great importance. Change is the norm rather than the exception. This includes change of all kinds and at all levels. For example, changes in VO membership are commonplace, but so are changes in goal or direction. In general, some change will occur that could not have been predicted.
2. Security is paramount. Companies are willing to share resources, but need quite fine-grained control over access. Virtual working raises additional security concerns: for example, some companies rate their business process as their major advantage and do not wish to publicise it to others. It is important that coalitions can easily build security contexts in which they can collaborate.
3. Most companies are unwilling to significantly change their modes of operation or to adopt new technologies, processes etc. in order to participate in VOs. They wish to carry on business as usual to the greatest possible extent, and yet flexibly cross organisational boundaries when necessary
4. Most companies are suspicious of virtual working, but recognise it as a major necessity in the future (eg REACH). They require an adoption path that is iterative, not overly disruptive to their culture, and is potentially reversible.
5. Companies show considerable interest in gradually changing to enable them to integrate more closely with other companies to improve efficiency, but are fiercely protective of their independence and their modes of working.
6. Companies wish to *co-build* solutions with their partners: they do not wish solutions or infrastructure to be imposed upon them
7. Every company's requirements are different

These requirements indicate that an application-level approach is not appropriate. GOLD has developed a *service-based infrastructural approach*, which provides essential facilities for the crossing of organisational boundaries. The expectation is that these will be used by collaborators to co-build an environment within which they can create and operate a VO. Given the relatively large amount of effort involved with this, it is likely that service providers will provide pre-built *hubs*, which can be configured to users' specific needs. They may also provide application-level support. GOLD research has shown that industry bodies may be keen to provide such hubs for their customers, along with additional value-added services, such as legal services, federation services (to allow their members to form VOs with members of other hubs and to use services operated by other hubs) etc. This tiered approach reduces complexity and increases opportunities for adoption, without reducing flexibility.

5. Revisiting the case study

Part of the case study involved building an application, which uses the GOLD services to simulate some stages of the CPD project described above. This provided proof of concept, demonstrating that GOLD can indeed be configured to reflect complex dynamic projects and providing evidence that it is suitable as an enabling technology for VOs in Chemical Process Development.

One of the major ways in which GOLD technology could have helped in the CPD project was in enabling and automating dynamism. When changes occurred in the project, one of the consequences was a sudden need to adapt very quickly by changing VO membership and altering the basis of communication between them. GOLD software greatly speeds this process by providing mechanisms for establishing the basis of trust, security contexts etc. and allowing these to be changed at will through simple policy exchanges. Moreover, GOLD is a very lightweight platform, which places very few requirements on the technical, cultural, procedural (etc.) of members and can be adopted piecemeal and as required.

The case study also reveals the potential benefits of VO software support such as that provided by the GOLD middleware (particularly when companies are involved with many projects) , and in particular to identify areas where VO technology would have helped significantly with the actual CPD project.

For example, one of the major problems that occurred was the withdrawal of the catalyst from the market. It was initially assumed that some other catalyst would prove suitable and decisions were made on this basis, which had a significant downstream effect. In particular, the pilot plant was designed, the basis of funding changed and the expected rate of progress accelerated. This decision proved to be only partially correct and may not have been made if Eau de Chem and other VO members had received faster feedback on the performance of the new catalysts.
These limitations were due partly to the resource limitations of the RE, the lack of management bandwidth owing to the unconstrained complexity of the project coupled with unexpected events, and partly due to lack of integration between VO members Part of the problem lay in the fact that there was no automatic mechanism by which this communication could take place and part by the fact that the parties involved did not appreciate what impact their actions and decisions might have on others.

Through careful configuration of the GOLD infrastructure, informed by use of the visualisation platform to create views that capture the expectations of all stakeholders, many of these problems could have been averted and accelerating process dynamics managed.

6. Conclusions

The case study illustrates that chemical development projects are highly complex and dynamic. A virtual organisation approach to management of these projects is particularly appropriate because it is conducive to the early identification of problems and their collective solution by appropriate teams of VO members. Since this is costly in terms of management effort, VO software is required to assist with this process. The service-based middleware infrastructure developed by GOLD is an example of such software. It meets the various requirements discovered during the industry interviews and ethnographic studies conducted by the GOLD project. The development of a demonstrator application using GOLD services and based on the CPD case study project illustrates the applicability of GOLD to real, complex, highly dynamic industrial projects.

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