European Symposium on Computer Aided Process Engineering – 15
L. Puigjaner and A. Espuña (Editors)

A Computer Architecture to Support the Operation of Virtual Organisations for the Chemical Development Lifecycle

Adrian Conlin[a], Philip English[b], Hugo Hiden[a+], Julian Morris[b], Rob Smith[a] and Allen Wright[b]

[a]Department of Computing Science
[b]Department of Chemical Engineering and Advanced Materials

University of Newcastle upon Tyne

United Kingdom, NE1 7RU

Abstract

Fine chemical and pharmaceutical manufacturers focus on new product development as a means of growth, with time to market as a key driver. Time to market improvements are, however, limited by a company's infrastructure; for example, in-house design and manufacturing capacity, ability to respond to a dynamic environment etc. In many marketplaces, there is an increasing trend towards outsourcing and operating networks of specialist providers. Different specialist companies may be involved at all stages in the R&D lifecycle, providing services ranging from basic research or safety testing, to industrial scale manufacturing. This outsourcing concept can be generalised to support advanced notions of collaboration such as loosely-coupled but highly integrated networks of companies cooperating as a single enterprise. These networks can be described as dynamic Virtual Organisations (VOs) (Demchenko, 2004). This paper will outline a computer based architecture developed to address the operational difficulties associated with the creation and operation of this type of VO and present it within the context of the chemical development lifecycle.

Keywords: Virtual Organisations, Chemical Development, Lifecycle Management

1. Introduction

An early example of a speciality chemical development VO, was reported by Wright (2004). The company employed chemists to develop synthetic routes, whilst most other functions were outsourced. This approach led to reported reductions of 92% in product development costs, and time to market savings of 66%. Although technically successful, this VO was not scalable due to the difficulties associated with the co-ordination of the individual companies and the management and distribution of the information generated during the process. To improve scalability, a improved infrastructure is required, which can provide services to address the problems reported during this virtual development

[+] Author to whom correspondence should be addressed: h.g.hiden@ncl.ac.uk

exercise. The architecture presented in this paper describes such an infrastructure, outlining a system that can demonstrate the following attributes:

- Security: Chemical companies participating in a VO may be mutually distrusting and security mechanisms must be provided to protect against misuse of shared resources and to form a basis for the establishment and maintenance of trust relationships.
- Auditability: In order to comply with statutory regulations and to monitor and manage interactions between collaborators, all actions performed within the system must be recorded and made available for audit.
- Flexibility: The chemical R&D lifecycle is highly dynamic and unanticipated direction changes can occur throughout the process. The infrastructure must provide mechanisms to recognise and respond to changes, including changes in VO membership, type and content of information managed, and business relationships.
- Usability: Companies typically have their own infrastructures: technical, procedural, cultural, etc. It is a requirement that they be able to participate in VOs without substantial changes to their legacy systems.

1.1 The Chemical Development Process and the Data it produces

Although the chemical development process is complex, it can be broken down into discrete stages, a representative selection of which, including the various forms of data generated, is shown below in Table 1.

Table 1. Example Chemical development stages and information requirements.

Stage	Generated Data Types	Data Scope	
		Local	Global
Chemical route development	Lab notes	X	
	References to previous work	X	
	Chemical route information		X
Business analysis and justification	Related patents	X	
	Competing companies	X	
	Economic information	X	
Scale up studies	Hazard/safety analysis		X
	Results data	X	
	Operational specification		X
Production	Equipment availability	X	
	Plant performance data	X	
	QA results		X

Table 1 also indicates specific cases where data has Global scope and may be shared between several stages within the development process. If the development is being performed within a VO, global data must be shared between different VO member companies. This implies a need for security and access control methods to be in place. Section 2.1.2 outlines some of the approaches that are relevant to the problem of securely transferring data between VO members.

2. Service Oriented Approach

In general, requests for information and action from one VO member to another should be trivial. However, fulfilling theses requests may require a complex internal process. Providers can hide that complexity by encapsulating it into a *service* with a simple interface defining how consumers can interact with it. This is referred to as a Service Oriented Architecture (SOA) (Erl, 2004).

The service-based approach conveys a number of important benefits. Most importantly, encapsulation, which can provide a solution to the problem of loose coupling but tight integration between organisations. Web Services (Skonnard, 2002) are a standards based approach to implementing a SOA, making it possible to leverage a wide variety of open standards and protocols and integrate different software applications running on different platforms. This helps to address the usability requirements for a VO, as described in Section 1.

2.1 Services to support Virtual Organisations

Two levels of infrastructure are required to support VOs: a basic level facilitating fundamental VO functionality, such as communication, coordination and accountability and an application specific level which, in this case, will allow VOs to be deployed within a chemical development context.

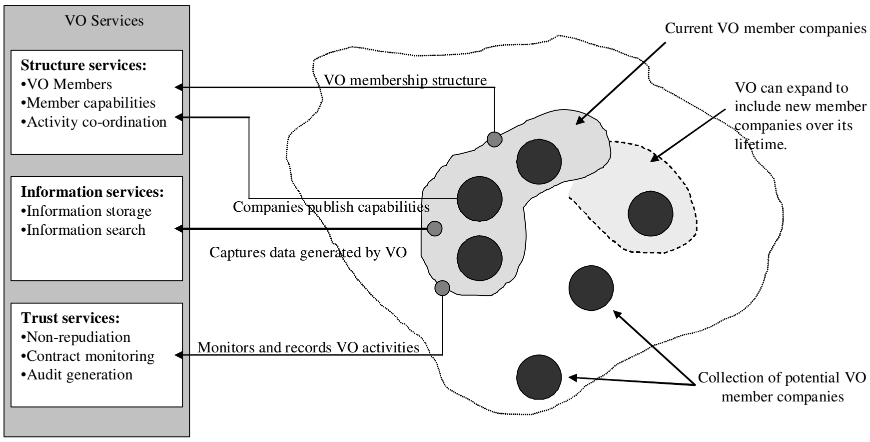

Figure 1: Services to support VO management and operations

Figure 1 illustrates a VO, comprised of a number of member companies being managed and controlled by the basic set of services described above.

2.2 Core VO functionality

2.1.1 Structure services

One of the key requirements for the operation of VOs is to be able to support a dynamic environment in terms of the participating member companies. For example, the companies involved during the initial investigative phases of the chemical development process are likely to be different to those involved during the final manufacturing stages. In order to monitor and control this dynamism, structural services should be provided to manage the VO and allow companies to coordinate their activities within it. In Figure 1, these structure services maintain information regarding the VO(s) that are currently operating, their member companies and additional potential member companies that can be invited to join.

2.1.2 Security and trust services

Security is a key concern when sharing information between VO members. Access to resources must be configured locally for security purposes but to prevent excessive management overhead in a dynamic environment it must be *policy based*. This removes the need for resource owners to possess information about individuals in other organisations and reduces the possibility of misconfiguration and error. Access control should be supported by authentication using digital certificates (for example, Choua and Yurovb, 2004) to provide a consistent security framework across organisational boundaries.

The basis of most business relationships is *trust*, however trust is difficult to achieve in a dynamic environment. This means that the facilities must be provided within the architecture to enable the establishment and management of trust relationships. These facilities should include electronic contracts for specifying interaction requirements (Molina-Jimenez et al, 2004), and need to be complimented by non-repudiable messaging (Cook et al, 2004) and audit trail generation to provide consistent, irrefutable evidence in the event of a dispute. The trust services in Figure 1 achieve this by monitoring the interactions between VO members and logging activities in a centralised location.

2.1.3 Information management

Sharing and integration of information is a key component of VOs. Member companies may store their information in very different ways and yet a VO must be able to integrate these heterogeneous data sources and provide a consistent interface across organisational boundaries, which behaves like a single database (see, for example, Chervenak, et al, 2003, who outline a grid enabled distributed data storage architecture). The information management services should also include features such as notification so that changes to information repositories and VO structure are propagated across organisational boundaries as appropriate.

2.3 Supporting the Chemical Development process

Creating and managing a VO is one aspect of a chemical development focussed VO. In addition, the VO must be able to support the various forms of data and business interactions that are anticipated within the chemical development process (Table 1). In accordance with the detailed discussion of the interactions and data types encountered during the chemical development process presented by Bayer and Marquardt (2004), we propose to build upon the Core VO functionality described in Section 2.2 in the following ways:

2.3.1 Extensions to handle chemical data types

A selection of data types that are encountered during the chemical development process are presented in Table 1. What is clear from this table is that there are a wide variety of different data formats and structures that must be managed by the VO. Some of this information, for example chemical route information, is available in a highly structured form (such as the Chemical Markup Language – CML (Murray-Rust et al, 1995) which can be used to describe chemical specific information) and can be supported and indexed directly by the information storage services provided within the VO. Other information, for example, laboratory notes may be available only in a proprietary format (such as MS Word), which must be stored as binary data within the information services. In these cases, additional Meta-Data (Date, 1999) can be attached to facilitate future search operations. Information regarding the capabilities of VO members to generate chemical development specific information is stored within the Member Capabilities service shown in Figure 1.

2.3.2 Trust and Security extensions to facilitate chemical business interactions

Whilst the business interactions occurring during the chemical development process are likely to be common to may types of business processes, the chemical industries have a higher than normal statutory duty for auditing and traceability. For example, the FDA regulations and 21CFR11 requirements for digital signatures (FDA, 2003). These capabilities are integrated into the core trust and security services (Section 2.1.2) in a manner that generates access logs that conform to FDA (and other relevant statutory) requirements.

3. Examples of VO Operations

This section presents some examples of the interactions between individual services during typical VO operations.

3.1 Creating a new VO

This example describes the steps required to create a new VO (assuming a suitable VO does not already exist) and invite a set of members to participate.

Table 4: Creating a VO

Action	Service Group	Services invoked
Create a new empty VO	Structure	Members
Search for potential member companies	Structure	Capabilities
Invite members to collaborate	Structure	Co-ordination
Members accept / decline invitation	Structure	Co-ordination

3.2 Requesting and storing data

This example describes the tasks performed when a VO member requests data to be generated by another VO member. This data is then stored and made available for other VO members to access.

Table 5: Requesting data from a VO member

Action	Service Group	Services invoked
Identify member that can produce the required data	Structure	Capabilities
Request data from member	Member	Data Generation
On completion the data is stored	Information	Storage
Notifies requestor when the data is complete	Information	Notification
Requestor retrieves the data from storage	Information	Storage

4. Conclusions and Further Work

This paper has presented an architecture to support the creation and operation of VOs for the purposes of collaborative chemical development. Although the services described in this paper have been presented in an implementation neutral fashion, they are currently being implemented using Web Services (Skonnard, 2002) which provide a widely used way of providing services over the internet. Once complete, the VO services will be used to perform an example chemical development process which will demonstrate both the chemical specific and more general business interaction features of the architecture.

References

Bayer, B. and Marquardt, W., 2004, Towards integrated information models for data and documents, Computers & Chemical Engineering, Volume 28, Issue 8, 1249 – 1266.

Chervenak, A.L., Atkinson M.P., Kunszt P., Narang I., Paton N.W., Pearson D., Shoshani A., Watson, P., 2003, Data Access, Integration and Management in The Grid 2: Blueprint for a New Computing Infrastructure Second Edition, November 2003.

Choua, D.C., Yurovb, K, 2004, Security development in Web Services environment, Computer Standards and Interfaces, Article in Press.

Cook, N.O., Robinson, P. and Shrivastava, S.K., 2004, Component Middleware to Support Non-repudiable Service Interactions, In Proc. IEEE Int. Conf. on Dependable Systems and Networks (DSN 2004), Florence, Italy, 28 Jun.-1 Jul. 2004.

Date, C.J., 1999, An Introduction to Database Systems, Addison Wesley Longman; 7th edition (October 1, 1999), ISBN 0201385902.

Demchenko, Y, 2004, Virtual organisations in computer grids and identity management, Information Security Technical Report , Volume 9, Issue 1 , January-March 2004, 59-76

Erl, T., 2004, Service-Oriented Architecture : A Field Guide to Integrating XML and Web Services, Prentice Hall PTR, 16th April, 2004. ISBN 0131428985

FDA, US Department of Health and Human Services, 2003, Guidance for Industry Part 11, Electronic Records; Electronic Signatures – Scope and Application, US FDA, August 2003.

Molina-Jimenez, C., Shrivastava, S., Crowcroft, J. and Gevros, P., 2004, On the Monitoring of Contractual Service Level Agreements, In Proceedings of the IEEE Conference on Electronic Commerce CEC\'04, The First IEEE International Workshop on Electronic Contracting (WEC), San Diego, 6-9, 2004

Murray-Rust, P., Rzepa, H.S., Leach, C., 1995, CML – Chemical Markup Language, Poster presentation, 210th ACS Meeting, Chicago, 21st August, 1995

Skonnard, A, 2002, The XML Files: The birth of Web Services, MSDN Magazine, Volume 17, Number 10, October 2002.

Wright, A.R., 2004, Turning Virtual Development Methods into a Reality, In BatchPro symposium on knowledge driven batch processes, Poros, Greece, 6th June 2004.

Acknowledgements

This paper was produced as part the GOLD project, which is funded by the EPSRC and operated in collaboration with Unisys, Lancaster University Management School, CPACT, BRITEST, SOCSA and the North-East Regional Development Agency Centre of Digital Excellence (Codeworks).