Linking Chemical Information with Geodatabase Features via Web Services

Eric A. Bernard[1], Daniel A. Andresen[2], Bhanuprakash Vanjaku [3], and Larry E. Erickson[4]
[1] *Kansas State University Department of Landscape Architecture Regional and Community Planning*
[2] *Kansas State University Department of Computer of Information Science*
[3] *Kansas State University Master's Student*
[4] *Kansas State University Department of Chemical Engineering*

Abstract

Information about chemicals' properties, potential hazards and regulations can be found in hundreds of Web sites from the EPA to state governments. Chemical information is critical for a multitude of business and government sectors in inventory management, environmental impact assessment, emergency response and public health. The Web-based Environmental Knowledge Assessment Tool (EKAT) developed for the United States Marine Corps catalogs more than 14,000 chemicals and queries policy and health regulations by jurisdiction via Web search. To leverage chemical information, Web services were developed in combination with an ArcGIS tool to integrate chemical knowledge with features stored in a geodatabase. Chemical information is linked to common features such as land parcels, buildings, soil or geologic formation, well/boreholes, streams/rivers, and transportation networks in existing data models. The power of ArcGIS spatial modeling and analysis can be harnessed for environmental modeling and assessment, hazardous substance inventory tracking and management, emergency and hazmat response.

Introductory Scenario

A laboratory, testing, and production facility in Kansas distributes chemical and solvent materials to clients worldwide. The process and products inherently pose a significant threat to humans and environment, but are critical to varied industries. The products are highly valued in the global market place, and given demand growth forecasts, management is proposing expansion facilities on the East and West Coasts, central Gulf region and upper Midwest. Their products are stored and applied in every state in the United States. Given the high risk-high reward nature of their business, they are seeking innovative ways to assist in critical planning and response decisions.

Posed this challenge, where would one begin to search for the information required to make critical planning or response decisions? Furthermore, how could one leverage material, process, transport, health, safety and policy information for: facilities management, emergency response, ecosystem and human contamination, and environmental assessment modeling and reporting? The Geographic Information Science (GIScience) community has realized the diverse and robust challenges and solutions possible given this scenario, and multitudes of others similar in nature, and responded with the geodatabase and data models to support such needs. Hereafter, foundational research is presented on one such approach to addressing the question of how to link material information with virtual spatial-temporal objects in data models to aid response and planning decisions.

Chemical/Solvent Material Information Assembly

The task of coalescing federal, state or jurisdictional information on chemical and solvent material regulations across diverse environmental and political landscapes is daunting in and of itself, let alone the coupling of material information with existing and future data and mathematical models. The Environmental Knowledge Assessment Tool (EKAT), available at http://www.ekat-tool.com is a web based tool designed to assist in locating, researching and evaluating environmental and safety-related issues for products and systems. EKAT has been developed for the United States Marine Corps via a partnership between M2 Technologies, Kansas State University (Hazardous Substance Research Center (HSRC)) and CABEM Technologies LLC. EKAT provides detailed guides on physical and chemical properties, hazardous waste management, particulates, and toxicology located directly in EKAT databases, or via links to other web based resources.

EKAT directly, or passively via web query, provides information on: Resource Programmatic Environmental, Safety and Occupational Health Evaluation (PESHE), National Environmental Policy Act (NEPA) requirements, jurisdictional regulatory requirements, potential air emissions from an operation, proper handling of waste products from an operation, a chemical spill, solvent use requirements associated with cleaning operations, proper reporting requirements, general chemical information, and available Department of Defense (DoD) environmental resources. Tools included via the web interface include: conversions, screening for chemicals for environmental,

regulatory, safety and health information, solvent screening, and TECCA, with additional resources planned and under development.

EKAT is accessed via web browser at www.ekat-tool.com. Once logged in, tools such as the screening tools are accessed from menus or tool buttons, and allow the user to input a CAS number or name to begin the screening process. Once the user executes the screening process a list of potential matches is presented. The user then selects the desired material(s) from a dialog window to obtain general material, safety and regulatory information for the selection(s). Screening results can be saved by a user into a project profile created by the user, then exported in a variety of formats for reporting purposes such as PESCHE and NEPA Environmental Impact Assessment and Statement documents.

EKAT's demonstrated ability to assemble and report valuable material information via a web interface offers great potential for the extension of ArcGIS applications to glean this information via web services. From web services provided by EKAT, an ArcGIS user would be able to link material information (or EKAT tool results) automatically with features contained in geodatabases, and extend existing data models to more completely describe the spatial-temporal aspects of a real world environment. The remaining text describes the process used to extend ArcGIS to infuse material information from EKAT with geodatabase objects or features.

EKAT Web Services and ArcGIS Extension Overview

While the information provided using EKAT screening tools is very useful for material understanding and generating reports, extending the information to features having those materials in geodatabases permits enhanced understanding through modeling spatial and temporal environments. To expedite this workflow requires the creation of a custom tool for ArcGIS applications to log into EKAT and perform the selected operations, then for EKAT to return requested results to the desired features or objects in an existing geodatabase. This process is best handled via web services and is diagrammed below.

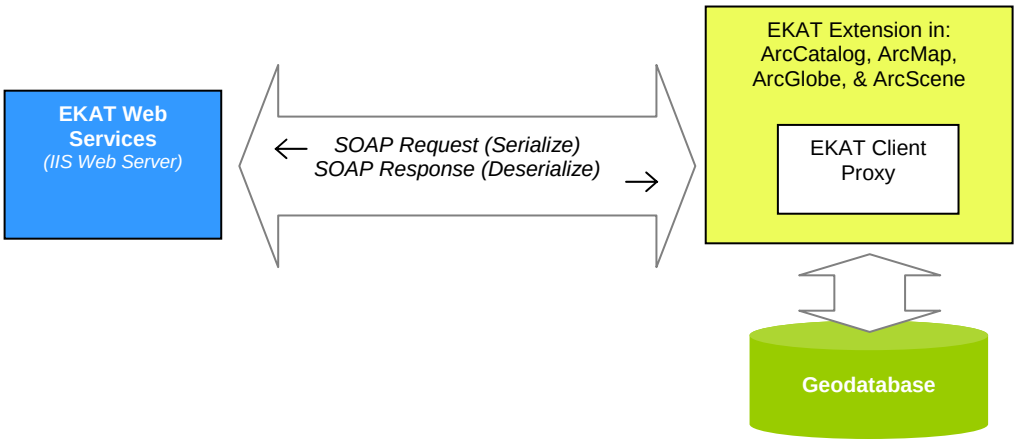

Figure 1: Architecture Design

As illustrated, the EKAT Web Services extension, accessed via tool button in ArcMap, ArcCatalog, ArcScene or ArcGlobe, contains the client proxy required to communicate with available EKAT Web services on the IIS web server. The Arc(Interface) client collects input parameters, serializes them into a SOAP request, and sends the SOAP request to the EKAT Web server, which deserializes it, invokes the method and sends the SOAP response back to the client and updates geodatabase with requested material information.

The EKAT tool conceptually is similar to the ArcWeb Toolbar in ArcGIS developed by ESRI. The ArcWeb toolbar has tools which extend ArcGIS Desktop applications to consume ESRI web services via shortcut tool buttons which evoke access to web services providing GIS resources. The major difference here is that the EKAT tool button interacts directly with a user's geodatabase and will automatically update or refresh chemical data if information in the EKAT database or reports is updated. Automatic updates of geodatabase features with chemical attributes is critical to first responders, for instance, that need the most current information available related to chemical and hazmat response. Because EKAT is querying the latest policy information from national and state repositories, the data delivered to the geodatabase features also provides necessary updated requirements for reporting and environmental assessment documentation.

Web Service Details

Web services provide a modular, distributed and platform independent application invoked by an ArcGIS user via XML based SOAP (Simple Object Access Protocol) to communicate with EKAT. As with the ArcWeb toolbar tools, the EKAT tool uses the SOAP standard. Both HTTP (Hyper Text Transfer Protocol) and SMTP (Simple Main Transfer Protocol) can be used for transporting encoded SOAP messages. The XML based Universal Description, Discovery and Integration (UDDI) is a directory for looking up web services similar in logic to a phone directory, and serves as the tool to locate EKAT web services. WSDI (Web Services Definition Language), also XML based, describes the operations and messages associated with the web service. Finally, Internet Information Services (IIS) Web server used for development of this application because this environment: is where EKAT web services are hosted, provides a fault-tolerant architecture, integration, scalability, security and management capabilities, and ease for deploying and accessing web services. The EKAT web service request and return provides all the content in a web template via a SOAP request and SOAP response illustrated on the following page.

SOAP Request:

```
POST /WebService2/Service1.asmx HTTP/1.1
Host: localhost
Content-Type: text/xml; charset=utf-8
Content-Length: length
SOAPAction: "http://tempuri.org/EKATWebService"

<?xml version="1.0" encoding="utf-8"?>
<soap:Envelope xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xmlns:xsd="http://www.w3.org/2001/XMLSchema" xmlns:soap="http://schemas.xmlsoap.org/soap/envelope/">
  <soap:Body>
    <EKATWebService xmlns="http://tempuri.org/">
      <s1>string</s1>
      <s2>string</s2>
    </EKATWebService>
  </soap:Body>
</soap:Envelope>
```

SOAP Response:

```
HTTP/1.1 200 OK
Content-Type: text/xml; charset=utf-8
Content-Length: length

<?xml version="1.0" encoding="utf-8"?>
<soap:Envelope xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xmlns:xsd="http://www.w3.org/2001/XMLSchema" xmlns:soap="http://schemas.xmlsoap.org/soap/envelope/">
  <soap:Body>
    <EKATWebServiceResponse xmlns="http://tempuri.org/">
      <EKATWebServiceResult>
        <response>
          <category>string</category>
          <results>string</results>
        </response>
        <response>
          <category>string</category>
          <results>string</results>
        </response>
      </EKATWebServiceResult>
    </EKATWebServiceResponse>
  </soap:Body>
</soap:Envelope>
```

Figure 2: SOAP Request and Response for EKAT Material Screening Results.

ArcGIS Applications Extension

To be able to evoke the EKAT web services a custom tool and tool button were created in ArcGIS applications such as ArcCatalog, ArcMap, ArcScene and ArcGlobe. The tool was built using ArcObjects (built on Microsoft's Component Object Model (COM)) which is commonly used to customize ArcGIS applications via DLLs (Dynamic Link Libraries). Given ArcObject's COM framework, C# and VBA were used to extend the ArcGIS Desktop applications to interface with EKAT and deliver the materials information to features or objects within a geodatabase. C# and the .NET Framework were used in this application as existing classes expedite development, efficient memory management and garbage collection, and .NET's language neutrality. A Microsoft Access database, the de-facto personal geodatabase format in ArcGIS Desktop applications, served as a test bed for proof of concept. Additionally, Access provides easy interaction with C# using the OLE DB connection. The diagram following provides a more detailed illustration of the architecture for the ArcGIS application extension.

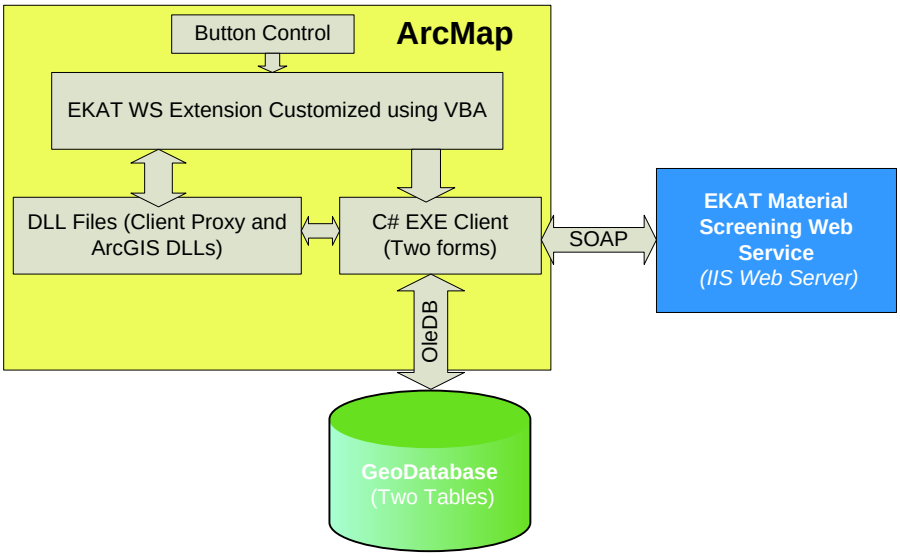

Figure 3: ArcGIS Application Extension Architecture

As illustrated the ArcGIS applications extension (ArcMap shown) accessed via a tool button, was customized with VBA, and uses DLL files which contain the client proxy required to communicate with the web service. A C# executable (exe) file is used to send the SOAP requests and process responses, as well as populate the geodatabase tables. Figure 4 illustrates the client extension interface in ArcGIS applications to login to EKAT and perform a screening respectively.

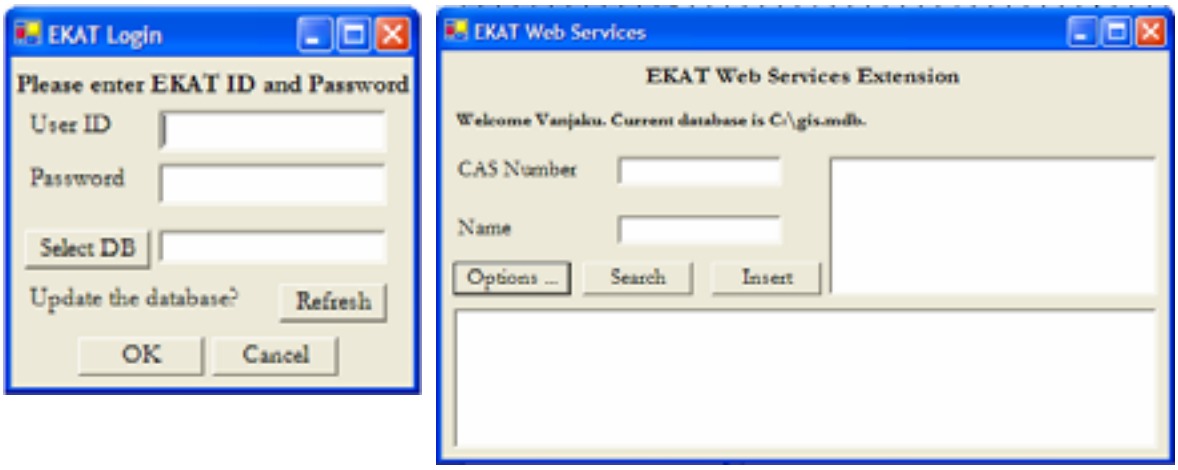

Figure 4: ArcGIS Applications Extension User Interface.

The results returned in the SOAP response, based on user input in the dialog boxes above, are used to populate tables in the ArcGIS user's geodatabase. The first table stores login information and the second material information returned by the EKAT Screening tool. A sample table design is shown in Figure 5.

users	
PK	id
	password selectedDB

gis	
	CASNumber Name lastUpdated category results

Figure 5: Sample Geodatabase Tables for EKAT Web Service Provided Information

The sample tables are intentionally simplified given the diversity of applications and means by which the GIS community would choose to relate the chemical or solvent material screening data to features or objects within data models. Whether the user intends to provide first responder information for a hazardous materials crisis, manage facilities storing materials, model groundwater contamination from a chemical spill, or prepare an EIS for a future development, data provided by EKAT web services and attached to geodatabase features provide critical current information and a fluid workflow. Existing data models provide excellent frameworks for numerous angles of the scenario presented and contain the relationship classes and schema to again expedite workflow.

Summary

The ArcGIS platform provides an easily extensible framework with ArcObjects and VBA and the .NET Framework to create custom interfaces to consume web services and populate geodatabase tables. EKAT Tools provide an excellent resource for material chemical and solvent information relevant to, or extending, existing data models. Chemical and solvent material regulatory, safety and health information attached to database objects can leverage both planning and response decisions for countless scenarios. As tools like EKAT, data models, and GIS tools continue to develop, opportunities to further enhance our virtual representations of real world environments and materials interaction within them will also grow making our world safer and further empowering decision makers.

Acknowledgements

Authors would like to thank the entire EKAT development team for support in this work and the Kansas State University Hazard Substance Research Center Staff for valuing GIS.

References

B. Vanjaku, “EKAT Web Services Extension for ArcGIS”, Master’s of Science Report, Kansas State University 2005

ESRI Documentation
http://www.esri.com/software/arcgis/

EKAT Tool Documentation
http://ekat-tool.com

Using OleDB Connections
http://msdn.microsoft.com/library/default.asp?url=/library/en-us/csref/html/ vcwlkadotutorial.asp

“ArcWeb Services”, ESRI Documentation, http://arcweb.esri.com/arcwebonline/index.htm

World Wide Web Consortium. “Extensible Markup Language”, visited 04-02-03. http://www.xml.org.

E. Christensen, F. Curbera, G. Meredith, and S.Weerawarana, “Web Services Description Language (WSDL) 1.1”, Technical Report, W3C, 2001.
http://www.w3.org/TR/2001/NOTE-wsdl-20010315.

F. E. Bustamante, G. Eisenhauer, K. Schwan, and P.Widener, “Efficient wire formats for high performance computing”. In Proceedings of the 2000 conference on Supercomputing, 2000.

D. Davis and M. Parashar, “Latency Performance of SOAP Implementations”, Proceedings of the 2nd IEEE/ACM International Symposium on Cluster Computing and the Grid, pages 407-412, 2002.
K. Devaram and D. Andresen. SOAP optimization via clientside caching. In Proceedings of the First International Conference on Web Services (ICWS 2003), pages 520–524, Las Vegas, NV, June 2003.

D. Andresen, K. Devaram, and V. P. Ranganath. LYE: a high-performance caching SOAP implementation. In Proceedings of the 2004 International Conference on Parallel Processing (ICPP-2004), Montreal, Canada, Aug. 2004.

K. Devaram and D. Andresen. SOAP optimization via parameterized client-side caching. In Proceedings of the IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS 2003), pages 785– 790, Marina Del Rey, CA, Nov. 2003.

V.P. Ranganath, D. Sexton, D. Andresen. LYE: High-performance SOAP with multi-level caching. In Proceedings of the IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS 2004)

“ArcGIS Desktop Developer Guide ArcGIS 9.1” Published by ESRI

“ArcGIS 9, What is ArcGIS 9.1?” Published by ESRI

S.Shin, “Web Services Overview”, http://www.javapassion.com/webservices/WebServicesOverview.pdf

Chitnis etal, “Introduction to Web Services”, http://www.developer.com/services/article.php/1495021

T Thagarathinam, “.NET Remoting Versus Web Services”,
http://www.developer.com/net/net/article.php/11087_2201701_2

“Microsoft.NET development, ASP.NET, VB.NET, C#.NET”,
http://www.cygnet-infotech.com/microsoft-dot-net-application-development.htm

N Bute, “Advantages of .Net”,
http://www.codeproject.com/Purgatory/Advantages_of_Net.asp

“What's New in Internet Information Services 6.0”, by Microsoft,
http://www.microsoft.com/windowsserver2003/evaluation/overview/technologies/iis.msp

Author Information

Primary Author
Eric A. Bernard
Kansas State University
302 Seaton Hall
Manhattan, KS 66506-2909
US
785-532-5961
ebernard@ksu.edu

Co-Author
Dr. Daniel A. Andresen
Kansas State University
234 Nichols Hall
Manhattan, KS 66506
US
785-532-6350
dan@k-state.edu

Co-Author
Bhanuprakash Vanjaku
Kansas State University
234 Nichols Hall
Manhattan, KS 66506
US
785-532-6350

Co-Author
Dr. Larry E. Erickson
Kansas State University
105 Durland Hall
Manhattan, KS 66506
785-532-4313
lerick@ksu.edu