A HYDRATE DATABASE: VITAL TO THE TECHNICAL COMMUNITY

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ABSTRACT

Natural gas hydrates may contain more energy than all the combined other fossil fuels, causing hydrates to be a potentially vital aspect of both energy and climate change. This article is an overview of the motivation, history, and future of hydrate data management using a CODATA vehicle to connect international hydrate databases. The basis is an introduction to the Gas Hydrate Markup Language (GHML) to connect various hydrate databases. The accompanying four articles on laboratory hydrate data by Smith et al., on field hydrate data by Löwner et al., on hydrate modeling by Wang et al., and on construction of a Chinese gas hydrate system by Xiao et al. provide details of GHML in their respective areas.

Keywords: Hydrate, Database, Gas Hydrate Markup Language, GHML, Laboratory data, Field data, Modeling, Simulation, Overview

1   INTRODUCTION: MOTIVATION FOR A HYDRATE DATABASE

Recent analyses by Bernstein (2004) and Sachs (2005) suggest that technology is a major driver of societal economies. In turn energy is a foundation of technology, and efficient access to data will enable effective use of energy. The thesis of this work is that an international hydrate database will enable efficient access to an important new energy source, and that the development of Gas Hydrate Markup Language (GMKL) is the first step in connecting the international databases.

Natural gas clathrate hydrates are ice-like compounds which form when water encages small (<0.9nm) guest hydrocarbon molecules in crystal cages, as reviewed by Makogon (1997) and by Sloan (1998). Recent estimates of the methane content of hydrates in nature range from 2.5×10^{15} m^3 STP (Milkov, 2004) to 120×10^{15} m^3 STP (Klauda

& Sandler, 2005). These estimates, while wide-ranging, are extremely large relative to the estimated conventional gas reserve of 0.15×10^{15} m^3 methane (STP) (Radler, 2000).

Hydrate knowledge is expanding exponentially, as shown in the semi-logarithmic plot of Figure 1 (Sloan, 2004). This plot gives the number of refereed hydrate publications in the last century, by decade; there were two publications from 1900-1910 and 3010 publications from 1990-2000. A semi-logarithmic extrapolation into the first decade of the 21st century leads to a staggering 7,500 publications - slightly more than two refereed publications per day, seven days per week.
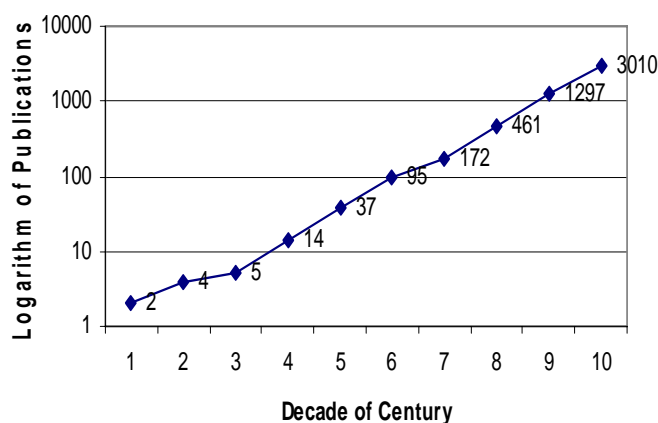

Figure 1. Number of refereed hydrate publications in the 20th century, by decade (Sloan, 2004)

With the above motivation and the expanding knowledge base, it is apparent that we need an efficient means of managing hydrate data. Through its multi-disciplinary worldwide network, CODATA has provided a convenient, internationally-sanctioned means of dealing with such information.

2   CODATA HISTORY OF HYDRATE DATABASE DEVELOPMENT

In 2000 CODATA authorized the first hydrate database Task Group, chaired by F. Kuznetsov. During this phase the Task Group met twice to organize the project and publicized the first local database, GASHYDAT (2001) developed by Drs. Klerkx and Dimitrov, with European Union funding. While the latter effort represents a landmark in hydrate databases, the database was initially small; it was limited by the funding, and work stopped in 2001. The GASHYDAT website domain has recently expired.

In 2002 a second CODATA Hydrate Task Group was again authorized, chaired by F. Kuznetsov. During the ensuing two years the Task Group held six world regional meetings shown in Table 1 to educate the hydrate community regarding the need for a database and to gain worldwide acceptance of the idea of an internationally-distributed database. The project was supported by several National and International bodies such as ICSU[1].

Table 1. Six regional worldwide hydrate database meetings

Region	Russia	North America	Japan	India	China	Europe
Meeting Place	Novosibirsk	Salt Lake City	Chiba	New Delhi	Beijing	Potsdam
Meeting Date	27/01/03	13/05/03	11/12/03	20/02/04	15/03/04	5/11/04

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[1] From 2002 to 2004, ICSU supported the CODATA gas hydrate initiative by providing a US$ 100,000grant over two years. It helped in organizing regional meetings in Russia, US, France, China and India (see Table1).

Also during their second period, the Task Group distributed a hydrate literature database of approximately 5000 articles, which contained authors, titles, page numbers, dates, and article abstracts relating to hydrates.

In 2004 CODATA gave the third charter to the Hydrate Task Group. It was during the third phase of the Hydrate Database Task Group effort that a need was recognized for Information Technology. That is, as nations began generating individual hydrate databases, a need was recognized to have a "common language" for communication among the hydrate databases. Information Technology experts, such as Jason Wang and Ralf Löwner, suggested that hydrates were sufficiently unique compounds to warrant a Gas Hydrate Markup Language (GHML). Fortunately Ralf Löwner had some expertise with hydrate databases – he had just completed the database for the Mallik2002 hydrate well described by Dallimore and Collett (2005).

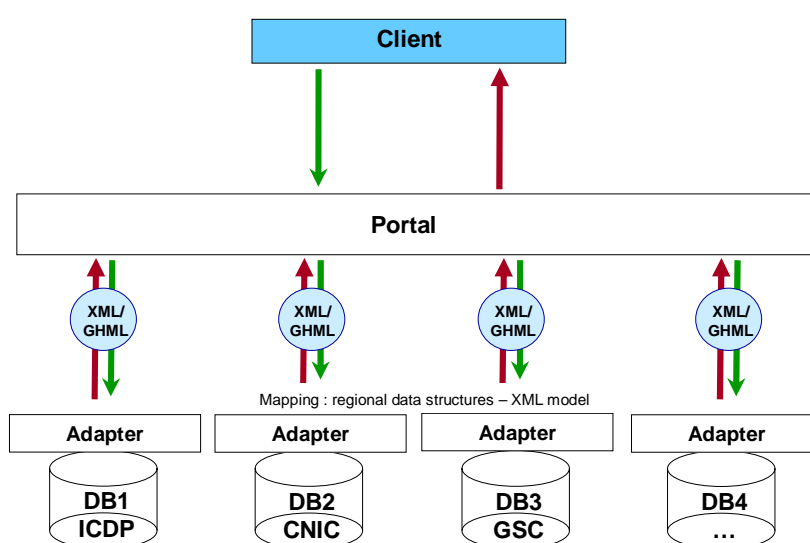## 3   HOW DOES THE GAS HYDRATE MARKUP LANGUAGE WORK?

Figure 2. A conceptual diagram for the working of the Gas Hydrate Markup Language and Portal

A conceptual understanding of the GHML is shown in Figure 2. The concept rests on the establishment of the databases (DBs at the bottom of the diagram) labelled ICDP (for InterContinental Drilling Program), CNIC (for Computer Network Information Center), GSC for the Geological Survey of Canada, etc. Without the foundation of these underlying databases, there would be no need for linking the communications.

At the top of Figure 2 is a Client who may request some information about hydrates. This client query is sent to a Portal, which communicates with the various databases through a common language – the Gas Hydrate Markup Language. Thus the client's query and response is communicated with each participating database, so that a number of data responses are obtained.

At this point, the reader may be asking, "Why do we need another Markup Language? Isn't this a fairly specific or niche application – too narrow to be general?"

It was desirable to use an existing Markup Language, but the field of hydrates is so general that it incorporates segments of several markup languages, without the entire language of any other. For example, when we studied the IUPAC standard Markup Language for thermodynamic data (ThermoML, as described by Frenkel, et al., 2006) there was no capability for inserting geological and geophysical data, such as well logs, which seemed vital to hydrates. Similarly other Markup Languages, were missing components for thermodynamic and kinetic data, so in

the end, a new language GHML was justified. However, a study of the existing Markup Languages provided valuable guidelines for our construction of GHML.

4   PUBLISHING GHML AND THE WAY FORWARD

The initial outline of the Gas Hydrate Markup Language was generated at the Computer Network Information Center at the Chinese Academy of Science (CNIC), by Willa Wang and Jason Wang in 2005. That initial effort was revised and set as database schemas in 2005 and 2006 with the entire Task Group, through intensified effort including a small steering committee composed of Ralf Löwner, George Moridis, Tom Smith, Willa Wang, Jason Wang, and Dendy Sloan. The Beta-version of the GHML was released at the Beijing CODATA meeting on October 23 with three components: (1) a laboratory data schema by Smith et al. (2007), (2) a field data schema by Löwner et al. (2007), and (3) a modelling/simulation schema by Wang and Moridis et al. (2007). The reader is referred to these three accompanying articles for the schema details of GHML.

For the first six months of 2007, comments from the user community will be solicited by placing the GHML, including a glossary and documentation, on the CODATA website. Revisions will be made to address the comments received. We anticipate an electronic, ever green publication of GHML, in which each revision will update, but not outdate, the earlier versions.

The next step for this project is to generate the Portal shown in Figure 2, as a means of connecting the client(s) to the databases via GHML. That is the intention of the CODATA Hydrate Task Group for the calendar year 2007. At the same time, national databases are continuing to be developed in parallel to this effort. The development of the GHML and Portal by CODATA should act to both enable and encourage these databases.

5   CONCLUSION

A Beta version of the Gas Hydrate Markup Language (GHML) has been developed and published in three parts: (a) laboratory data, (b) field data, and (c) simulations. This is a first step, to be followed in 2007 by the development of a Portal to connect the hydrate databases which are growing in various parts of the world. Individual database developments are proceeding in parallel to this connection effort, with CODATA encouragement to use GHML as a common language.

6   ACKNOWLEDGEMENTS

7   REFERENCES

Bernstein, W. (2004), *The Birth of Plenty*, New York: McGraw-Hill Co.,

Dallimore, S.R., Collett, T.S. (Eds.) (2005) *Scientific Results from the Mallik 2002 Gas Hydrate Production Research Well Program, Mackenzie Delta, Northwest Territories, Canada*, Ottawa, Canada, Geological Survey of Canada Bulletin 585, including CD

Frenkel, M., Chirico, R.D., Diky, V.V., Dong,Q., Marsh, K.N., Dymond, J.H., Wakeham, W.A., Stein, S.E., Königsberger, & Goodwin, R.H. (2006) XML-based IUPAC standard for experimental predicted and critically evaluated thermodynamics property data storage and capture (ThermoML), *Pure Appl. Chem.,* 78(3), 541-512, doi:10;1351/pac200678030541

GASHYDAT (2001) initial hydrate database generated by J. Klerkx and J. Dimitrov. Retrieved from the WWW April 18, 2007: http://www.gashydat.org/

Klauda, J., B., Sandler, S.I. (2005) Global distribution of methane hydrate in ocean sediment, *Energy & Fuels*, 19, 459-470.

Löwner, R. Cherkashov, G., Pecher, I.,. Makogon, Y. F (2007) Field Data and the Gas Hydrate Markup Language, *This Journal (submitted)*

Makogon, Y.F. (1997) *Hydrates of Hydrocarbons*, Tulsa, Oklahoma: PennWell Books

Milkov, A.V. (2004) Global estimates of hydrate-bound gas in marine sediments: How much is really out there?, *Earth Science Reviews*, 66 (3-4) 183-197.

Radler, M. (2000) World crude and natural gas reserves rebound in 2000, *Oil and Gas J*., 98(51) 121-123

Sachs, J.D. (2005) *The End of Poverty*, New York: Penguin Press

Sloan, E.D., (1998) *Clathrate Hydrates of Natural Gases*, (2nd Ed.) New York: Marcel-Dekker, Inc.

Sloan, E.D., (2004) Introductory overview: hydrate knowledge development, *American Mineralogist*, 89, 1155-1161

Smith, T., Ripmeester, J., Sloan, D., Uchida, T. (2007) Gas Hydrate Markup Language as it pertains to laboratory data, *Data Science Journal,* 6, GH18-GH24.

Wang, W., Moridis, G., Wang, J., Xiao, Y., & Li, J. (2007) Modeling hydrates and the gas hydrate markup language, *Data Science Journal,* 6, GH25-GH36.