# VIRTUAL MOLTEN SALT LABORATORY: DREAM OR REALITY?

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**Abstract**

The genesis of the Molten Salt Database, realized as early as 1967 with the publication of the Molten Salt Handbook by George Janz is as relevant today as it was over 30 years ago.

Building a world-class critically, evaluated database is a difficult and complex process, involving considerable time and money. Ultimately, the success of the project depends on positive interactions between a diverse group of people – support staff to identify and collect relevant literature, scientists to extract and evaluate the data, database experts to design and build the necessary data architecture and interfaces, database reviewers to ensure that the database is of the highest quality, and marketing staff to ensure the widest dissemination of the database. The advent of the World Wide Web (WWW) has provided another exciting component to this paradigm – a global database structure that enables direct data deposition and evaluation by the scientific community. Also the new concepts in engineering data information system are emerging and make it possible to merge people, computers, databases and other resources in ways that were simply never possible before.

Ongoing efforts in this respect will be described with the ultimate goal of building a *Virtual Molten Salt Laboratory*.

**Historical Overview**

The genesis of the Molten Salt Database was realized as early as 1967 with the publication of the Molten Salt Handbook by George Janz. The preface of the Handbook is as relevant today as it was over 30 years ago.

> *"The field of molten salts has been the subject of renewed interest over the past 25 years and has attracted the attention of scientists in research and technology from such diverse fields as: theoretical and applied electrochemistry, inorganic coordination chemistry, transition metal chemistry, preparative and process chemistry having melts as catalysts or as reaction media, nonaqueous solvents, thermochemistry, fuel cells and batteries, nuclear technology, analytical principles of chromatography and liquid-liquid +solvent extraction, corrosion science, and the principles of liquid structure, theoretical chemistry and physics." George J. Janz, Molten Salt Handbook, 1967.*

The first volume of the National Standard Reference Data System (NSRDS) molten salt data series was released in 1968 and was followed by 9 more volumes. The original computerized database was compiled in the late 1980's to provide engineers and scientists' rapid access to critically evaluated data for inorganic salts in the molten state. Properties for 320 single salts and 4000 multi-component systems included density, viscosity, electrical conductivity, and surface tension. Up to 1990, this database represented a significant portion of the critically evaluated data that was available in the literature from 1890-1990. However, during the last ten years, there has been a considerable increase in the amount of data available on molten salts. This explosion in the amount of data is due to the emergence of molten salts into new applications, such as waste processing, energy storage and metals electrodeposition. In addition, classes of salts that are liquid at room temperature are receiving renewed attention for applications in both catalysis and energy storage. The addition of new salts and data properties provides a propitious time to evolve the existing database into a modern on-line database and to provide new features such as, data visualization, modeling and simulation and collaboration tools.

**Building Databases**

First, it is important to define what a database *is* and *is not* and secondly, distinguish between compiled and evaluated databases. In the most simplistic terms, a database is a collection of related information, stored on a computer in such a way that different applications may use it without knowledge of the storage details. This definition provides no restrictions on the type or quality of data that is included in the database. In general, scientific databases fall into two categories – data impartially compiled from the known literature and data that is critically assessed by independent experts. There are merits to both database systems; however, critically evaluated data has an inherent value to the non-expert, in that the data has been reviewed and confirmed by experts in the field of research.

For over 30 years, NIST Standard Reference Data Program (SRDP) has been an international leader in producing high quality evaluated scientific and technical data. To maximize the impact of this public investment, NIST has been a long-standing advocate in using the most advanced technology to make these data widely and easily available. Today, NIST disseminates its data through two major publications, over 40 PC databases and via at least 12 online systems. NIST supports data evaluation activities in about 40 disciplines (http://www.nist.gov/srd/) in partnership with many industrial, national and international organizations.

Building a world-class critically, evaluated database is a difficult and complex process, involving considerable time and money. Ultimately, the success of the project depends on positive interactions between a diverse group of people – support staff to identify and collect relevant literature, scientists to extract and evaluate the data, database experts to design and build the necessary data architecture and interfaces, database reviewers to ensure that the database is of the highest quality, and marketing staff to ensure the widest dissemination of the database. The advent of the World Wide Web (WWW) has provided another exciting component to this paradigm – a global database structure that enables direct data deposition and evaluation by the scientific community.

IUSTI has established links for many years with the international molten salt community through :

- the edition of MOLTEN SALT BULLETIN. This quarterly newsletter, published since 1968, has a distribution of 600. It consists of an Editorial written by an expert and aiming to highlight new developments in the field, recent bibliography, reports on conferences and announcement of forthcoming meetings. A Web-based version was developed recently (http://iusti.univ-mrs.fr/IUSTI_EDITION/bulletin.html) that makes dissemination of information more effective (e.g. HTML links provide an immediate connection to the source of information).

- the direct organization (or involvement) of international research programs and conferences

These established activities is one of the reasons that the current Molten Salt Database Project will be able to expand rapidly and maintain the links with the molten salt community.

**The Current Molten Salt Database Project**

Molten salts are salts that are liquid typically at elevated temperatures; although, room- temperature molten salts and ionic liquids are also well known. Investigations have been conducted either at the fundamental level (a physical and chemical approach dealing with the liquid state of matter) or at an applied level, in support of the large number of industrial applications. Some important applications include:

- Electrodeposition of common or less common metals (Al, lanthanides,...), of inorganic materials (carbides, borides) as an economic alternative to PVD, CVD and conventional routes; …
- Environmental issues, especially molten salt waste processing, recycling as also catalytically-induced desulfuration of fumes; …
- Non-nuclear energetic issues, such as carbonate fuel cells, thermal storage of energy in solar energy plants; …
- Nuclear energetic issues, for example, waste processing (fast reactors), fuel recycling, spallation neutron driven system for weapon-Pu burning and energy production; …
- Molten salt catalysis of important industrial processes, for instant the vanadium oxide supported oxidation reaction SO2->SO3 for the production of sulfuric acid; …

- Technical applications, including casting cleaning, paint stripping, descaling of steels, superalloys, nitriding of ferrous components for mechanical properties optimization;
- Etc.

The current database project between IUSTI and NIST has been developed as a multi-stage effort to build a molten salts database that will contain evaluated data for a variety of applications. This database will build upon the work done by Professor George Janz (deceased) at RPI and supported by the NIST Standard Reference Data Program. The molten salts database is envisioned as a Web-based database that provide rapid access to reliable data on the physical and chemical property data for all molten salt systems. The original proposal defined the project into three phases:

*Stage one*: Planning and Design - The specification of the Database can only be decided after a clear identification of the objectives (content, dissemination method) that determine the technical details of implementation. The following features must be taken into account :

- type of data: factual (numerical and graphical)
- content: numerical data, experimental techniques reported, literature
- reference, data evaluation when possible
- structure: modular
- Dissemination: World Wide Web
- Interface: user-friendly graphical user interface with graphics capability
- Built-in software: data estimation or interpolation should be possible
- Security: for data input and data access
- Online data deposition: from specialized cooperating research groups

*Stage two:* Implementation, including loading of old data as well as more up to date data and establishment of a network to collect and evaluate data generated after 1990 and

*Stage three:* Data collection and evaluation on a steady state.

Initial portions of *Stage one* have been completed. Both graphical and numerical data will be included in the database. In addition, bibliographical data will also be included to provide original sources for the data. Where possible, tools that enable graphical representation and direct manipulation of the data will be provided. The content of the database will evolve over time. It is anticipated that the first release of the database will include the data from the original NIST/RPI database. Subsequent versions of the database will focus on new collections of data contributed and reviewed by the molten salt community. Dissemination of the database will be via the World Wide Web and is anticipated to be free. However, the nature of the staged development allows for portions of the database to be fee-based if it is deemed necessary to continue the project. Software tools are currently under investigation that will enable direct deposition of data sets and real-time data evaluation by the community. All data included in the database will be critically assessed and a final determination will be made as to the accuracy of the data before final inclusion into the database.

**The Future Molten Salt Data Project**

During the last ten years, there has been a significant increase in the amount of data available on molten salts. This explosion in the amount of data is due to the emergence of molten salts into new applications, such as waste processing, energy storage and metals electrodeposition. In addition, classes of salts that are liquid at room temperature are receiving attention for applications in both catalysis and energy storage. The addition of new salts and data properties provides a propitious time to further evolve the existing database into a database that will provide new data visualization, modeling and simulation and collaboration tools. The new database will emerge as the Virtual Molten Salt Laboratory (VMSL) and will enable researchers in the field to have expanded design and experimental capabilities.

**Proposed Plan for the VMSL:**

Development an open and flexible distributed architecture to support the implementation of a multidisciplinary database utilizing metadata tools

developed as part of the Globus Data Grid (http://www.globus.org/documentation/papers.html) and the NPACI Data Technical Thrust Area (http://www.npaci.edu/Thrusts/DI/index.html). Specifically, metadata strategies, as well as evaluating the underlying technologies necessary for working with metadata and for working with distributed collections of data, will need to be developed. In addition, the open architecture and the multi-user data tools, i.e. data input, data evaluation, and inclusion into master database, will necessitate the development of a "collabotorium" for accessing, evaluating, and utilizing the data. This effort will have an immediate positive impact on the molten salt community and is likely to also serve as a model for other multi-disciplinary scientific areas.

Building on the individual strengths of each team member, the Alliance, NIST, and IUSTI, propose to build a common, flexible architecture that would be used to build the on-line access component for the VMSL. The Alliance would be the hub for the technology elements of the collaboration, NIST would aid in the development of data evaluation tools for the collabotorium and in the final dissemination of the database and IUSTI would serve as the scientific lead for the project.

An important and vital component to this project is the inclusion of the user community early in the development of the architecture. Utilizing IUSTI's experience and long history within the molten salt community, a guest researcher (Prof. Marcelle Gaune-Escard) will spend 3-6 months at NCSA in the initial stages of the project to assist in the scientific aspects of the development. In addition, NIST will actively seek out opportunities to partner with societies and other agencies, such as the Minerals, Metals & Materials Society (www.tms.org), to avoid duplication of efforts, broaden the scientific base of the project and to aid in dissemination of results. Finally, since the mid-70's, NIST has served as a focal point for critically evaluated data to the molten salt community; therefore, it is a logical extension of their past efforts to provide a home for maintaining the VMSL after the completion of this effort.

**Inclusion of Room-Temperature Molten Salt Data:**

As mentioned above, the recent resurgence of interest in room-temperature molten salts, or ionic liquids as they are sometimes referred to, has provided the opportunity to build a component of the database to

support room-temperature salt data. This presents new challenges to the project mainly the absence of critically evaluated data on the emerging salt systems. However, this serves to focus the research community on data quality and quantity issues. Moreover, the critical analysis of existing room-temperature data may reveal new areas of research and discovery. The next steps in realizing the inclusion of room-temperature molten salt data must come from the research community. This Conference represents a significant step in recognizing data needs and soliciting community involvement. Volunteers are needed to serve as leaders in focusing data retrieval activities (from the literature and ongoing work) and to forge data links between diverse technologies areas, i.e. catalysis and batteries. The upcoming CODATA Workshop on Building Information on Molten Salts in Marseille, France, September 18-20, 2000 provides a logical opportunity to coalesce future data activities and finalize the involvement of room-temperature data in the VMRL design.

The CODATA Molten Salt Working Group was established in 1999 with the objectives of developing the criteria for evaluating molten salt data including estimation procedures based on research results, and eventually improving the accessibility of these data in an internally consistent database. Coordination and standardization of existing molten salt data is essential to this activity. The goal of this first Workshop is to discuss the barriers to and propose solutions for bringing together the vast amounts of data in the molten salt literature into a "Virtual Molten Salt Data Laboratory". The Workshop will be divided between individual presentations and panel discussions. Following the completion of the workshop, a summary of the discussions will be posted on the Internet and a working model will be proposed for the creation of a centralized Virtual Molten Salt Data Laboratory.

The workshop will consider two main issues:

- The large amount of data available in the literature and
- The effective use of the Internet to link together the different communities of data generators and data users.

Other topics to be addressed include:

- What community action, if any, is needed to retrieve the older data both in the open and "grey" literature?
- What databases exist currently and are there gaps in the data that need to be filled?

- What additional standards are needed to facilitate the building of a “Virtual Molten Salt Data Laboratory”? Delivery? Integration?
- What actions are needed to sustain the molten salt data community, especially as the WWW promotes individual actions?
- Additional information or questions concerning this Workshop should be addressed to Marcelle Gaune-Escard, mge@iusti.univ-mrs.fr or Joan Fuller joan.fuller@nist.gov .

The NATO Advanced Study Institute on “Molten Salts ; from Fundamental to Applications” ( 4-14, May 2001 –Kas, Turkey) will include a related session and thus provide the next opportunity to follow on and to review advances along these lines. Additional information or questions concerning this Workshop should be addressed to Marcelle Gaune-Escard, mge@iusti.univ-mrs.fr .

A copy of the slides presented at the present Sixth International Conference on **Molten Slags, Fluxes and Salts** ( Stockholm - Helsinki June 12-16, 2000) are included for information in the following.

# The Challenges of Building a Molten Salt Database

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# Historical Overview

*"The field of molten salts has been the subject of renewed interest over the past 25 years and has attracted the attention of scientists in research and technology from such diverse fields as: theoretical and applied electrochemistry, inorganic coordination chemistry, transition metal chemistry, preparative and process chemistry having melts as catalysts or as reaction media, nonaqueous solvents, thermochemistry, fuel cells and batteries, nuclear technology, analytical principles of chromatography and liquid-liquid solvent extraction, corrosion science, and the principles of liquid structure, theoretical chemistry and physics."*

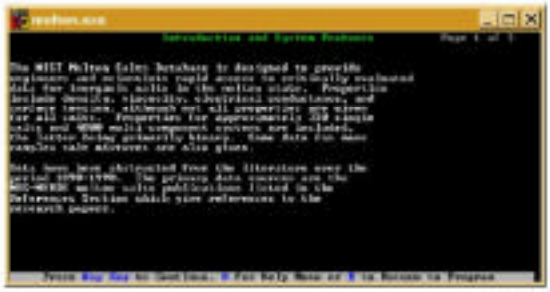
*George J. Janz, Molten Salt Handbook, 1967.*

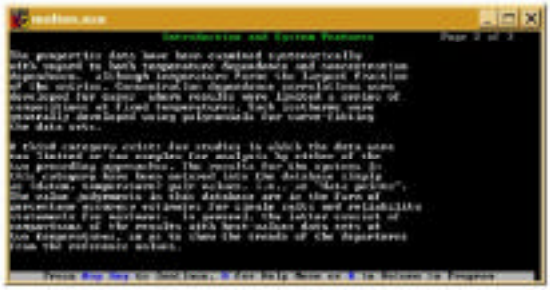
## *Initial efforts*

- The first volume of the National Standard Reference Data System (NSRDS) molten salt data series was released in 1968 and was followed by 9 more volumes.
- The original computerized database was compiled in the late 1980's

## *Initial efforts (..)*

- critically evaluated data for inorganic salts in the molten state : density, viscosity, electrical conductivity, and surface tension.
- Up to 1990, a significant portion of the critically evaluated data available in the literature from 1890-1990.





## Then ...

**Explosion in the amount of data due to :**

- **Emergence of molten salts into new applications**
- **Classes of salts that are liquid at room temperature receiving renewed attention for applications in both catalysis and energy storage.**

## Building Databases : what a database *is* and *is not*

*In general, scientific databases fall into two categories*

- **data impartially compiled from the known literature**
- **data that is critically assessed by independent experts.**

## NIST SRD Systems

- *11 web based – FREE*
- *http://www.nist.gov/srd/online.htm*
- *NIST Chemistry WebBook & NIST Ceramics WebBook*
- *10,000s users per month*
- *Data is added continuously*
  - *46 PC based databases*
  - *Updated 12-24 month cycle*
  - *Over 5000 databases distributed last year*
  - *Use third party distributors*

# Molten salt data

- Molten salts :
  - High temperature liquids
  - room temperature molten salts
- Investigations conducted
  - at the fundamental level *(physical & chemical approach dealing with the liquid state of matter)*
  - at an applied level *( support of the large number of industrial applications).*

# The Current Molten Salt Database Project

- **The current project between IUSTI and NIST : a multi-stage effort to build a molten salts database that will contain evaluated data for a variety of applications.**
- the success of the project depends on positive interactions between a diverse group of people – support staff ***to identify and collect relevant literature***, scientists ***to extract and evaluate the data***, database experts ***to design and build the necessary data architecture and interfaces***, database reviewers ***to ensure that the database is of the highest quality.***

# The Current Molten Salt Database Project (…)

- The advent of the World Wide Web (WWW) has provided another exciting component to this paradigm – a global database structure that enables direct data deposition and evaluation by the scientific community.

# The Future Molten Salt Data Project

- It is the time to evolve the existing database into a modern on-line database
- to provide new features such as,
  - data visualization,
  - modeling and simulation
  - collaboration tools.
- The new database will emerge as the Virtual Molten Salt Laboratory (VMSL) and will enable researchers in the field to have expanded design and experimental capabilities.

# New concepts in engineering data information systems

## 1. Managing Data Collections in Persistent Archives

- Development of an appropriate information model for describing data. Technology based on the eXtensible Markup Language (XML) can provide a common information model for describing data structure and data set context.

## 2. Data Grids

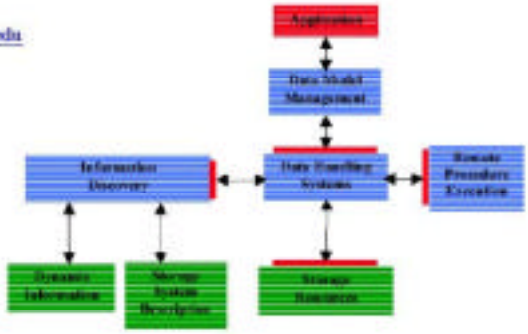
- In the US, the National Partnership for Advanced Computational Infrastructure (NPACI) is building a national data grid through the integration of local data caches, distributed data collections, and distributed archives.

# Introduction to The Grid

- With the advent of new high-speed research networks, linking together high-performance resources is now possible.
- The Grid merges people, computers, databases, instruments, and other resources in ways that were simply never possible before.

# Persistent Archives for Data Collections

*(from NPACI)*
*Info* http://www.npaci.edu

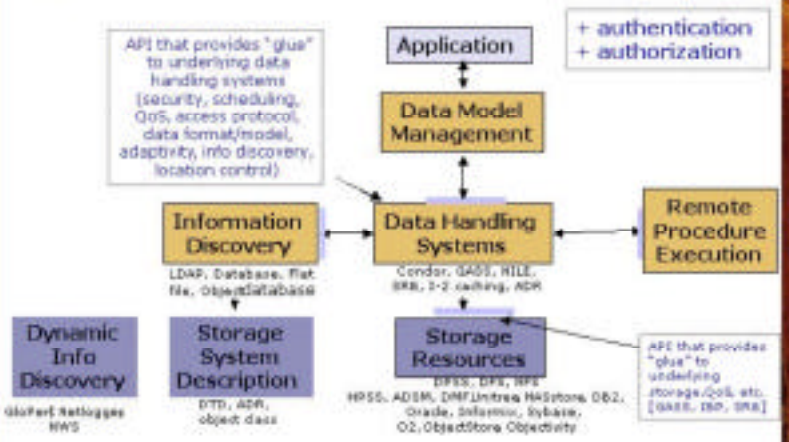


Data access architecture for Open Grid Architecture

National Partnership for Advanced Computational Infrastructure

# Grid Forum Data Access Architecture

*(from NPACI)*
*Info* http://www.npaci.edu




National Partnership for Advanced Computational Infrastructure

# Information Management Architecture

- **Grid Forum**
  - **Support for distributed services / procedures**
  - **Inter-realm authentication**
    - GSI Grid Security Infrastructure
  - **Data handling system**
    - Storage Resource Broker, Meta-data Catalog
- **Digital library community**
  - **SDLIP interoperability protocols**
    - Distributed information resources
  - **Mediation of information using XML - MIX**

# Some examples ...

- Computer-enhanced instruments, such as in microtomography
- Collaborative engineering, such as creating a collaborative learning environment for young children
- Very large-scale simulation, such as vehicle simulation
- *Browsing of remote datasets*
- *Use of remote software*
- *Data-intensive computing*
- Large-scale parameter studies

# Now is the time that we need your input.

*High temperature*

&

*lower temperature systems*



# Now is the time that we need your input.

- **None**
- *At least send your paper list (we'll pay for postage ... e-mail is free !)*
- **Moderate**
- *You're an expert in your field and nobody but you can do data evaluation*
- **Intense**
- *Join the developing group (NIST, NCSA, IUSTI) and be a partner Molten Salt Data Center!* *VMSL*

## Now is the time that we need your input.

- *Direct submittal*
- *Literature surveys*
- *Molten salts data expertise*
- *Data assessment*
- *Development of database tools*

## Now is the time that we need your input.

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FROM MARSEILLE

TO CORSICA

Workshop Secretariat :
E-mail: molten.salts@luminy.univ-mrs.fr

CODATA Molten Salt Working Group

*workshop on*

**BUILDING INFORMATION**

**ON MOLTEN SALTS**

Marseille to Corsica,
France
18-20 September 2000

NATO - ASI - 2001

## *NATO Advanced Study Institute*
## "Advances in molten salts : from fundamental to applications"