Supercritical Fluid Database for practical applications of supercritical fluid technology

Yoshiaki Kurata
Supercritical Fluid Team, Research Center for Compact Chemical Process

A tool for promotion of supercritical fluid research

Supercritical fluids are non-condensing; its density may change in a wide range depending on the pressure. This and other exotic characteristics of supercritical fluids has long been known, but it began to attract attention as a new class of solvents only recently. Once brought to the supercritical state, the naturally abundant water or carbon dioxide acts as an innovative medium for energy-saving, safe and environment-friendly chemical processes for the future.

Japan Chemical Innovation Institute (JCII) has been leading a NEDO joint research program called “Development of Technology to Reduce the Burden on the Environment” since 2000. We attempted to make its accumulated results, ranging from fundamental to application research, open to public for widespread practical use of the technology and provide a basis for more systematic presentation of related data and methodology.

This task was achieved by the compilation of Supercritical Fluid Database (SCF-DB).

The database is provided on the Internet as a convenient tool for R&D activities related to supercritical fluids.

Structure of SCF-DB

SCF-DB has two objectives: making research results accessible to the public and assisting practical application of the technology through systematic representation of relevant knowledge. In order to deal with research results including numerical values and graphic representations, and to integrate information needed for industrial use of the technology ranging from the basics of supercritical fluids to intellectual properties information, SCF-DB was constructed as an aggregate of six segments:

1. Supercritical Fluid Research Database, comprising abstracts, figures and citations of research reports.
2. Corrosion Database, designed for numerical search and two-dimensional representation of corrosion data.
3. High-Pressure Gas Database, a collection of safety data, accident reports, and related regulations.
4. Intellectual Property Database, providing recent information on intellectual properties related to supercritical fluids.
5. Simulations, providing examples of simulations using estimated data including those on properties of polymers.
6. Research Results of The Society of Chemical Engineers, Japan, a collection of bibliographic data compiled by the Division of Supercritical Fluids of the society.

Fig. 1 shows a procedure of searching the Supercritical Fluid Research Database and an example of results obtained (taken from AIST Web site, RIO-DB page).

Fig. 2: Two- and three-dimensional movie representations of simulation results.
Development of "Claist", a Flexible, Heat-Resistant Inorganic Film

Takeo Ebina
Material Processing Team, Research Center for Compact Chemical Process

"Claist" is a film under development in the Research Center for Compact Chemical Processes. It has both plastic-like flexibility, workability, and ceramic-like characteristics. The membrane is manufactured by densely laminating clay crystals about 1 nm (1 nm is one billionth of 1 m) in thickness, together with a small amount of additives, if necessary to improve flexibility and for other purposes. The total thickness of the membrane can be controlled in a range from 10 to 100 µm, maintaining flexibility comparable to that of a sheet of copying paper.

Permeability (cc/m²/24 hr/atm) of dry Claist to inorganic gases such as helium, hydrogen, oxygen or nitrogen was under detection limit at room temperature. This is far lower than conventional engineering plastics (e.g. Nylon-6 with an oxygen permeability of 18 cc/m²/24 h/atm) and comparable to that of aluminum foil (oxygen permeability = 0). Currently samples of standard type (usable at temperatures up to 350° C) and heat-resistant type (up to 600° C) are available from AIST innovations. Other possible modifications include reinforcement with heat-resistant fibers, lamination with heat-resistant cloth, surface treatment for higher thermal resistance, and water-proof surface treatment.

Claist is an environment-friendly product because it consists principally of clay and no byproduct is formed in its production process. Its production cost is comparable with that of general engineering plastics. Claist, with its thermal resistance and gas barrier characteristics, is a promising material for gaskets in automotive engines, sealing of the piping in chemical plants, fuel cells and flexible circuit substrates. Developments are planned for expansion of applications by improving moisture resistance, surface flatness, and mechanical properties.

result, the database contains drawings of testing and measuring apparatuses, providing useful information for developing new research programs. The Society of Chemical Engineers data can also be utilized in the same way.

The main content of the Corrosion Database is numerical data on the corrosion behavior of metallic materials in supercritical water, collected from a variety of reports and articles published in and outside Japan. These data should be helpful for preliminary screening of materials for apparatuses.

The High-Pressure Gas Database aggregates safety data (such as ignition of materials in high-pressure oxygen), important standards in selected countries, and accident reports, thus providing useful information for safety design of experiments. The database also contains Japanese regulations and related legal procedures.

Fig. 2 shows an example of two- and three-dimensional movie representations of simulated dissolution and distribution of carbon dioxide in a polymer. The file can also be used for new analysis using retrieved data.

While data in SCF-DB are still behind the target to build a comprehensive information basis for the supercritical fluid technology, links to "SCF-related Web sites" are provided as supplements.

Supercritical Fluid Database in future

While being expected as an innovative way of chemical reactions, the supercritical fluid technology has suffered from lack of organized knowledge needed as the basis for research and development. SCF-DB aims at fill this gap by providing information that assists in appreciation of possibilities of the technology and promotion of its industrial applications in a new way.

Future plans for SCF-DB include addition of estimation formulas for properties of supercritical fluids and for behavior of polymers in supercritical atmospheres. Efforts will further be intensified to collect relevant data, material, news and related technical information.