New Analytical Method that Measures Fluid Properties within Closed Container Helps Verify Chemical Weapons Compliance

Ausgangssituation
Ein Verfahren zur Bestimmung der Zusammensetzung von Flüssigkeiten innerhalb eines geschlossenen Behälters zu entwickeln war das Ziel an den Los Alamos National Laboratories.

Fragestellung
Mit Hilfe einer akustischen Methode lassen sich die Eigenschaften einer Flüssigkeit bestimmen. Diese Daten liegen jedoch in Rohform vor, erst durch die Auswertung des Resonanzspektrums muss mit Hilfe mathematischer Funktionen (Peak Fitting, Integration) vorgenommen werden. Daneben war eine gut lesbare und detaillierte Darstellung der Daten gefordert, um Abweichungen im akustischen Spektrum erkennen zu können.

Lösung
Mit Origin und Origin Pro lassen sich beliebige Datenformate beliebigen Umfangs einlesen und verarbeiten. Vor allem die mathematischen Funktionen, die Automatisierbarkeit und die umfangreiche Diagrammbibliothek sprachen für den Einsatz von Origin und Origin Pro als Analysewerkzeug**.**

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The ability of a new analytical method to measure fluid properties within a closed container will help to verify compliance with the chemical weapons treaty. The new method will make it possible for inspectors to determine whether artillery shells and other sealed containers are filled with chemical warfare compounds without the time and expense of opening them. Called Swept-Frequency Acoustic Interferometry (SFAI), the new noninvasive method shoots sound waves through the liquid to measure its sound speed, sound attenuation, density and viscosity. The method was developed by researchers using data analysis and technical graphics software to correlate the characteristics of the resonance peaks of sound waves to the liquid's physical properties.

SFAI is a novel adaptation of an ultrasonic interferometry technique developed decades ago for determining sound velocity and absorption in liquids and gases. The underlying principle is the establishment of a standing acoustic wave inside a resonator cavity, using external excitation and simultaneous detection. It works through the application of swept frequency electric excitation, in a frequency range from 1 kHz to 15 MHz, to a piezoelectric transducer attached to the outside of the container. At certain frequencies, the signal produces acoustic resonance in the liquid inside the container. The result is a series of resonance peaks in a spectrum. These are detected by a second piezoelectric transducer that works as a receiver.

Information about the contents is derived from an analysis of the spectrum of resonance peaks. A single sweep measurement can be used to derive liquid properties that include sound speed, sound absorption, frequency dependence of sound absorption, and liquid density. Sound speed is determined from the spacing of the peaks. In a non-invasive measurement, sound waves inside the container are attenuated because of the absorption of the sound, which is frequency-dependent, and also due to the acoustic impedance mismatch between the container wall and the liquid inside. Sound attenuation at a given frequency is determined by the width of the resonance peak. Density is determined from measurements of peak width over a wide band of frequencies followed by extrapolating the peak width to zero frequency, giving the value of the acoustic impedance ratio of the wall to the material. Viscosity is determined from the interference of sound waves that go around the circumference of the container and appear superimposed on top of the liquid spectrum. In SFAI, deriving so much information from the one measurement is important, particularly in the area of chemical diagnostics. Many chemical compounds can have the same sound speed, for example, but none is identical across all four parameters.

In the development of the SFAI process, the task for researchers was to create algorithms that would derive sound velocity, attenuation, density, and viscosity from the spectrum. To do this, literally thousands of data sets from tests were plotted against theoretical predictions. Each new data set had many subtle variations some of which hid patterns that could be used to determine the properties of the fluid inside the sealed container. Data analysis software, ORIGIN from OriginLab Corp., Northampton, Massachusetts, was selected to analyze the data because it provided all the advanced data analysis routines required to detect underlying patterns. In addition, its ability to easily visualize data turned out to be critical to this work.

With ORIGIN, it was possible to adjust virtually any component of a plot through interactions with the mouse and dialog boxes. As a result, instead of poring over tables of data or rudimentary plots and missing important information, researchers were able to easily create thousands of highly informative plots, some of which uncovered vital aspects of the SFAI process. For example, in a plot of an acoustic spectrum, one would anticipate seeing regularly spaced peaks. Using ORIGIN's zoom feature, however, it was sometimes possible to pick up unexpected and subtle variations in the spectrum. These slight variations could indicate some new physics that was then incorporated into an algorithm to extract one of the target parameters

The analysis software's peak fitting feature was first used to derive the liquid's speed of sound and attenuation of sound (see Fig. 1). It was used to find the maxima of resonances, for example, and the differences between them is what indicates sound speed. A width measurement, also obtained from a peak fit, relates to absorption and attenuation of the sound. Rather than requiring weeks of writing subroutines to fit peaks to the data, the process with ORIGIN was simply "point and click." ORIGIN's peak-fitting module included all the necessary spectroscopic fitting equations. It also provided time-saving tools such as automatic determination of peak centers, half-widths, heights, and areas. The simplicity of the peak-fitting process allowed researchers to evaluate many algorithms quickly.

In several cases, the right graphics helped researchers make sense of apparently random data. In one instance, researchers noticed fluctuations on the right side, the high frequency side, of the peaks, and originally believed them to be noise, a nuisance to be smoothed out or tossed out. However, an autocorrelation done with ORIGIN detected a periodic pattern that turned out to be related to shear modes which propagated along the circumference of the container (Fig.2). These shear modes were later directly related to the viscous coupling of the liquid. The result was a unique way to determine viscosity of liquids inside sealed containers. After all the required algorithms for SFAI were determined, they were rewritten as FORTRAN or Quick BASIC programs for use in the detector that is used in the field. The instrument weighs about six pounds, and feeds data into a 486 PC with a customized digital synthesizer and analyzer board from Neel Electronics, Laguna Niguel, California. The computer memory contains a database of the physical properties of all primary chemical warfare compounds. To use the system, an operator simply places the transducers on the item to be tested and presses a button.

All measurements and analysis are done automatically. The detector can safely analyze a container in approximately 20 seconds, a significant improvement over early monitoring systems.

In the area of chemical weapons compliance, SFAI is a very needed technology. The Chemical Weapons Convention treaty calls for the eventual destruction of all chemical weapons, making it essential that there is some technique that can quickly and easily monitor compliance. The US Defense Special Weapons Agency has funded this development effort for use in such treaty compliance. This technique can allow "challenge inspections" of suspect munitions without opening or drilling a hole into artillery shells or containers. At this time, SFAI has been successfully tested on a large variety of chemical munitions at government storage depots. During those trials, a developer of the system was on hand to assist with the operation of the detector. Operators who have had no previous experience with the technology will perform the next stage of field trials.

SFAI has other applications besides determining the content of sealed munitions. It has been shown to be a good technique for characterizing petroleum products and also for detecting spoiled milk in sealed containers such as paper cartons, plastic bottles, and Tetra Pak pouches.

In the development of SFAI, nearly every capability of ORIGIN was used on a daily basis. When the software did not contain a certain analysis, it was either created in-house through ORIGIN's built-in scripting language or OriginLab provided it. The company was very responsive to the needs of this project, to the point of delivering a new feature only a day after it was requested. Without ORIGIN, it would have been very difficult to develop the algorithms for this technique.

(SFAI is a technology developed and patented by Los Alamos National Laboratories)