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Sandia National Laboratories

Computer Simulation Improves Design of Hand-Held Chemical Analysis System

THE CHALLENGE

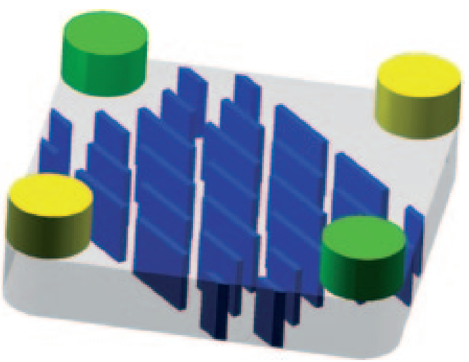
- Designing a micro-electro-mechanical system (MEMS) that operates on too small a scale to measure
- The preconcentrator needs to collect as much analyte as possible and release most or all of it in a very short period of time

THE STORY

Sandia Corporation, a Lockheed Martin Company, has developed a hand-held chemical analysis system designed to be used by first responders for the detection of toxic agents. The first stage of the ChemLab system is the preconcentrator which samples and collects analytes from an inlet gas stream and ejects them on command into the separation stage. Due to difficulties associated with measuring flow on a micro scale, designing the preconcentrator was challenging. Sandia engineers worked with consultants at ESI Group to simulate fluid flow and chemical reactions through the preconcentrator with ESI's CFD-ACE+ computational fluid dynamics (CFD) software. The simulation results showed that in the initial concept design flow rushes along the sides of the preconcentrator with poor wetting of the adsorbent pillars resulting in inefficient adsorption of analyte. Sandia and ESI engineers modified the design by rearranging the pillars to improve wetting and optimize the adsorption and desorption phases.

THE BENEFITS

- Sandia substantially improved the preconcentrator design
- Simulation reduces the number of prototypes that were needed.



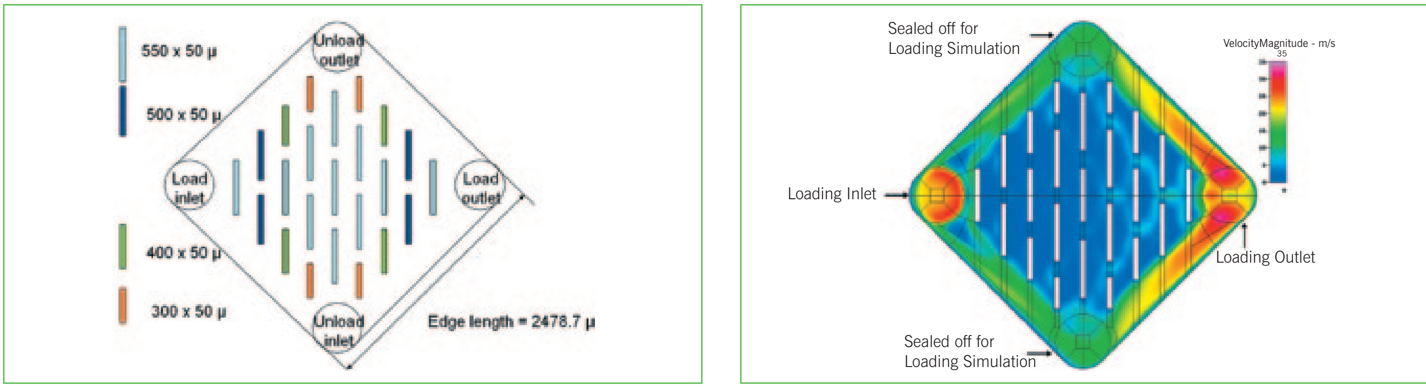
Sandia's ChemLab is a portable, handheld chemical-analysis system for homeland security, defense, and environmental and medical applications that can detect chemical warfare agents and toxic industrial chemicals. The planar preconcentrator consists of a thin silicon nitride membrane supporting a patterned metal film heating element. The membrane is coated with a templated porous sol-gel to selectively and reversibly absorb analytes of interest while allowing interferents to pass by. In the collection phase, a gas stream containing target analytes flows through the preconcentrator chamber and adsorbs to the preconcentrator film. The adsorbent surfaces are then heated using thin-film resistor micro-heater while the carrier gas is flowed into the device. This thermally desorbs the collected analytes in a narrow concentrated chemical pulse over approximately 0.2 seconds.

DESIGN CHALLENGES

The challenges to the engineers designing the preconcentrator were to collect as much of the analyte as possible on the adsorbent surfaces in the least possible time and provide a sharp peak of analyte flux for detection by the sensor. The design parameters included the geometry of the preconcentrator, the mass flow rates during the adsorption and desorption phases, the carrier gases during adsorption and desorption phases, adsorption and desorption kinetics, and the desorption temperature profile. Microfluidic devices such as the _ChemLab are not well suited to traditional build and test design methods. The small size of the devices makes it nearly impossible to instrument them with sensors that would be required to evaluate local fluid flow. Without quantitative information, engineers normally are left to rely upon on their instinct and guesswork in attempting to optimize the design.

A substantial improvement over the conventional design methods was achieved in this application by simulating the performance of the preconcentrator using CFD-ACE+. The CFD simulation showed that in the original design, flow rushes along the edges of the preconcentrator to avoid the obstructions presented by the pillars. The result was that there was very little contact between the flow and pillars. Engineers rearranged the pillars in an effort to solve this problem. The basic idea was to position the pillars to block off the escape route around the sides of the preconcentrator. They accomplished by running the pillars all the way across the preconcentrator so that the gas flow was forced to go through the rows of pillars. Re-running the analysis using this geometry showed a greatly improved flow profile with much more wetting of the adsorbent pillars.

After the optimal flow geometry was determined, four simulations were performed to measure the surface reactions involved in adsorption and desorption of the analyte. Two different flow rates were used for the adsorption phase and two different gases and two different flow rates were used for the desorption phase. The simulation results showed much more analyte is adsorbed with a flow rate of 300 mL/min. Analyte concentration drops dramatically across the chip for the 60 mL case with virtually no analyte found on the pillars away from the inlet.



Original design showed poor wetting of pillars

"The cost of designing, fabricating and testing micro devices can often be prohibitive. So the ability to simulate the behavior of the micropreconcentrator was critical to advancing new designs quickly and affordably. To this end, working with ESI Group was a very beneficial since their experience in CFD simulation of microfluidics, chemical reactions, flow, etc permitted us to rapidly make a model, validate it and use it to predict improved designs. We are now implementing the recommended design changes." - Ron Manginell, Principal Member of the Technical Staff, Sandia National Laboratories

CFD helped improve flow through preconcentrator

ABOUT ESI GROUP

ESI is a world-leading supplier and pioneer of digital simulation software for prototyping and manufacturing processes that take into account the physics of materials. ESI has developed an extensive suite of coherent, industry-oriented applications to realistically simulate a product's behavior during testing, to fine-tune manufacturing processes in accordance with desired product performance, and to evaluate the environment's impact on product performance. ESI's products represent a unique collaborative and open environment for Simulation-Based Design, enabling virtual prototypes to be improved in a continuous and collaborative manner while eliminating the need for physical prototypes during product development. The company employs over 750 high-level specialists worldwide covering more than 30 countries. ESI Group is listed in compartment C of NYSE Euronext Paris. For further information, visit www.esi-group.com.

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