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DESIGN OF AN ASYMMETRIC WAVEFORM SPECTROMETER

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Abstract

A design for a handheld MEMS chemical detector is proposed. The detector will be used to detect trace amounts of chemicals in air. It can detect drugs, toxic chemicals and/or explosives. The proposed detector will use ion mobility spectrometry (IMS), a technique that is well known for accuracy and has been used in the past in suitcase sized chemical detectors. The separation and detection of the chemicals occurs in the drift channel and the process was modeled using the finite element method and CoventorWare modeling software. A manufacturing process sequence for the drift channel is proposed and was demonstrated.

Introduction

The goal of this effort is to design, model, and prototype a MEMS chip that will be the key component in an ion mobility spectrometer (IMS). This technique uses an asymmetric potential to separate the various ion species in a stream of incoming air [1-4]. One advantage of IMS is its ability to separate chemical species from air at atmospheric pressure and temperature. This is a requirement for a simple to use handheld drug or chemical detector. IMS can be used to detect drugs, toxic chemicals and explosives and it is well known for accuracy in detecting very small amounts of chemicals. This chemical detection technique has been used in the past, but not in handheld detectors.

One variant of IMS is the high-field asymmetric waveform ion mobility spectrometry or FAIMS [3]. The FAIMS process, shown in Figure 1, works as follows: a gas sample is admitted into the instrument where gas molecules are ionized, typically by a weak radioactive isotope source, ultraviolet light source, and more recently through field emission. The ions move along the length of a channel while they are separated in the transverse direction by an asymmetric electrical potential. The potential, in the form of an asymmetric waveform, causes relative motion between the various chemical species. The species that hit the charged top and bottom plates are neutralized and only those ions that move along the center are detectable as charged chemical ions at the end of the channel.

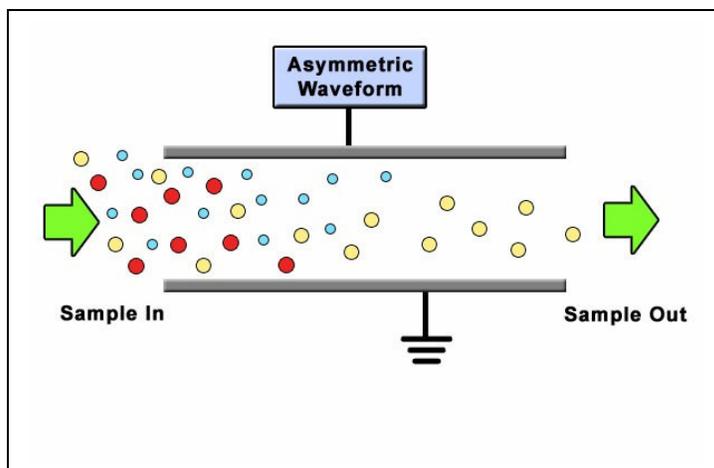


Figure 1 – FAIMS Drift Channel

One important assumption is that ions produced in the ionization chamber are created in the same proportion as their concentration in the air stream. Thus, because air is mostly Nitrogen and Oxygen, if we can measure the ratio of Nitrogen and/or Oxygen ions to ions of a species such as CO₂, we can tell the concentration of the species of interest in the air stream. This is a two-step process where first, the Nitrogen or Oxygen ions are channeled through the center of the drift channel and counted, and then the process is repeated for the species of interest. It is important to note that the ability to separate the various species is the key to the operation this type of instrument.

Chemical Specie Separation

Species separation occurs because different molecules move at different velocity under the influence of the electrical field created by the charged top and bottom plates. Larger, heavier molecules have higher inertia than smaller, lighter molecules. If the electrical field is changing strength and polarity, the effect of inertial mass is to make the lighter molecules respond faster to the changes. The result is that the movement of the different ions is dependent on the frequency and amplitude of the asymmetric waveform, especially at very high frequencies of more than 10⁶ Hz. In addition, to the field strength, the size of the ions and molecules of the carrier gas (i.e. air in our example), and their concentration are important because they dictate how many collisions take place as the ions move towards the charged top and bottom plates.

The resulting velocity as the ions move towards the charged plates is called drift velocity (V_d) and is defined as [1]:

$$V_d = K \times E \quad \text{Eq. 1}$$

where

$$K = \text{ion mobility in cm}^2/\text{volts}\cdot\text{sec}$$

and

$$E = \text{electric field strength in volts/cm.}$$

The ion mobility (K) is a function of the molecule's weight, size, effective cross section and the same properties of the molecules in the carrier gas. In most cases, K is an experimental value as defined by Equation 1, but there are theories that attempt to predict mobility from first principles. It can be estimated from Equation 2 by Mason and McDaniel [1,5]

$$K = \text{drift velocity/electrical field} = (3e/16N)(2\pi/\mu k T_{\text{eff}})^{1/2} [(1+\alpha)/\Omega_D(T_{\text{eff}})]. \quad \text{Eq. 2}$$

The variables are defined in the references. If the ions and molecules are rigid spheres that interact in elastic collisions, Mason's equation can be simplified to

$$K = \text{drift velocity/electrical field} = (3e/16N)(2\pi/\mu k T_{\text{eff}})^{1/2} Q_D. \quad \text{Eq. 3}$$

$Q_D = \pi d^2$ is the collision cross section and d is the average diameter of the ions and molecules.

When experimental data are collected, it is observed that the mobility can increase with increasing field strength, or decrease with increasing field strength, or it can be independent of field strength [5]. This difference in behavior facilitates the separation of the ions, especially at high field intensities of 10,000 Volts/cm and higher typical of FAIMS. Increasing mobility as a function of field strength allows ions to move farther during the high voltage part of the cycle than during the low voltage part resulting in “drift” relative to ions that have decreasing or no change in mobility.

There are no easy and direct ways of predicting what type of oscillating electrical field will cause separation of ions of different species. It is easier to separate ions with a large difference in their ion mobility, but even a small difference can be enough if the right waveform and voltage is used. Asymmetric square waveforms as represented in Fig. 2 have been used in the past [2,3] to achieve species separation. This type of waveform is defined by four variables: 1)the frequency, 2)the peak value, 3)the asymmetric ratio and 4)the offset. In addition, 5)the length of the drift channel and the velocity of the carrier gas are important variables that can be controlled to achieve separation of the species. Thus seven variables are available (including the mobility of two or more species). The optimum combination can be discovered by modeling the process.

Modeling the Drift Channel

The function of the drift channel is to separate the various species in the air stream. This is accomplished by applying a variable potential to the top and bottom plates of the channel. The only way to determine what potential will be successful in separating two species is to experiment with the variables until the best potential is found. This can best be accomplished by creating a model of the drift channel. Hence, a model was built using Coventorware software by Coventor, Inc. using the finite element method.

The software used to model the drift channel was Coventorware by Coventor, Inc. Modeling begins by defining a process plan. The process plan lists the steps required to fabricate the structure. Figure 3 lists the steps and Figure 4 is a simple depiction of the various components needed to manufacture a drift channel. The steps are: 1)begin with a Pyrex glass wafer, 2)use vapor deposition to coat one side of the Pyrex wafer with gold, 3)bond a silicon wafer with the channel shape etched away and 4)bond another Pyrex wafer also coated with gold on top. Step 3, etching the channel shape in the silicon wafer, requires a mask with the channel dimensions 10mm X 100mm.

With the process plan and the mask outline we can generate a solid model of the drift channel in Figures 5 and 6. Figure 6 is the cross-section of the channel with the top wafer removed to show the air passage. Finally, the fluid can be meshed for analysis as shown in Figure 7. In this example, the elements used are Manhattan bricks with 4 nodes.

The analysis was performed using the Coventorware Netflow module, normally used to model electrophoresis processes. The boundary conditions are 4 sidewalls, an inlet mass flow rate, inlet concentration for all species, and the voltages of the top and bottom walls. The top wall was subjected to the asymmetric waveform potential. Finally, the information necessary for the transient analysis included the time step and the convergence requirements.

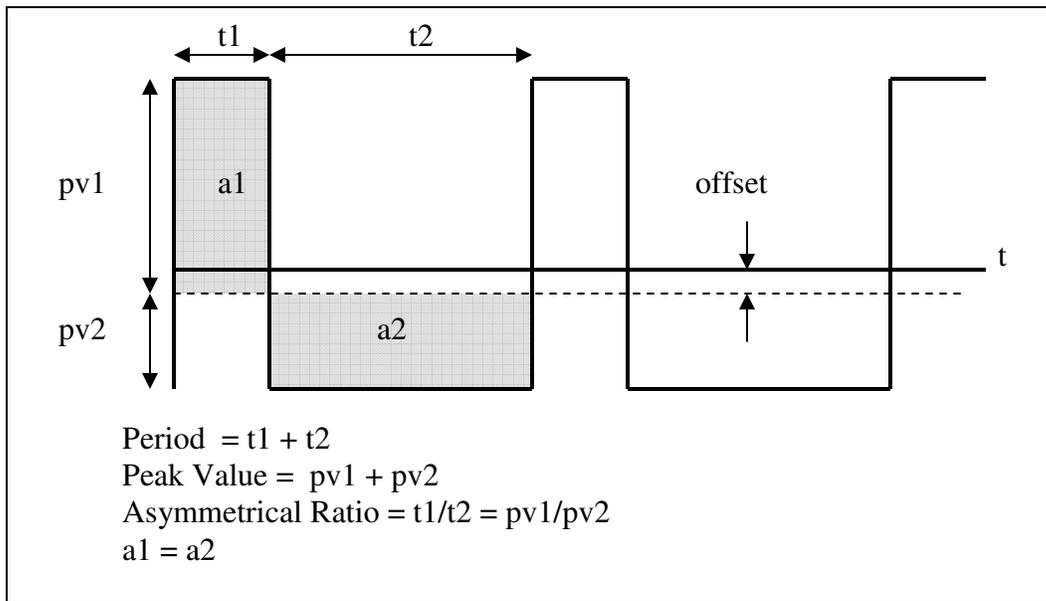


Figure 2 – Asymmetric Square Voltage Waveform

ProcessEditor: C:\Coventor_Design_Files\ctc_spectrometer2D\Devices\channel2.proc

File Edit View Help

Step	Action	Type	Layer Name	Material	Thickness	Color	Mask Name/ Polarity	Depth	Offset	Sidewall Angle	Comment
0	Base		bottom	GLASS	500.0	yellow	GND				
1	Deposit	Planar	electro...	GOLD	1.0	green					
2	Deposit	Planar	channel	SILICON_100	100.0	orange					
3	Etch	Front, Last Layer				cyan	channel2 -	100.0	0.0	0.0	
4	Deposit	Planar	air	AIR	0.0	blue					
5	Deposit	Stacked	electro...	GOLD	1.0	red					
6	Deposit	Planar	top	GLASS	500.0	yellow					

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Figure 3 – Process Plan for Drift Channel

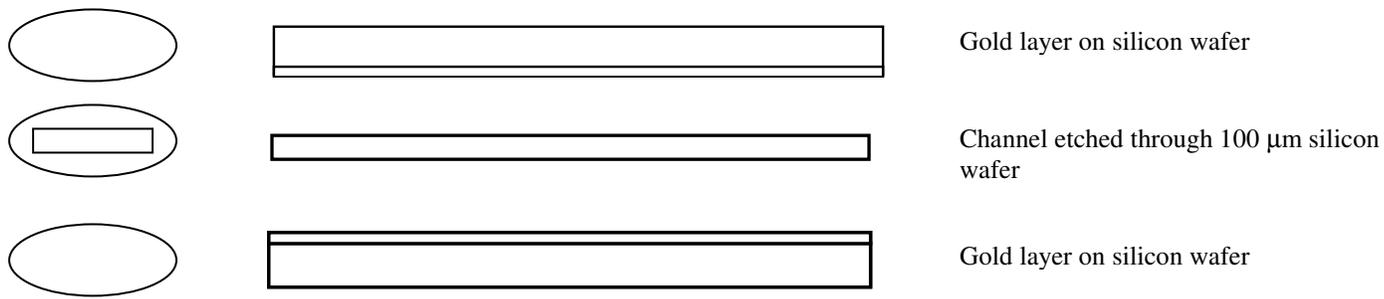


Figure 4 – Drift Channel Components

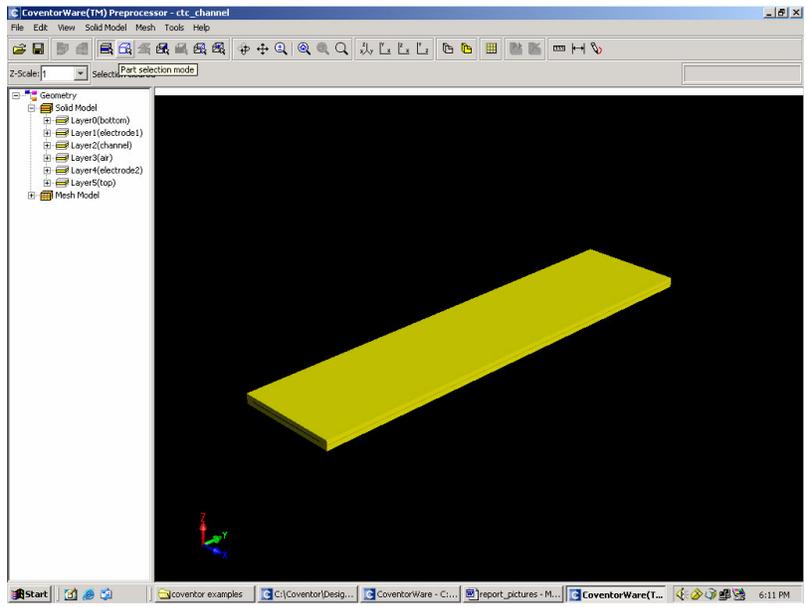


Figure 5 – Solid Model of Drift Channel.

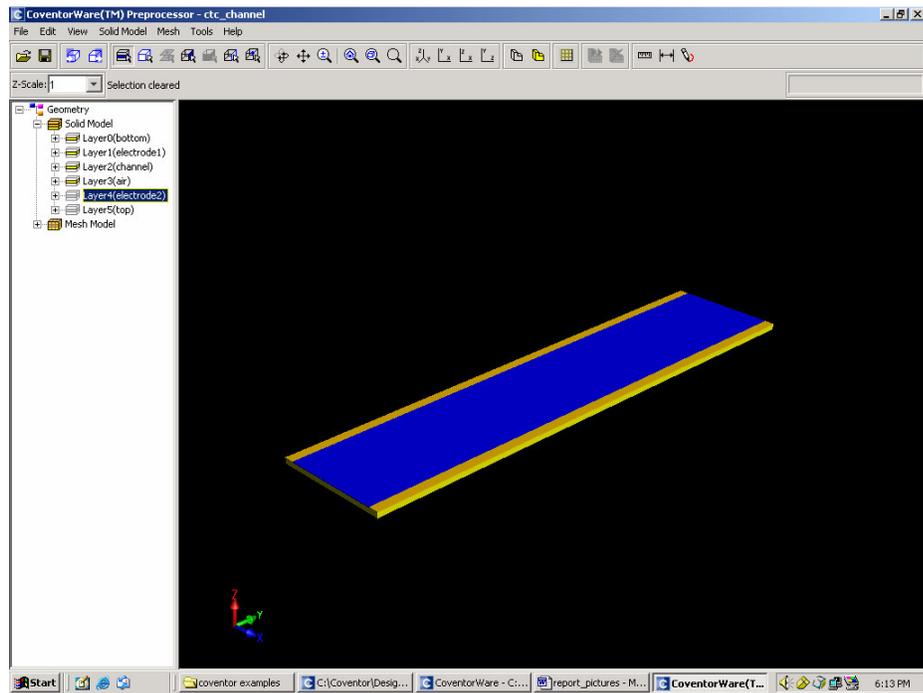


Fig. 6 – Solid Model of Drift Channel Showing Internal Air Flow.

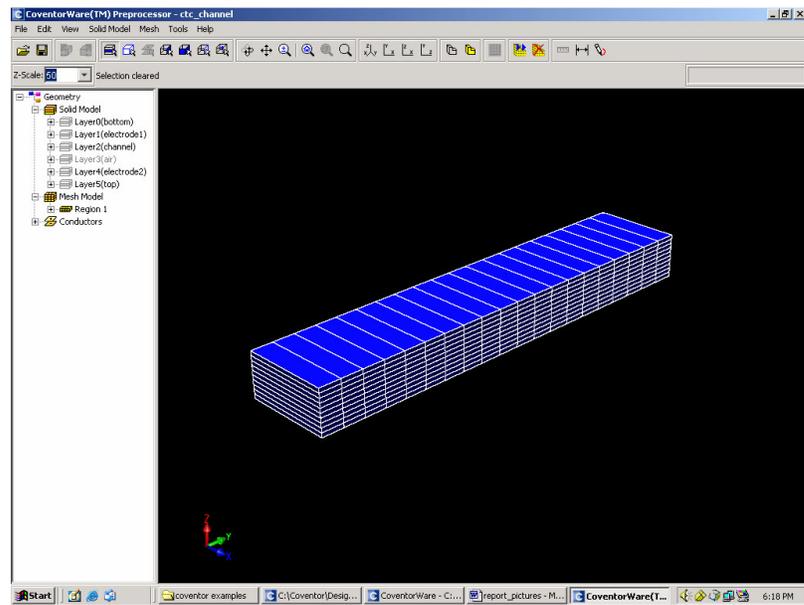


Figure 7 – Finite Element Mesh of Fluid in Drift Channel.
Thickness scaled 50X.

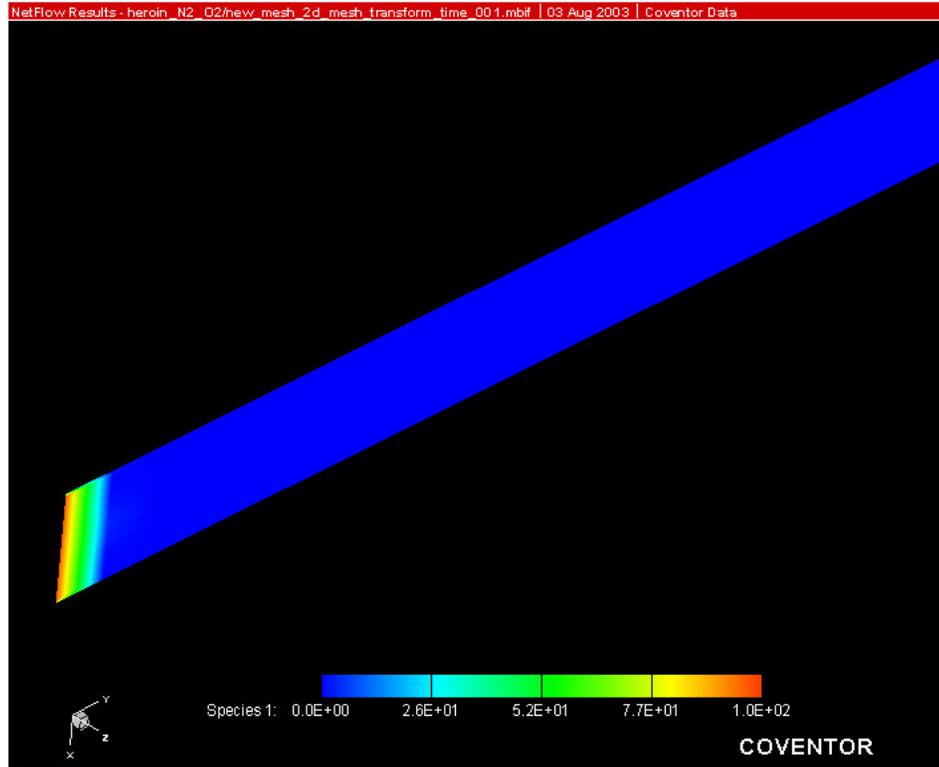


Figure 8a – Heroin Vapors in Drift Channel Cross-Section at t=0.001 secs.

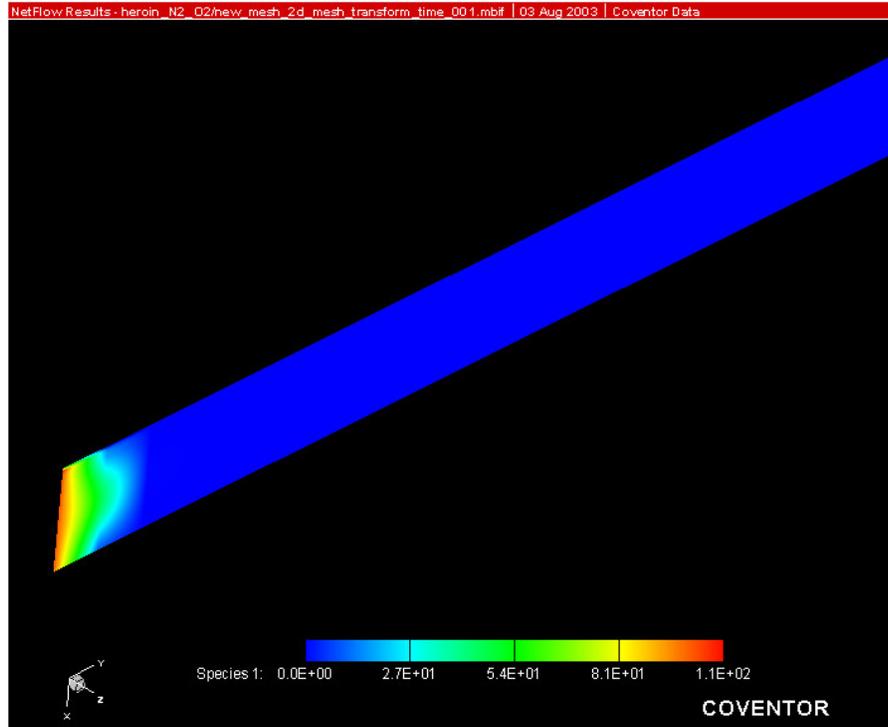


Figure 8b – Heroin Vapors in Drift Channel Cross-Section at t=0.003 secs.

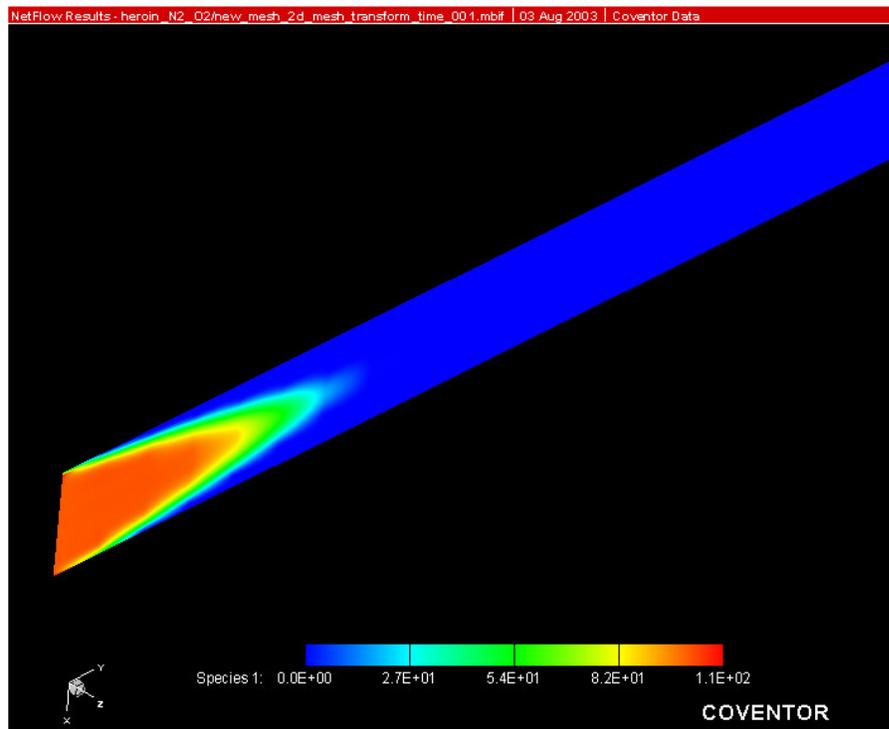


Figure 8c – Heroin Vapors in Drift Channel Cross-Section at t=0.01 secs.

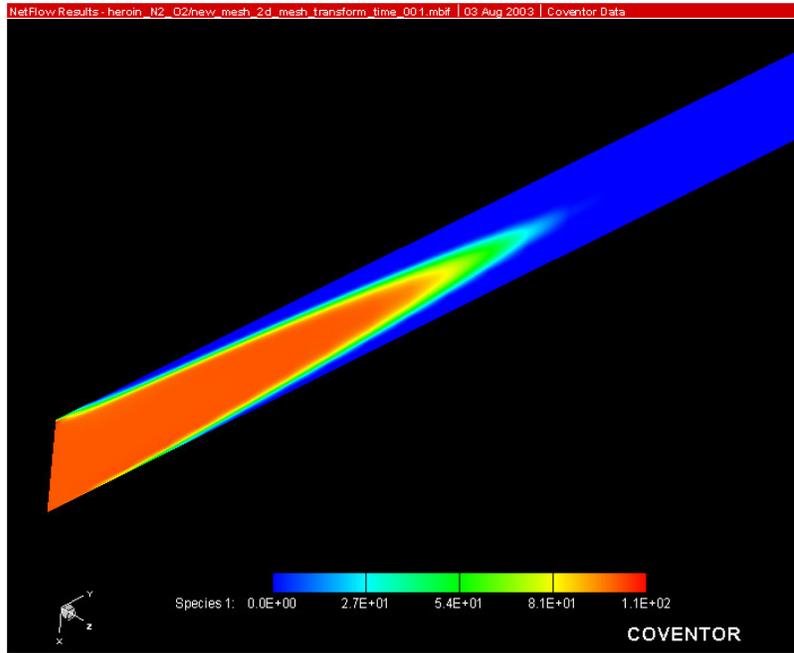


Figure 8d – Heroin Vapors in Drift Channel Cross-Section at t=0.05 secs.

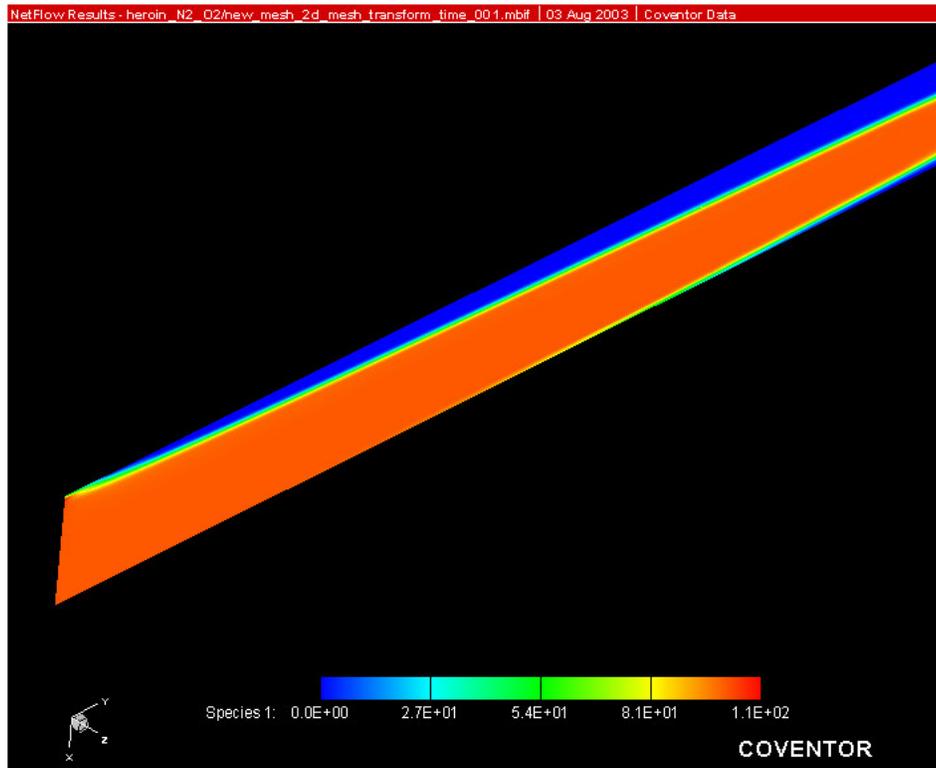


Figure 8e – Heroin Vapors in Drift Channel Cross-Section at t=0.1 secs.

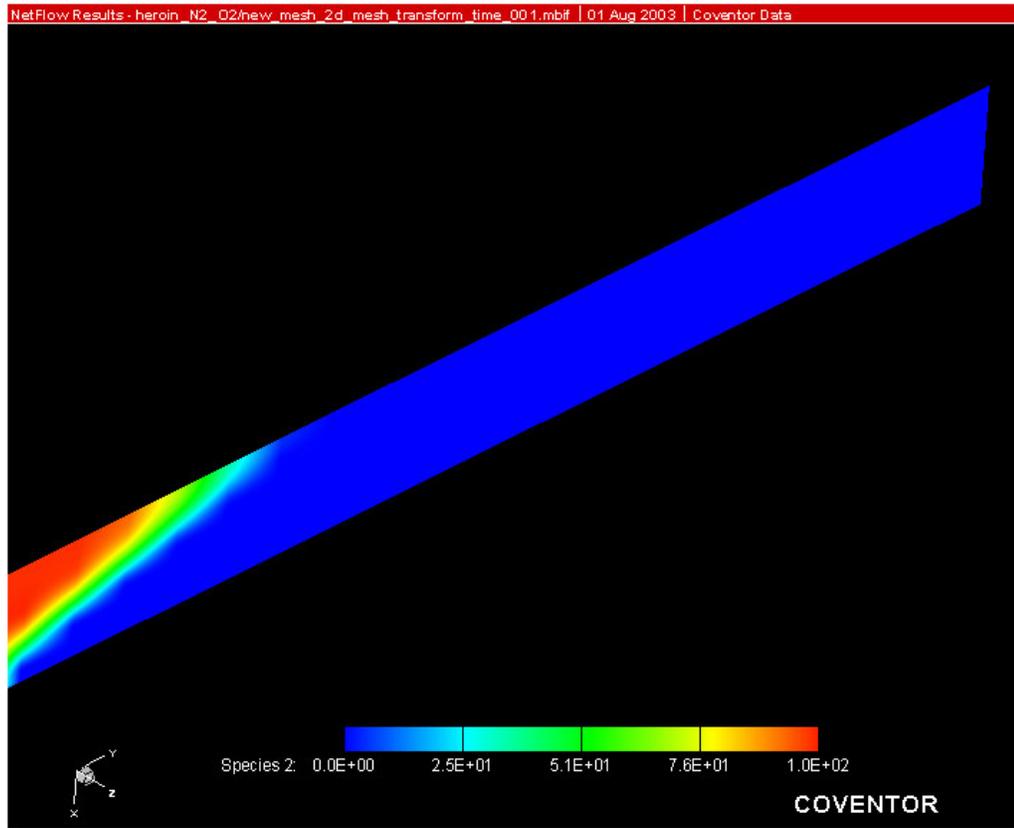


Figure 9 – Separation of Nitrogen Ions. Channel Length=100 mm.

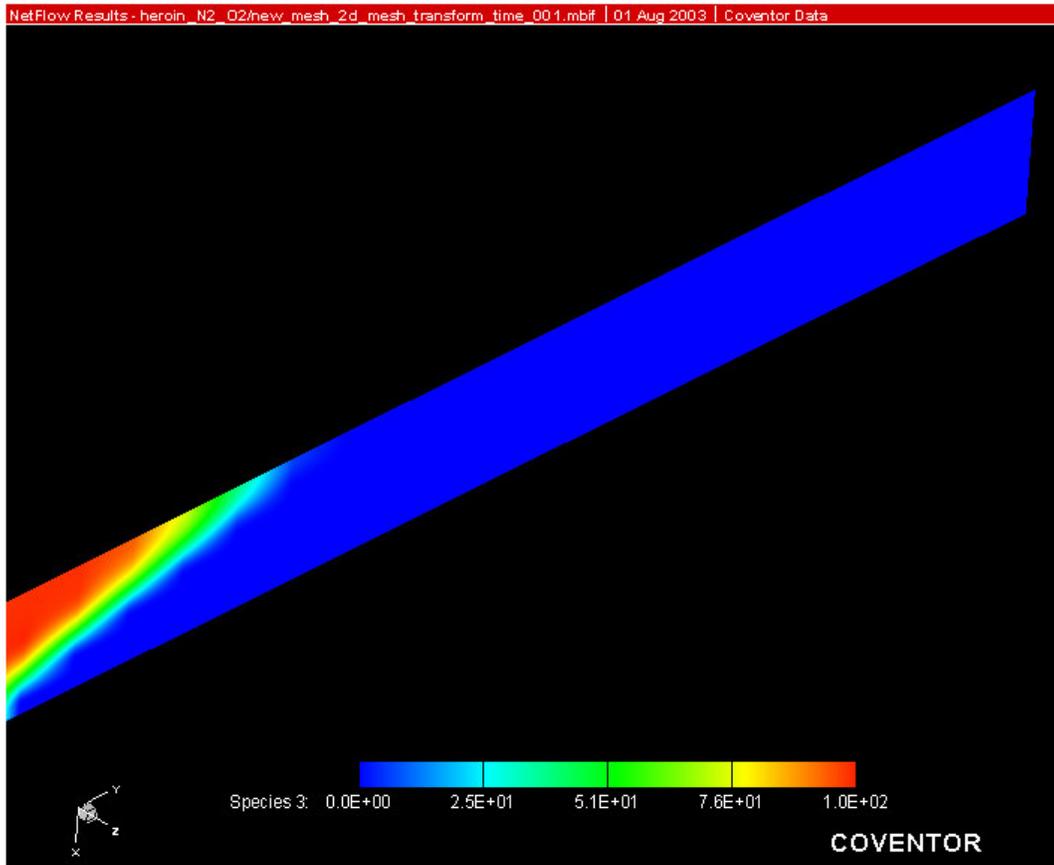


Figure 10 – Separation of Oxygen Ions. Channel Length=100 mm.

Typical analysis results are shown in Figure 8 for Heroin. For ease of interpretation, a cross section of the channel is shown in time-lapse scenes. For similar asymmetric waveforms, Nitrogen and Oxygen ions are attracted by the charged wall and neutralized while the Heroin remains along the center of the channel. The separation was accomplished with a square wave with a period of 0.0001 sec, peak voltage of -8 volts, an asymmetric ratio of 0.8 and a +3 volts offset. In this example the mobility of the Heroin ions is $1.05 \text{ cm}^2/\text{volts-sec}$ and remains constant for all field intensities [1], the mobility of the Nitrogen ions is $1.87 \text{ cm}^2/\text{volts-sec}$ at 760 volts/cm and 0.87 at 228,000 volts/cm [4] and the mobility of Oxygen is $2.24 \text{ cm}^2/\text{volts-sec}$ at 760 volts/cm and $1.25 \text{ cm}^2/\text{volts-sec}$ at 228,000 volts/cm [5].

Conclusion

This effort was successful in building a finite element model of the drift channel and in simulating the separation of chemical species with different ion mobility by using a square asymmetric potential waveform. In addition, a MEMS process sequence was developed to fabricate the drift channel modeled.

References

- [1] "ION Mobility Spectrometry" by G. Eiceman and Z. Karpas, by CRC Press (1994).
- [2] <http://www.grasebydynamics.com/ims.htm>.
- [3] <http://www.faims.com>
- [4] Miller, R.A., Eiceman, G.A.,Nazarov, E.G. and King, A.T, "A MEMS Radio-Frequency Ion Mobility Spectrometer for Chemical Agent Detection," Proceedings of the 2000 Solid-State Sensor and Actuator Workshop, Hilton Head Island, SC, 2000.
- [5] "Transport Properties of Ions in Gases" by E.W. McDaniel and E.A. Mason, John Wiley and Sons, New York (1987).