Chapter 3 Hybrid Array Architectures

The combination of homogeneous and heterogeneous sensors into a hybrid array architecture is just as important as the choice of signal processing for chemical sensing microsystems. Intuitively, arrays of sensors have many inherent advantages over individual sensors. A heterogeneous array that contains many different types of sensors improves the system selectivity while a homogeneous array that contains several of the same type of sensor operating under identical conditions improves the robustness of sensory data. The more robust aggregate output of a homogeneous cluster of sensors can be used as a single input to the heterogeneous portion of a hybrid array. In this chapter, the combination of homogeneous and heterogeneous chemical sensors is evaluated for optimizing hybrid array architectures for chemical sensing. A number of questions must be answered in choosing such an array architecture:

- Homogeneous array: How many sensors per homogeneous array?
- Heterogeneous array:
 - Which parameters establish the heterogeneity (e.g. physical properties, temperature)?
 - How many heterogeneous sensors or clusters of homogeneous sensors make up the array?
 - How are these heterogeneous sensors spaced (e.g. temperature range)?
- Given a fixed number of sensors, how should the homogeneity and heterogeneity in an array be split to optimize the advantages of the hybrid array?

3.1 Homogeneous Arrays

In the homogeneous array, the component sensors are of the same type and operate under identical conditions. Ideally, the outputs of a homogeneous array of sensors should be identical. Because of variations within the sensors themselves and in the sensor heaters, however, the outputs of homogeneous sensors may be different. As a result, the outputs of individual sensors within the array can be averaged or pre-processed into an output that is more robust than the output of any of the individual component sensors. Averaging inherently screens out random fluctuations in sensor operation, thereby generating an aggregate output that is more stable and accurate than the output

of any single sensor. Since many variations in mature fabrication processes are considered random [50], averaging techniques are an effective way to minimize the effects of individual sensor variation on subsequent signal processing stages. Non-random (systematic) variations such as sensor drift and chemical concentration changes are accommodated in subsequent signal processing of the heterogeneous portion of a hybrid array and therefore, are not influential in determining the architecture of the homogeneous section of the array. In this section, a simple model for evaluating the effect of the size of the homogeneous cluster on the variation and robustness of the cluster outputs is presented.

Considering only random variations, assume that the output of any individual sensor is normally distributed with mean μ and standard deviation σ . Assume also that the preprocessing of a homogenous cluster of *M* sensors involves computing the mathematical mean of the individual sensor outputs as follows:

$$\sum_{cluster} V_n = \frac{n=1}{M}$$
(3.1)

where $V_{cluster}$ is the output of a homogeneous cluster of sensors and V_n are the individual sensor outputs. To improve the performance of homogeneous processing, outliers in the homogeneous cluster may also be removed before averaging. The straightforward calculation of the mean as well as removal of outliers have been implemented in analog VLSI as part of this research and are covered in detail in Chapter 4. This analysis, however, focuses on the simplest preprocessing task of calculating the mean of individual sensor outputs. The standard deviation, σ , associated with the mean of these homogeneous clusters is:

$$\sigma_{cluster} = \sqrt{\frac{\sigma_n^2}{M}}$$
(3.2)

where $\sigma_{cluster}$ is the standard deviation of output of a homogeneous cluster and σ_n is the standard deviation of each of the individual sensor outputs. The relationship between cluster size *M* and

variation in the cluster output is shown in Figure 3.1 for a typical tin oxide sensor with mean of $36k\Omega$ and a standard deviation of $3.4k\Omega$ [51].



As seen from the relationship shown in Figure 3.1, the performance improvement gained by adding sensors to a homogeneous cluster decreases with an increasing number of sensors M per homogeneous cluster. As the standard deviation of the cluster output decreases, the potential for error in subsequent signal processing also decreases. It stands to reason that for a fixed size array, a hybrid architecture exists that optimizes the trade-off between improving robustness through the use of homogeneous clusters and improving discrimination capability through the use of heterogeneous clusters.

3.2 Heterogeneous Arrays

The counterpart to the homogeneous cluster in a hybrid array is the heterogeneous array that consists of sensors who are different from each other in some way. Differences among sensors may be loosely classified as follows:

- Heterogeneous Differences
 - fundamental changes in physical properties such as dopant level and grain size
 - cannot be altered after fabrication
- Pseudo-heterogeneous Differences
 - changes in operating conditions such as temperatures and filter type
 - can be altered after fabrication

While limited in their scope, pseudo-heterogeneous differences can provide chemical sensing systems with a great deal of flexibility. Since pseudo-heterogeneous parameters may be altered after fabrication, systems can be designed that modify these parameters during operation or calibration in order to suit a variety of discrimination tasks; such flexibility in the sensing requires only semicustom rather than custom fabrication of sensor arrays. This flexibility has significant economic benefit for the unit cost of both prototyped and production parts.

When broad selectivity and sensitivity ranges are required of a chemical sensing task, it may be necessary to use a truly heterogeneous array. Modification of grain size during fabrication of chemically sensitive materials is known to provide a great deal of flexibility in sensitivity range for the chemical sensors made of these materials [27]. Likewise, the inclusion of various catalysts in the chemical sensors themselves can significantly improve the discrimination capability of a heterogeneous array [52].

3.2.1 Temperature as a Heterogeneous Parameter

By far, the most common of the parameters for heterogeneous arrays has been the control of operating temperature of chemical sensors. Unlike most other pseudo-heterogeneous parameters, the control of temperature allows relatively broad flexibility in sensitivity range and selectivity. Consider, for example, the tin oxide, thin-film chemical sensors. The response of the sensor at a particular temperature to a reducing chemical can be affected by any of the following:

- The nature of oxygen present on the sensor surface [43]:
 - Physiosorbed oxygen at temperatures below 300° C

- Chemisorbed oxygen at temperatures between 300 and 600° C
- Lattice oxygen (generated by thermal reduction of sensor surface) at temperatures > 600°C
- Rates of Reaction at the sensor surface [54]:
 - Reaction of reducing chemical with O₂⁻
 - Reaction of reducing chemical with O⁻
 - Adsorption rate of O2
 - Generation of O⁻
- Formation of secondary products that interferes with the primary chemical reaction between the reducing chemical and the sensor surface material

The responses of a tin oxide chemical sensor to two reducing chemicals, isopropanol and carbon monoxide, is shown in Figure 3.2. The differences in these two chemical signatures are primarily caused by the formation of a secondary product, water vapor, when isopropanol reacts with the sensor surface at high temperatures. Water vapor, in turn, reacts with the sensor surface as well; when both water vapor and isopropanol react with the sensor surface, the total response is stronger than that for carbon monoxide whose secondary product, carbon dioxide, does not react with the sensor surface. Carbon monoxide also reacts more strongly with O⁻, which predominates at lower temperatures, than O_2^{-} , which predominates at higher temperatures. Similar differences in the rate and type of reaction with sensor surfaces occur among many other reducing chemicals and contribute to the uniqueness of a chemical's signature over temperature.

The testing of architectures developed in this research focuses on operating temperature as a heterogeneous array variable because of the flexibility that temperature provides in discriminating a variety of chemicals. Since fabrication capabilities are not within the scope of this research, it has not been possible for the signal processing architecture described herein to be tested on integrated and continuous heterogeneous arrays of chemical sensors. Rather, operating temperature has been varied across arrays of discrete sensors. The sensor data generated by these discrete arrays has proven sufficient to accomplish many discrimination tasks using the signal processing techniques described in later chapters.



3.2.2 Evaluating the Robustness of the Heterogeneous Array

In order to evaluate the robustness of a heterogeneous array of size N in discriminating among chemicals, some assumptions about sensor behavior and modelling of sensor response are needed. For an array made up of a single sensor technology, the following form of the sensor response is assumed since it is a simple but realistic model of many thin-film and MOSFET-based chemical sensors:

$$S_i = a_{i1}x_1^k + a_{i2}x_2^k + \dots + a_{in}x_n^k$$
(3.3)

where S_i is the output of a chemical sensor operating at temperature T_i , x_n is the concentration of chemical n in the sensing environment, and k is a constant dependent on the sensing technology with value 1 for a linear sensor and between 0.3 and 0.8 for many common thin-film sensors [55]. While saturation effects common to many chemical sensor technologies can be included in the above model by adding a Langmuir adsorption isotherm to equation (3.3), these effects are not

included here to maintain clarity and simplicity of explanation. Using the simplified response, the general response S of the entire sensor array can then be written in matrix form as follows:

$$\begin{bmatrix} S_1 \\ S_2 \\ \vdots \\ S_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{11} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1^k \\ x_2^k \\ \vdots \\ x_n^k \end{bmatrix} = Ax$$
(3.4)

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where ideally, the coefficients in the matrix A are linearly separable so that in an array of N sensors, N different chemicals can be distinguished. When only a single chemical j is present in the sensing environment at concentration x_j , this equation reduces to:

$$S_i = a_{ij} x_j^k \tag{3.5}$$

Given this form of the solution, some relationship among the coefficients in matrix A needs to be determined that will generate responses S_i that contain the key features of the actual sensor responses shown in Figure 3.2. The key features in the response of the array to a single chemical are, by observation:

- Response contains a single peak.
- Response decreases monotonically on either side of the peak.
- Response saturates at some minimum value far away from the peak.
- The second derivative of the response decreases with increasing distance from the peak.

Several relationships have been investigated that approximate the actual response curves of chemical sensors over temperature. The key features of the actual response are well modelled by calculating the coefficients a_{ii} using the following relationship (similar to the normal distribution):

$$a_{ij} = \frac{1}{q} \exp\left[-\frac{1}{2}\left(\frac{y_i - y_{max}}{q}\right)\right]$$
(3.6)

where y_i are the sensor outputs along the array, y_{max} is the peak output, and q is a measure of how quickly the response curve saturates on either side of the peak. The points y_i are equally spaced between 2q below to 3q above the peak location y_{max} . This asymmetry guarantees some skew to the response curve. A sample response curve using this model where the scaling constant q is 0.5 and y_{max} is located at point 40 in the array is shown in Figure 3.3. By observation, the response curve is similar to the actual response of a chemical sensor (Figure 3.2) across temperature and because of this similarity, equation (3.6) is used as a model for further analysis of heterogeneous arrays.

In order to evaluate the trade-off between robustness and discrimination capability of the heterogeneous array, it is assumed that some signal processing technique has been applied to the array of sensor outputs modelled in Figure 3.3. This analysis applies a thresholding technique across the sensor response curve using the mean output value as the reference for thresholding. After thresholding is performed, the binary outputs of the sensor array are as follows:

$$f(S_i) = \begin{cases} 0 & \text{if} \quad S_i < \frac{1}{N} \sum_{\substack{k=1\\N}} S_k \\ 1 & \text{if} \quad S_i > \frac{1}{N} \sum_{\substack{k=1\\N}} S_k \end{cases}$$
(3.7)

where N is the total number of points or heterogeneous sensor outputs in the array and the reference value used for thresholding is the mean value of the inputs S_i .



Figure 3.3: Model of a Typical Chemical Sensor Array Response

Shown above is a modelled response curve S_i for a typical reducing chemical which contains all the key features of the actual response curve. For this curve, q is 0.5 and y_{max} is located at point 40 in the array. The 100 points shown above are evenly spaced in operating temperature across the hypothetical sensor array.



array of analog sensor outputs is thresholded according to the mean value in the array (0.5) and the resulting output is high or low for sensor outputs lying below and above the mean respectively. The sensor outputs, N, in the array are evenly spaced from points 0 to 100 in Figure 3.3. As N increases, the resolution and discrimination capability of the array also increase.

In order to make a comparison of response curves containing a varying number of points N, the mean of the inputs S_i is normalized to a value of 0.5 by choosing the concentration of the chemical of interest x_i according to the following equation:

$$x_j = \frac{0.5N}{\sum a_{ij}} \tag{3.8}$$

Using equations (3.7) and (3.8), the binary representation of the response curve shown in Figure 3.3 is shown in Figure 3.4 for various values of *N*. This response pattern is an example of an ideal response for a particular chemical and can vary during actual sensing tasks due to error in the individual sensors. It is important to evaluate the impact that this error has on the overall sensing performance.

In order to analyze the effect of error in individual sensors on the overall system performance, each individual sensor S_i is assumed to experience random variations according to a standard normal distribution with standard deviation σ . For this preliminary analysis of purely heterogeneous arrays, the standard deviation is assumed constant and independent of the number and type of heterogeneous or homogeneous sensors in an array, The Gaussian integral limit is defined as follows:

$$\varphi(i) = \frac{0.5 - S(i)}{\sigma} \tag{3.9}$$

where S(i) is the mean output of the *i*th point in the array, 0.5 is the mean of all the sensor outputs, and σ is a constant standard deviation at each array point. Using this limit, the probability, p(i), that a sensor output S(i) will fail to produce the ideal binary value (Figure 3.4) after thresholding is calculated from the definition of the normal distribution as follows:

$$p(i) = \left[1 - \int_{-\infty}^{\varphi(i)} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy\right]$$
(3.10)

where p(i) is the probability that the *i*th sensor in the array will fail. This expression for probability of failure comes directly from the definition of the Gaussian distribution. The probabilities p(i)are calculated for every point in the array and combined to generate the total probability of zero thresholding failures in the array. This probability of failure can be calculated for all *N* points in the array. The probability of zero failures in the thresholding process for an array of sensory outputs *S*(*i*) is then calculated as follows:

$$P(0,N) = \prod_{i=1}^{N} (1-p(i))$$
(3.11)

where P(0,N) is the probability of zero failures in a heterogeneous array of N sensors.

Similarly, the probability of a single thresholding failure in array of sensor outputs S(i) can be calculated using:

$$P(1,N) = \sum_{i=1}^{N} \left(\prod_{i=1}^{N} \left[(1-p(i))p(j) \right] \right) (\text{ for } j \neq i)$$
(3.12)

where P(1,N) is the probability of one thresholding failure in an array of N sensors.

Likewise, the probability of exactly two thresholding failures is then:

$$P(2,N) = \sum_{i=1}^{N} \sum_{i=i}^{N} \left(\prod_{k=1}^{N} \left[(1-p(i))(1-p(j))(p(k)) \right] \right) \text{(for } k \neq i,j)$$
(3.13)

and so on for any number of failures in a heterogeneous sensing system. After thresholding the response model of Figure 3.3, the probabilities of exactly zero, one, two, three, four, five, and six failures are calculated and shown in Figure 3.5a for a constant standard deviation, σ , of 15% which is typical of tin oxide chemical sensors.

As expected, the maximum probability of exactly k failures in the array decreases with increasing k. Likewise, the maximum probability of failure shifts to the right as the number of allowable failures increases. This result implies that the larger the number of sensors N in a heterogeneous array, the more likely multiple failures are in that array. The probability of more than 6 simultaneous failures is not calculated here, because, for heterogeneous arrays sizes up to 80 sensors, the primary contributors to the expected error in these arrays are the probabilities of six or fewer failures.





Using these five failure rates, the expected error for an array of size *N*, with constant standard deviation σ can be computed as follows:

$$\langle E \rangle = P(1, N) + 2P(2, N) + 3P(3, N) + 4P(4, N) + 5P(5, N) + 6P(6, N)$$
 (3.14)

The expected error for this heterogeneous array example is plotted in Figure 3.5b based on the failure probabilities in Figure 3.5a. Expected error is a weighted probability of error. It is inversely proportional to the robustness of the system; the higher the expected error for an array, the less robust the array is. The more error that is present in a system, the less likely the overall system response will be consistent and reproducible.

Whether the expected error is considered large or small for a particular sensing system depends largely on the way in which the processed output for these systems is interpreted. For example if the sensing system used to process this sample array can only tolerate a single error in the output pattern, a maximum of 30 heterogeneous sensors may be used in that particular system. In most practical systems, however, the number of errors that can be tolerated is not necessarily constant. In these practical systems, it is important to devise a metric for evaluating the trade-off between decreasing robustness and increasing discrimination capability that occurs as the number of heterogeneous sensors in the array in increased.

If the sole objective of our chemical sensing systems is to minimize the probability of thresholding failure, the ideal number of sensors N would be 1, where the probability of failure is the lowest in all cases. However, since practical chemical sensing systems must be able to discriminate among a variety of chemicals, they require more than a single heterogeneous sensor to narrow the selectivity of the overall system. Therefore, to gain an understanding of the optimal size of the heterogeneous array N, the expected error can be compared to the discrimination capability gained by increasing the size of the heterogeneous array.

In order to quantify the benefit gained by increasing the size of the array, the discrimination capability D(N) is introduced and defined as the relationship between the number N of heterogeneous sensors in an array and the number of chemicals that can be distinguished using N sensors. For

example, an ideal sensor array that generates heterogeneous outputs that are completely linearly separable has the following discrimination capability function:

$$D(N) = N \tag{3.15}$$

The function D(N) varies with the sensor technology and operating parameters of the heterogeneous array and can be calculated empirically in most cases. In order to evaluate the trade-off between increasing discrimination capability and increasing error in arrays of increasing size N, the robustness R of the array is defined as $R = 1 - \langle E \rangle$ where $\langle E \rangle$ is the expected error calculated according to equation (3.14). The robustness R compared to the discrimination capability of a heterogeneous array with a constant standard deviation of 15% is plotted in Figure 3.6 for two discrimination functions D(N). The first function (Figure 3.6a) uses the discrimination function of (3.15) and the second (Figure 3.6b) uses a function D(N) that varies as the square root of N.

For this particular example, it is assumed that the decrease in robustness caused by increasing the size of the heterogeneous array is equivalent to the increase in discrimination capability caused by this same increase in size. If robustness were considered more important than discrimination capability (e.g. a toxic gas sensing application), it would be weighted more in the analysis, causing the robustness curves in Figure 3.6 to drop off more steeply. Likewise, if robustness were considered less important than discrimination capability (e.g. on-line monitoring of perfume manufacturing), the robustness curves would drop off less steeply than the curves shown in Figure 3.6. With equal weighting given to robustness and discrimination capability, however, the optimal architecture for these arrays is found at the intersection of these two curves and is 30 and 22 heterogeneous sensors for Figure 3.6b respectively.





Shown above are the robustness vs. discrimination capability of a sensor array of size N for two different discrimination functions D(N). The first function D(N) (a) assumes that for N sensors, N chemicals can be discriminated (a linearly separable array). The second function D(N) assumes that for N sensors, the square root of N chemicals can be discriminated. The optimal number of sensors in the array is the intersection of the two curves (30 sensors for (a) and 22 sensors for (b)). The flatness of the robustness curve as the array size approaches 80 is a result of computation error arising from including only the first six failure probabilities in calculating the expected error.

In a truly hybrid array containing both heterogeneous and homogeneous sensors, the assumption of constant standard deviation made in this analysis is not a valid one. Such a hybrid array contains a fixed number of sensors M^*N that are divided into N heterogeneous sensor clusters and M homogeneous sensors per cluster. For a fixed number of sensors in a hybrid array, increasing the number of heterogeneous sensors or points in the array occurs at the expense of sensors within homogeneous clusters. While the analysis presented in this section is valid for heterogeneous arrays of individual sensors, the next section analyzes hybrid arrays containing both heterogeneous and homogeneous sensors.

3.3 Optimizing the Hybrid Array Architecture

In practical chemical sensing systems, the number of chemical sensors in an array are limited by the available space on a particular substrate. M*N sensors can be arranged in architectures ranging from M*N homogeneous sensors provided a single aggregate output to M*N sensors providing M*N heterogeneous outputs. At some point between these two extremes lies the optimal architecture for given array parameters and signal processing structures. To illustrate this trade-off, assume that the sensor outputs in a homogeneous cluster of sensors are aggregated into a single output using the simple averaging algorithm of (3.1). Assume also that M*N sensors are uniformly distributed into N heterogeneous clusters and M homogeneous clusters the resulting standard deviation of a homogeneous cluster output is as described in (3.2):

$$\sigma_{cluster} = \sqrt{\frac{\sigma_n^2}{M}}$$
(3.16)

Probabilities of zero, one, and multiple failures can be calculated using the relationships developed in the previous section by replacing a constant standard deviation σ with the variable standard deviation, $\sigma_{cluster}$ In this analysis, the maximum standard deviation is chosen to be that of the typical individual tin oxide sensor, 15%, used in the analysis of the previous section. Furthermore, the total number of sensors in the array is set at 100, split between *N* heterogeneous sensors and 100/*N* homogeneous sensors. Probabilities of 0 through 6 failures can be calculated using equations (3.9) - (3.13) and are plotted as a function of heterogeneous sensors *N* in Figure 3.7. The expected error of this hybrid array is plotted in Figure 3.7b. As expected, the homogeneous clusters used in these hybrid arrays are generating a more robust output after the thresholding process (smaller $\langle E \rangle$) than individual sensors. This decrease in expected error should cause the optimal number of heterogeneous sensors (related to discrimination capability) in the array to increase with the hybrid array architecture. This is indeed the case, as the robustness and discrimination capability curves in Figure 3.8 illustrate. As in the example presented in the previous section, it has been assumed for this example that robustness and discrimination capability are equally weighted in the constraints of the overall sensing system. Using this equal weighting, it can be seen that, for a completely linearly separable sensor technology (D(N) = N), the optimal architecture for the hybrid array is 40 heterogeneous clusters consisting of 2 homogeneous sensor each (for a fixed array size of approximately 100 sensors). For the less separable sensor technology, where the discrimination capability of the array varies as the square root of the number of heterogeneous outputs in the array, the optimal number of heterogenous clusters is 33, each containing 3 homogeneous sensors each.

Through the examples presented in this chapter, the feasibility of determining analytically an optimal hybrid architecture for an arbitrary chemical sensing system has been established. This analysis can be repeated for any sensor technology and array architecture for which the following parameters are known:

- A signal processing metric for differentiating ideal output from actual outputs with errors
- Variation (standard deviation) in individual chemical sensor outputs
- An estimate of the discrimination capability (*D*) of the array that is dependent on:
 - array parameters
 - degree of separability among neighboring heterogeneous sensors in the array

In the following chapters, experimental results for homogeneous clusters of sensors are presented in addition to the corresponding results for heterogeneous arrays of sensors that use discrete tin oxide sensors whose operating temperatures vary across the array. In future chemical sensing systems developed beyond this research project, these signal processing techniques will be combined into hybrid arrays where the discrimination capability and robustness of the array are key factors in determining the optimal ratio of heterogeneous to homogeneous sensors required for a particular sensing technology.





Shown above are the (a) probabilities of zero, one, two, three, four, five, and six failures for a typical hybrid array of tin oxide chemical sensors containing N heterogeneous sensors and 100/N homogeneous sensors. The (b) expected error, shifts to the right as compared to the expected error of a purely heterogeneous array whose individual sensors have a constant standard deviation of 15%.





Shown above are robustness vs. discrimination capability of a hybrid sensor array of size 100 for two different discrimination functions D(N). The first function D(N) (a) assumes that for N heterogeneous sensors, N chemicals can be discriminated (a linearly separable array). The second function D(N) assumes that for N heterogeneous sensors, the square root of N chemicals can be discriminated. The optimal number of heterogeneous sensors in the array is the intersection of the two curves (40 sensors for (a) and 33 sensors for (b)).