

MONTE CARLO SIMULATION AS PROCESS CONTROL AID

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ABSTRACT

Field emission from carbon nanotubes (CNT) for display purposes was optimized using Design of Experiments (DOE). The brightness was improved by three orders of magnitude but the achieved gains could not be sustained in the “Control” phase of a DMAIC project and the process reverted to poor performance. It took an intense effort of circa two months to recover the process. Monte Carlo simulations were used to provide an excellent fit to all the measured emission data over the course of eight months in both range and shape. The simulations were also indicating the cause of the process drift. A hidden factor that was too time- and labor-intensive to measure in real-time was responsible and uncovered. With the aid of the simulations the process could have been recovered within days instead of months.

1 INTRODUCTION

Statistically designed experiments have become the essential tool in many fields of research and industry for rapid learning, optimization and to minimize the use of time and resources (Fisher, 1925; Box and Wilson, 1951; Box, et al., 1978; Montgomery, 1976). The rapid increase in computer technology has led to the merging of statistically designed experiments with powerful computer simulations. The Monte Carlo method, a technique that uses a large set of random numbers to measure uncertainty, was named after the casino in Monaco due to its random nature and was applied during the Manhattan project at Los Alamos National Laboratory (Metropolis and Ulam, 1949).

Often Monte Carlo simulations are used as a powerful tool in the “Analyze” or the “Improve” phase of a Six Sigma DMAIC (Define, Measure, Analyze, Improve, Control) project. For instance, Monte Carlo simulations can be used to improve the capability of processes. If the response surface of the process is well mapped out, i.e. via a Response Surface Method (RSM), Monte Carlo simulations can quickly predict the expected process variability. To improve the capability the process can be moved into a region of the response surface which is more robust to process input variation. The Monte Carlo simulations can quantify the expected variation improvement. However, simulations are not only very powerful when utilized in the earlier phases of a DMAIC project, they are also a powerful tool in statistical process control, as demonstrated in this paper.

2 METHODOLOGY

Carbon nanotubes (CNTs) have become the basis of intense research due to their intriguing mechanical and electrical properties (Iijima, 1991). In Motorola’s Embedded Research Systems Laboratory, CNT’s electrical conductivity and high aspect ratio (length in the μm , diameters in the nm range) have been utilized in one particular application for field emitter displays. Figure 1 shows a 4.6” display where millions of CNTs have been selectively deposited on a glass cathode while their emission has been regulated for display function (Dean, et al., 2005).



Figure 1: A 4.6-inch display using the emission properties of millions of CNTs from Motorola’s Nanoemissive display (NED) group.

Fully processed displays such as the one shown in Figure 1 represent a considerable resource commitment due to their manufacturing complexity. Therefore, blanket, non-patterned, diode samples were initiated as test and optimization vehicles. CNT growth was achieved by a two-step deposition process; first, a metallic catalyst is deposited in a separate tool, followed by the deposition of the CNTs in a chemical vapor deposition (CVD) reactor. After deposition of the CNTs, the emission properties were investigated by extracting the emission current on an anode and exposing the CNTs to an electric field of ca. $6 \text{ V}/\mu\text{m}$. The current density, thus measured, was an indicator of brightness, convoluted by the phosphorus efficacy of the anode.

The brightness of the display was maximized using a classical Design of Experiments (DOE) approach in what is called subsequently the “Laboratory phase.” The most efficient method for optimization is a sequential approach that is partitioned into three separate components: screening DOE, Path of steepest Ascent (PoA) and Response Surface Method (RSM), as illustrated in Figure 2.

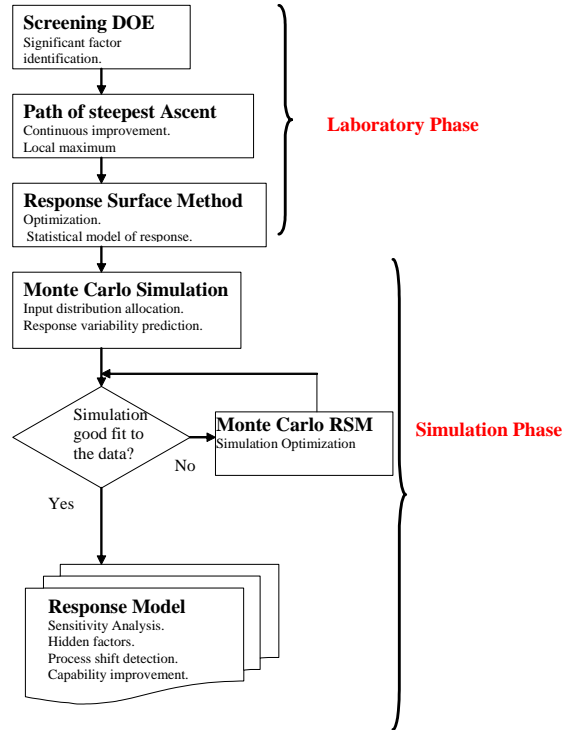


Figure 2: Flowchart of the experimental procedure

Minitab[®] software (<http://www.minitab.com>) was used for the statistical analysis in this particular case although other statistical software packages could have been used similarly. The sequential experimental approach allowed for resource efficient optimization of the emission current density. Typically, this three-tiered approach is now used in Monte Carlo simulation to predict the process variability followed by laboratory verification runs. In the approach below, it is demonstrated that the Monte Carlo simulation in what is termed the “Simulation Phase” can also be used as process troubleshooting tool and may lead to discoveries of hidden influential factors. Crystal Ball[®] software (<http://www.crystalball.com>) was used to carry out the Monte Carlo simulation, although other simulation software packages could be used as well.

The statistical model obtained from the “Laboratory Phase” was used as a transfer function to calculate the expected emission output current density. Since the control of the significant factors is limited, their variation led to a distribution of the resulting emission current density. The DOE demonstrated that the output distribution is critically dependent on the input variation distributions. By systematically changing the significant factor distribution in a computer experiment, a good fit to the measured emission current density was obtained. Then the obtained response model can be analyzed for its sensitivity to the input distributions. The response model can also be used to detect significant deviations, for example, deviations caused by a process shift, from the expected output curve.

3 LABORATORY PHASE

A screening DOE ($\frac{1}{2}$ fraction of a 2 level, 4 factor resolution IV, 2^{4-1}_{IV}) was carried out in the initial phase to reveal what factors had significant influence on the emission current. The Pareto chart in Figure 3 identifies the two most significant factors, A and B, whereas D had only a minor influence. It also shows that some interaction between A and B was present and Factor C had no impact. The inset displays the residuals of the statistical model plotted against the most significant Factor A. The response surface was curved; therefore a RSM was required for true optimization.

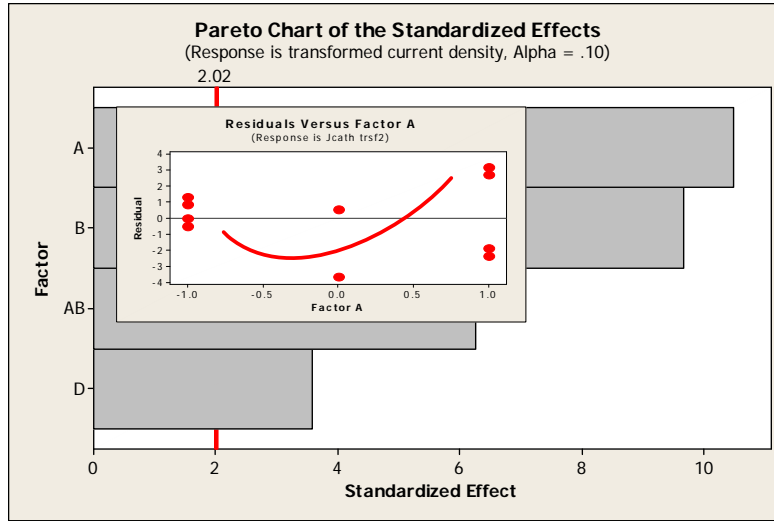


Figure 3: Pareto chart of factor effects indicating the significance level of the different factors. An alpha value of 0.1 was used to determine the significance. The inset graph shows the residuals plotted versus the most significant Factor A indicating a curved response surface

In the contour plot of Figure 4, an inverse square root transformation was used on the emission current density to normalize the data and plotted versus the two most significant factors, A and B. The Analysis of Variance (ANOVA) table is given in the inset. Results of Figure 4 indicated that in order to improve emission current density Factor A should be increased and Factor B decreased. This course was pursued with the PoA.

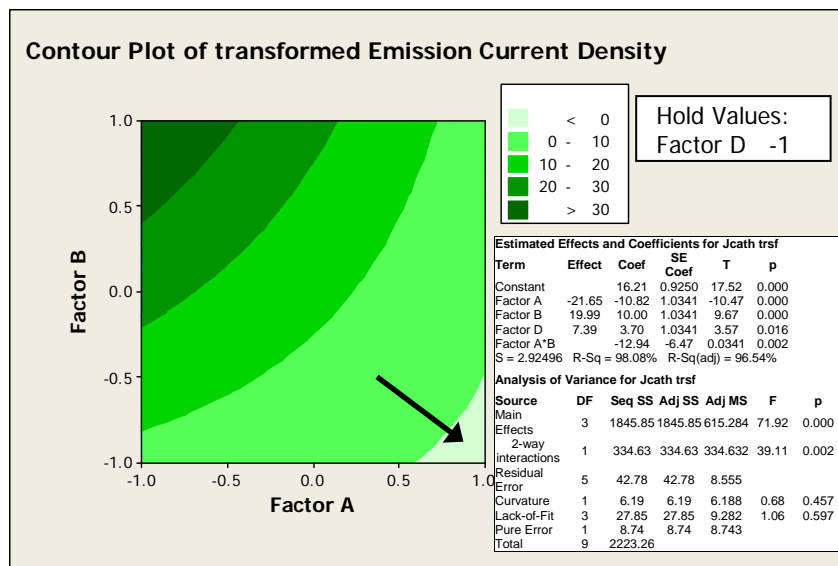


Figure 4: Contour plot of transformed emission current density from the screening DOE. The Factors are displayed in coded units. An inverse square root transformation was used, i.e., higher emission is in direction of arrow. Inset shows the ANOVA table.

It rapidly became clear that while Factor A was easily controlled and increased, Factor B was not. Lowering Factor B below a certain threshold resulted in loss of controllability and a compromise had to be found. Therefore the most flexible and most important factor was Factor A. As Factor A was steadily increased a local maximum for emission current was found with the RSM centered on that new high point.

The results of the RSM are shown in Figure 5 with the ANOVA table as an inset. The contour map of the model obtained by the analysis indicates the region of maximized emission current. Figure 6 illustrates the effect of the optimization experiments. The box plot summary of the emission current density is shown over time grouped by month. The current density is plotted on a logarithmic scale (each of the dashed lines representing one order of magnitude), and the median values for each month are indicated in bold numbers. It can easily be seen that the improvement equates to more than 3 orders of magnitude (from ca. -1.25 to ca. to +1.3, averaged over the last 6 months).

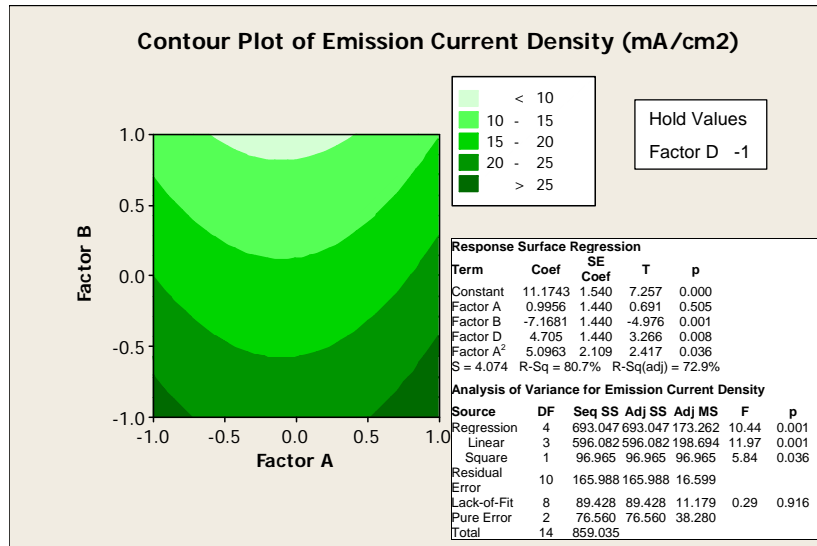


Figure 5: Contour plot of the emission current density from the RSM, darker regions represent higher current density. Inset shows the ANOVA table.

The two images of the inset of Figure 6 illustrate the increase in brightness. The shutter speed of the camera had to be reduced by ca. 100x due to the much higher emission after the RSM. If the camera shutter speed had been left the same, the right image would have been overexposed. Nonetheless, the improvement is not only noticeable in the brightness but also in the much higher density of emitters.

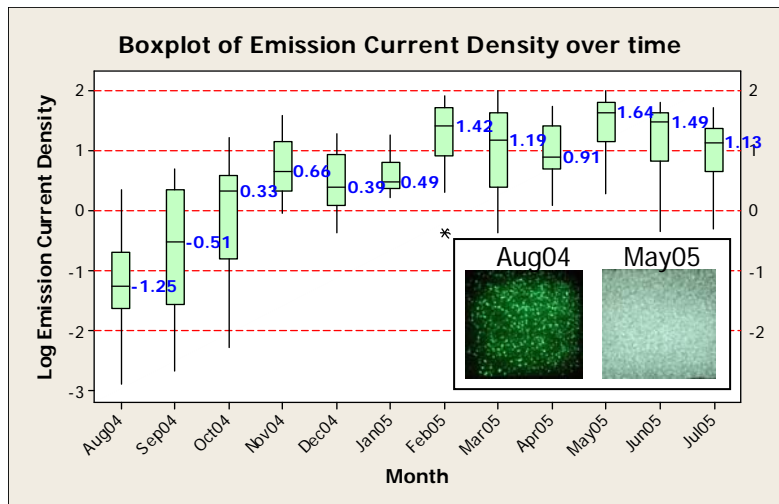


Figure 6: Box plot summary of emission current density over time. The numbers indicate the median value for the respective month. The dashed lines indicate one order of magnitude. The inset shows visual images of the emission before (left) and after the (right) the improvement process (camera shutter speed reduced by ca. 100x to prevent overexposure).

To this point, the CNT growth project appeared to be a conventional Six Sigma DMAIC project with significant and quantifiable improvement. The control phase started and for several months the emission stayed at a high level. However, in the 4th quarter of 2005, the process unexpectedly underwent a shift to lower emission. Since Factor A had been identified as most important and controllable factor, initial investigation focused on this factor, however, it was found that it was within the expected fluctuations. No clear explanation could be derived from the inherent variations of the other significant factors either.

After a more thorough investigation, the root cause was identified as an underlying factor relating to the catalyst thin film surface morphology that had not been measured directly. The characterization required to obtain the film surface morphology data on a regular basis had been excessively time and labor intensive. It took nearly two months of thorough experimentation and painstakingly characterization to bring the process back into control. The question became if this shift could have been prevented. One obvious answer was that the correct parameter needed to be tracked, however, in this case the parameter was unknown. Could the shift of the process still have been prevented, and if so how?

4 SIMULATION PHASE

In a typical DMAIC improvement project the process improvement is followed by some experimental verification runs followed by the capability analysis. The proposed method is to have the laboratory phase followed by a simulation phase to aid in the “Control” phase and to avoid costly process shifts even when hidden factors are important.

Optimized process conditions had been obtained and implemented, but how robust was the emission current density due to process input parameters, Factors A, B and D? If no variation to the optimized process parameters existed, the transfer function, obtained from the statistical model, could simply be used - taking into account the model error - to accurately calculate the expected emission current density output. As that is an idealized scenario even with the best controls in place, it becomes critically important to study the effect of process input fluctuations on the output.

No historical data for any of the factors existed. However, during the improvement project, data collection on the most significant factor, Factor A, was initiated (after some hardware modification on the tool). Since it took considerable time to collect enough data to be statistically viable, best guess estimation for all three significant factors, A, B and D had to be done. Normal distributions with standard deviations of 20%, 20% and 10% of the respective means were assigned to the three factors (the latter variable was more effectively controlled), as shown in the model in Figure 7.

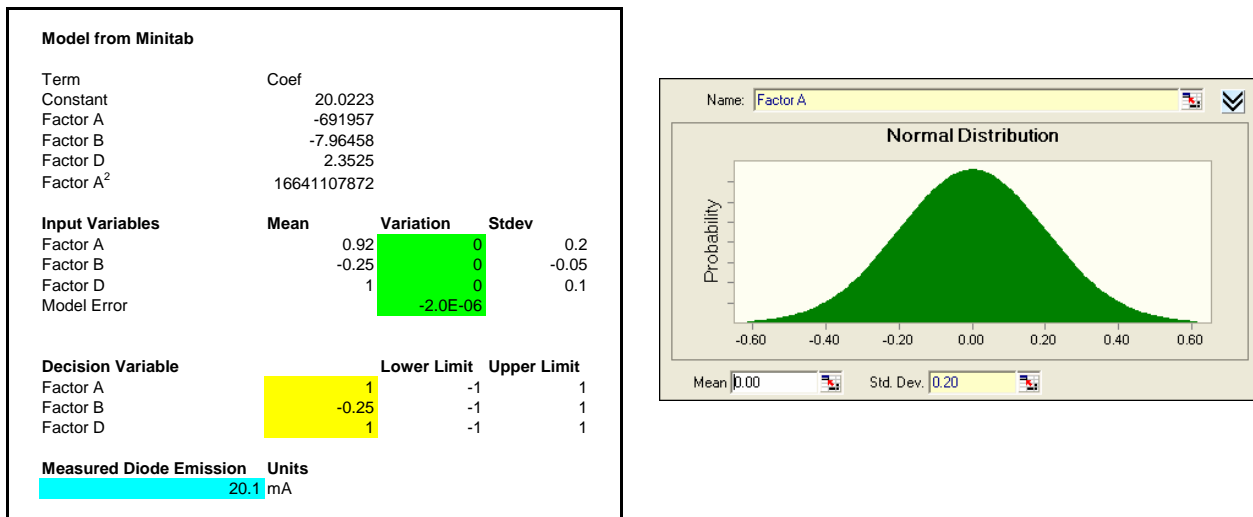


Figure 7: Crystal Ball model from a Microsoft[®] Excel[®] worksheet. The right-hand figure shows the Factor A variation distribution as an example. The yellow-highlighted cells in the distribution window indicate that the displayed values are linked to the respective Excel cells allowing for easy modification of the model. The same model was also used to find optimized process parameters using Optquest[®].

After Monte Carlo simulation was carried out, the resulting output emission current distribution was then compared to the measured data, as shown in an example in Figure 8.

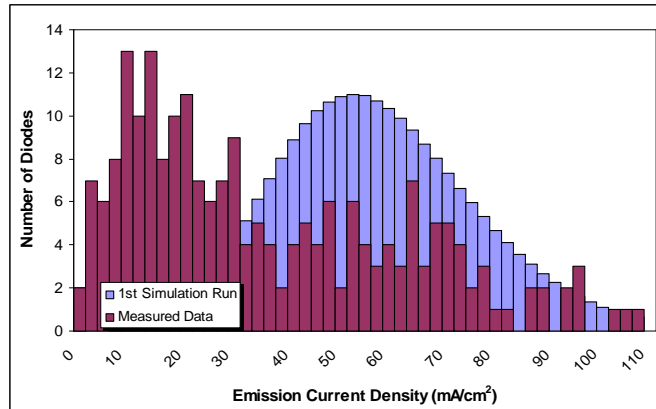


Figure 8: Comparison between a first set of simulated and the measured data.

Obviously, the first run provided a fairly poor fit to the measured data. To obtain a better fit, both the simulated and measured data were equally divided into equivalent bins and the difference for each bin calculated. The sum of squares (SS) of these bins was then used as the response in an optimization Monte Carlo RSM, as outlined in the flowchart of Figure 2.

Factor A was identified in the very first screening DOE as the most significant factor on the emission current density and Figure 9 shows several graphs overlaid with Factor A input variation from 5% to 50%. It can be seen that this variation has a substantial effect not only on the range but also on the shape of the current density distribution. The smallest variation in Factor A resulted in the sharpest peak with a very high kurtosis. As the variation is increased it can be seen that the curve broadens considerably. However, the broadening disproportionately occurs at the upper end of the emission curve while no important effect is observed at the low end of the spectrum.

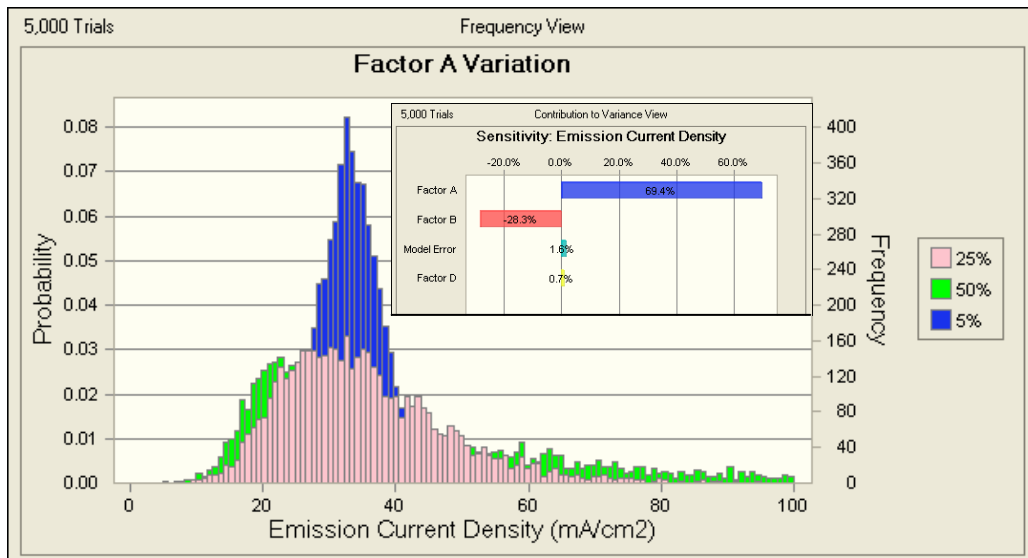


Figure 9: Overlaid simulations from Crystal Ball software with varies degrees of variation of Factor A which is shown in the Sensitivity chart to be the most significant factor.

Only the introduction of a much higher value than the experimental set point in combination with greater variation of Factor B, as seen in Figure 10 allowed for the extension of the emission current histogram towards zero emission and thus achieve a good fit to the measured data.

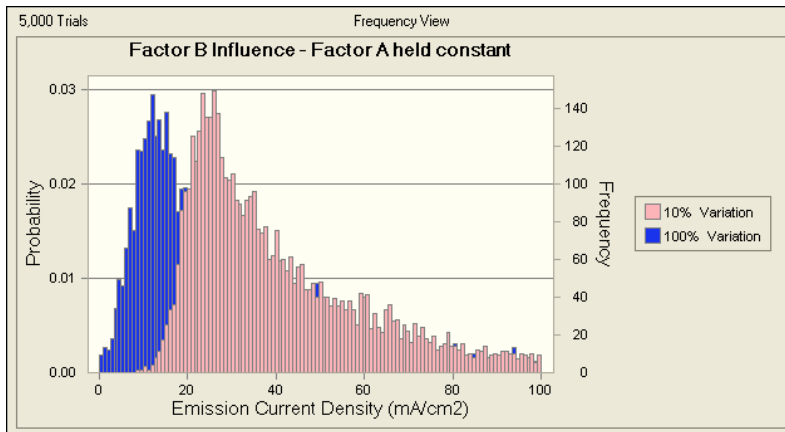


Figure 10: Crystal Ball software output showing the influence of Factor B and its variation on emission current density curve from 5000 simulation trials. Factor A variation was held constant at 50%.

Thus, for the Monte Carlo RSM Factor B, Factor B variation and Factor A variation were considered as variables. A central composite design was used and statistically analyzed, with conditions found that minimized the total SS and were then used as a best fit to the measured data.

The resulting final fit to the measured emission current density output distribution is shown in Figure 11. The fit was obtained with a 50% variation of the most significant Factor A, 78% variation of Factor B and Factor D stayed at 10% variation.

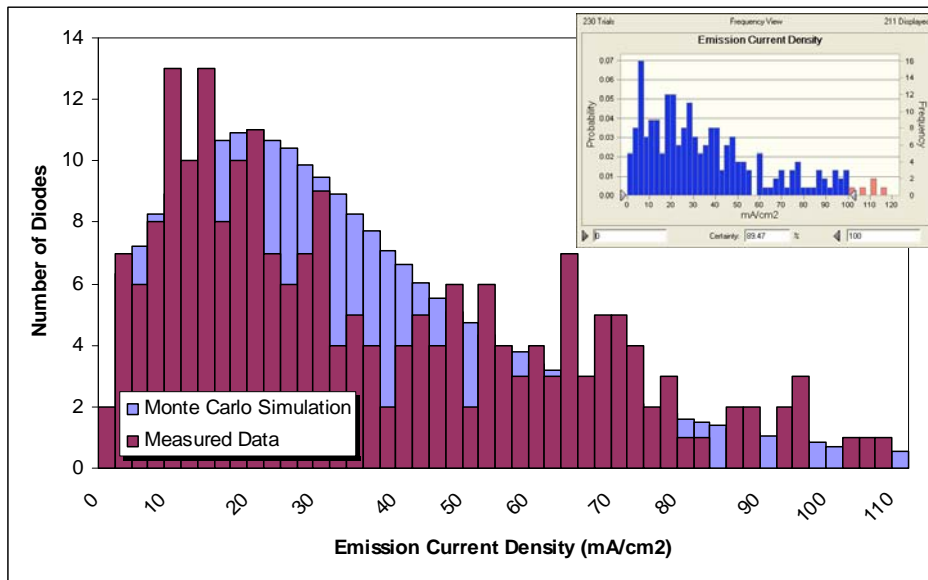


Figure 11. Overlay plot of Monte Carlo simulation of emission current density and measured data. Inset is a simulated run with the same amount of runs as the measured data.

The curve of measured data appear somewhat serrated compared to the fitted curve which may be explained by the limited number of 230 data points when compared to about four million simulated data points. The inset of Figure 11 shows the result of a simulation with only 230 runs (i.e., the equivalent number of measured data). The graph is very similar to the measured data, as it displays again a certain degree of unevenness and some bins that are not occupied.

Therefore, the discretization of the data seems to be due to the low number of measured data relative to the simulation. As mentioned above, during the improvement process the measuring of Factor A run-to-run variation was initiated. As illustrated in Figure 12, the measured Factor A variation has a standard deviation of 42% of the mean and agrees quite well with the 50% of simulated curve. Also shown are the Factor B and D variation.

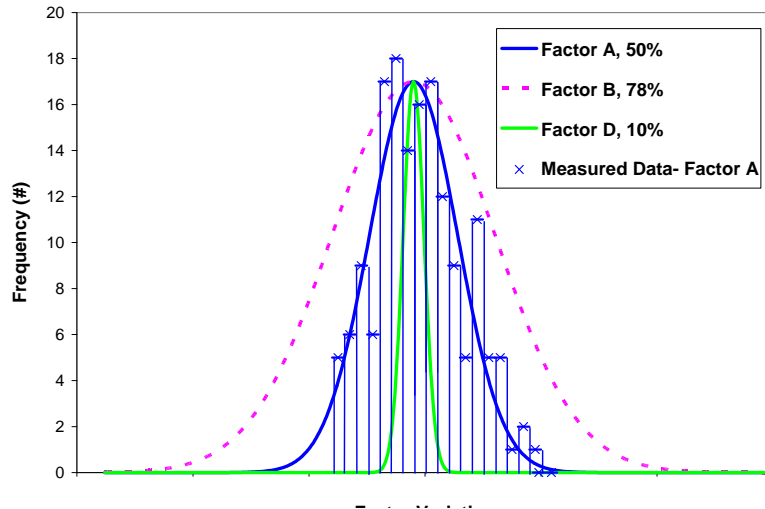


Figure 12: Distributions of all the process input factors after a good fit to the measured data (displayed as a histogram) had been obtained.

The high Factor B variation was unexpected. The large fluctuation of Factor B was directly related to an underlying factor that dramatically decreased the emission current density. The morphology was crucially influenced by any fluctuations or drift in Factor B. The instrumentation that controlled Factor B was indicating no drift, and the important influencing underlying factor was not known at the time, thus leading to the drift.

5 CONCLUSIONS

The importance of the Monte Carlo simulation is demonstrated by the fact that the cause of the process shift was evident without any further follow-up investigation. The simulation showed that even extremely large fluctuations of Factor A could not cause the low tail end of the emission whereas large fluctuation of Factor B could cause low emission. This would have led immediately to the discovery of the important underlying factor without expenditure of any resources. Instead, it took nearly two months of thorough experimentation and characterization whereas the Monte Carlo simulations could have been concluded in only one or two days.

In a typical DMAIC improvement project, Monte Carlo simulation may be used in the “Analyze” or in the “Improve” phase, particularly when it is combined with Design of Experiments. The power of Monte Carlo simulation lies in the ability to use a statistical model, take realistic variation into account and display the process output both in range and shape. Both range and shape can provide valuable information on the process and its underlying dynamics. A stochastically confirmed response model through Monte Carlo simulation can be used to increase the process capability since its relationship to input variation is known. However, it can also serve to detect hidden factors that are not directly controlled and measured but may be indirectly linked to the process inputs. This will lead to increased understanding and process control at a minimum of expenditure of resources. However, for this method to be successful a good statistical model must be obtained through meticulously designed experiments in the “Analyze” and “Improve” phases.

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REFERENCES

- Box, G.E.P. and K.B. Wilson. "On the experimental attainment of optimum conditions" J.Roy. Stat.Soc. B 13:1-45, (1951)
- Box, G.E.P., Hunter, W.G., and J.S. Hunter, "Statistics for Experimenters", John Wiley, New York, (1978).
- Dean, K A., Coll, B.F., Dinsmore, A., Howard, E., Hupp, M., Johnson, S.V., Johnson, M.R., Jordan, D.C., Li, H., Marshbanks, L., McMurtry, T., Tisinger, L.H., Wieck, S., Baker, J., Dauksher, W.J., Smith, S.M., Wei, Y., Weston, D., Young, S.R., and J. E. Jaskie, "Color Nanotube Field Emission Displays for HDTV", IMID 2005, 1003 (2005).
- Fisher, 1925; Box and Wilson, 1951; Box, et al., 1978; Montgomery, 1976).
- Iijima, S. "Helical Microtubules of Graphitic Carbon", Nature 354, 56-8 (1991).
- Montgomery, D.C. "Design and Analysis of Experiments", John Wiley, New York (1976).
- Metropolis, N. and S. Ulam, "The Monte Carlo Method", J. Am. Stat. Assoc. 44, 335 (1949).

BIOGRAPHY

Dirk Jordan (dirk.jordan@motorola.com) received a Ph.D. and M.S. in physics from Arizona State University, following a B.S. in physics from the University of Heidelberg in Germany. He was a post-doctoral researcher in the Electrical Engineering department at Arizona State University before joining Motorola in 2000. He became a Motorola Six Sigma Green Belt in 2003 and Black Belt in 2005 and is responsible for quality and Six Sigma implementation at Motorola Labs in Tempe, AZ.