

# PEP-II Vacuum System Pressure Profile Modeling Using EXCEL\*

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## Abstract

A generic, adaptable Microsoft EXCEL program to simulate molecular flow in beam line vacuum systems is introduced. Modeling using finite-element approximation of the governing differential equation is discussed, as well as error estimation and program capabilities. The ease of use and flexibility of the spreadsheet-based program is demonstrated. PEP-II vacuum system models are reviewed and compared with analytical models.

## INTRODUCTION

Vacuum systems for particle-beam accelerators, storage rings, and synchrotron light sources are characterized by long tubes of variable conductance and gas desorption rate, with both lumped and distributed pumping. Because of ever more demanding requirements for beam lifetime and radiation background, the pressure profiles and expected performance of these vacuum systems must be well understood.

To adequately characterize such complex vacuum systems, all variables must be included in a model. However, since these variables do, indeed, vary, the resulting piecewise continuous system cannot be modeled analytically. An alternative solution method involves approximating the system as the sum of a series of smaller subsystems. One such modeling method is finite-element analysis (FEA). This is a discretization process whereby a piecewise-continuous problem is divided into discrete, linearly-varying pieces, or "finite elements."

## DERIVATION OF SYSTEM OF EQUATIONS

The finite-element discretization method (FEM) for molecular flow is derived from the second-order differential equation which describes such flow:

$$\frac{d}{dx} \left[ c(x) \frac{dP}{dx} \right] = f(x), \quad (1)$$

where  $c$  is the specific conductance of the vacuum chamber (L-cm/s),  $P$  is the pressure (torr), and  $f$  is the gas-production rate per length of chamber (torr-l/s-cm). Equation (1) is the "strong form" of the descriptive equation in that it describes the system at every point. Alternatively, the "weak form" describes the behavior of the system as a whole, including both the domain and boundaries [1]:

$$\int_{\Omega} c \frac{dP}{dx} \frac{dP^*}{dx} d\Omega - \int_{\Gamma_2} Q_2 P^* d\Gamma_2 + \int_{\Gamma_3} s_3 P P^* d\Gamma_3 = \int_{\Omega} f P^* d\Omega. \quad (2)$$

Here,  $P^*$  is analogous to "virtual work" in the structural mechanics realm,  $Q_2$  signifies a constant gas flow out of the system, and  $s_3$  is a pressure-dependent pumping speed at the system boundary. The domain integrals are evaluated over the domain  $\Omega$ , while the boundary integrals are evaluated over their applicable boundaries,  $\Gamma_2$ , and  $\Gamma_3$ .

To approximate the weak form equation, the integrals over the entire domain are transformed into discrete integrals over individual finite elements, then the element integrals are summed over the domain. Finally, the integrals over each finite element are approximated using the element's shape function. The shape function describes the assumed linear variation of the pressure over the element with respect to the edges, or nodes of the element. The resultant equation is a matrix equation, with  $2 \times 2$  matrices representing the element:

$$\sum_{e=1}^E \frac{c}{L} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{Bmatrix} P_1 \\ P_2 \end{Bmatrix} + \sum_{e=1}^{E_1} \frac{s_3 L}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} P_1 \\ P_2 \end{Bmatrix} + \sum_{e=1}^{E_2} s_4 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} P_1 \\ P_2 \end{Bmatrix} = \sum_{e=1}^{E_1} \frac{fL}{2} \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} + \sum_{e=1}^{E_2} Q_{2e} \begin{Bmatrix} 1 \\ 0 \end{Bmatrix}. \quad (3)$$

Each element matrix equation is then assembled into an overall stiffness matrix and force vector. These have a rank equal to the number of nodes in the model and contain all element connectivity, gas loads, and pumping. The global matrix equation:  $[K]\{P\} = \{F\}$  can then be solved for the pressure vector  $\{P\}$ .

## THE VACPAC FEM PROGRAM

The finite-element formulation described above produces a system of equations which approximate the vacuum system being modeled. This method has been used in the program called VACPAC. It is based on the spreadsheet program EXCEL, from Microsoft Corporation, Redmond, WA, USA, which provides a good combination of availability, ease of use, and power for VACPAC.

Since a real beam line vacuum system is never standard, VACPAC allows most parameters to be defined uniquely for each element. These parameters include: element length, temperature, conductance, gas desorption rate, pumping speed, and gas load. Because most vacuum systems are topologically one-dimensional, VACPAC has been designed to solve only one-dimensional problems. Furthermore, because VACPAC is built on a standard spreadsheet, it can be expanded to pre-process the input. For example, the desorption rate may depend on the geometry of the chamber. This can be calculated, then input into the appropriate column. Or side calculations of pump Tee

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conductance or pump speed versus pressure can be performed in the same spreadsheet as the main program.

Also, standard formulas for chamber conductance are available as formula macros to preclude hunting through reference books. This library of formulas was generated from standard texts by Roth and Dushman [2,3] and can be easily expanded using the EXCEL function macro language. All of these features aid in "pre-processing" the data before the program solves the system of equations.

The VACPAC solver uses the one-dimensionality of the vacuum system to speed the pressure calculations. Such a one-dimensional system produces a tri-diagonal matrix which is very sparse and, consequently, very fast to solve using Gaussian elimination and back-substitution [4].

An iterative solution method is used to solve "linked" systems. Systems are linked when, for instance, periodic boundary conditions exist. Alternatively, two independent piping systems can be modeled separately, then linked at a single node, signifying the intersection of the two systems. Clearly, the pressure at the intersection node must be identical when it appears in both system models. To produce this, the "goal-seeker" feature of EXCEL is used to drive the pressure differential between the coincident nodes at the intersection point to zero, by varying the throughput out of one pipe and into the other. This iterative process preserves the "tri-diagonality" of the system(s), while still producing accurate results.

Finally, the results of the VACPAC program can be "post-processed" using the variety of spreadsheet features available in EXCEL. Pressure and throughput can be graphed, or the process can be iterated to optimize a dependent variable by altering an independent one. Furthermore, scenarios can be stored for comparison, such as pressure profiles for varying pump speeds or various gas species, or pump throughput as a function of chamber temperature. Since input parameters such as conductance or gas load can be varied easily, these scenarios can be tried and compared quickly, and the results can be compared graphically.

## PROGRAM VERIFICATION

The PEP-II High Energy Ring (HER) straight section half-cell vacuum system can be used as a straightforward sample problem both to verify the accuracy of the program, and to demonstrate some of its features. In the straight sections, the beam pipe is a 9.5 cm diameter stainless steel tube, with a single 220 l/s ion pump located every 7.6 meters. Gas is desorbed off the surface of the tube at a rate of  $2 \times 10^{-11}$  Torr-l/s/cm<sup>2</sup>. The pressure profile of this simple system can be described by the parabolic equation:

$$P = q_0 BL \left[ \frac{1}{S_p} + \frac{x}{c} + \frac{x^2}{2cL} \right], \quad (4)$$

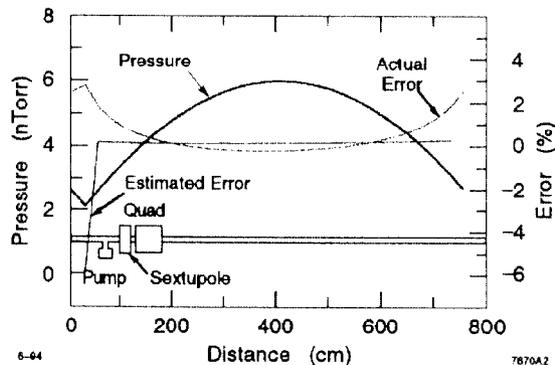


Figure 1: Pressure profile and error in a HER straight section half-cell

where  $qD$  is the desorption rate,  $B$ , the perimeter,  $L$ , the length,  $S_p$ , the pumping speed, and  $c$ , the specific conductance. Using VACPAC, the system is divided into 25 elements of uniform length. Since a half-cell is repeated sixteen times in each straight section, the boundary conditions for a single half-cell model are periodic, with the pressure the same at both ends. To model this, the linking feature will be used.

Figure 1 shows the pressure profile for a half-cell generated by VACPAC and the percent error with respect to the actual value at each node. The estimated error is an approximation of the "discretization error" [5]. This is the error introduced by transforming a continuous system into a discrete, linear one. It is proportional to the square of the element length and to the second derivative of the function. Graphically, this error is the length of the sagitta between the linear discretized value, and the smooth curve of the actual function. Note that, since the estimated error is just an approximation it, also, is not exact. Comparing the errors above, the estimation gives an idea of the areas in which the model will see the largest error.

For most physically realistic vacuum systems, this estimated error provides an indication of the actual error of the model. However, if the error approaches the limit of acceptability, a new model should be generated with a finer mesh. In regions where the slope of the function is changing quickly, such a finer mesh will offset the increased error brought on by the larger second derivative. This will produce a more accurate model.

## PEP-II HER VACUUM SYSTEM MODELING

The VACPAC program was also used to model the gas desorbed and the resultant pressure profile for the HER arc vacuum chambers. As with any high-current storage ring, most of the gas produced in the system results from the synchrotron radiation (SR) impinging on the wall of the chamber. SR is emitted by the beam as it travels in an arc through the dipole bend magnets. In the HER arc sections, the five meter long bend magnets are separated by a two meter long straight

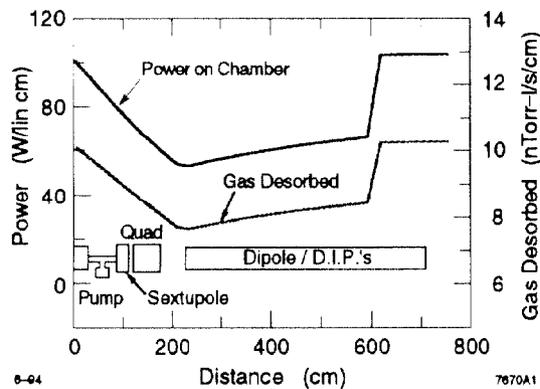


Figure 2: Synchrotron radiation and resultant gas desorbed in a HER arc half-cell.

region. Thus, both the SR incident on the chamber and the gas desorbed off the chamber wall vary with location [6]. Figure 2 shows this variation for a typical arc half-cell.

This power curve was actually computed by augmenting the VACPAC program. For every element, the synchrotron radiation impinging on the element and the gas produced by the element were calculated using the location of the element with respect to the beam as it curves through the dipole magnet. Thus the messy trigonometry was calculated automatically, based on the beam line location of the element centroid. Beam parameters such as energy, current, critical energy of the electrons, and bending radius were also included in this calculation.

Finally, Distributed-Ion Pumps (DIPs) were located throughout the length of the dipole magnet, and a single 60 L/s sputter ion pump was located just upstream of the sextupole magnet.

Figure 3 shows the results of the VACPAC pressure calculation. It shows the pressure profile for a nitrogen-equivalent molecular weight gas, and a nominal chamber temperature of 60°C [7]. The linking feature of VACPAC was used since the profile repeats itself every half-cell, with the end of one running into the start of the next. Thus, the pressure is equal at the first and last nodes.

The average pressure of 11.1 nTorr was found by weighting the pressure values at each element by the element length. VACPAC estimates the maximum error to be 3.6%, which is far better than the possible error of the desorption coefficient, so the results are about as accurate as possible, given the accuracy of the input.

The VACPAC model brings to light a few interesting results. First, as expected, the pressure is highest in the quad chamber, where there are no distributed ion pumps. However, the sputter ion pump actually does very little to affect this hump. A 120 l/s or even 240 l/s pump does not significantly reduce the peak pressure, and does almost nothing to reduce the average pressure of the system. Thus, money is better spent on improving

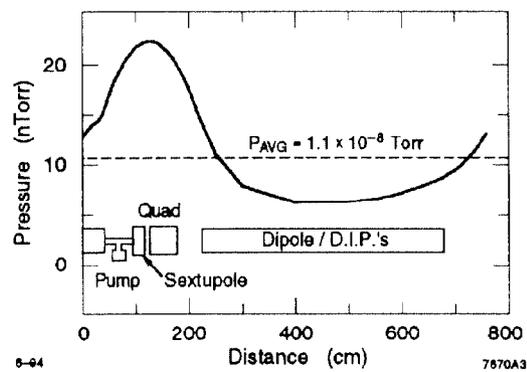


Figure 3: Pressure profile in a HER arc half-cell.

the DIP pumping speed, and not by putting in bigger lumped ion pumps.

The second result brought to light by the VACPAC program is the factor of two variation in the DIP pump gas load. The DIP modules nearest the quad chamber see twice the load as those in the middle of the dipole chamber. This is because the modules near the end of the dipole chamber are pumping gas from the quad chamber, and are in a region of higher SR power and, thus, higher gas desorption. They combine to produce double the gas throughput and, possibly, half the life of the DIPs in the center of the chamber.

## CONCLUSION

The modeling of the PEP-II HER arcs shows one example of the power of the finite-element analysis method when applied to vacuum system modeling. Furthermore, when using EXCEL, powerful features such as goal-seeking, scenario-management, iteration, and graphing can be brought to bear on the problem. All of these features were used to model the relatively complex variations of the HER arc vacuum system. The results of this modeling have subsequently been used to size both the lumped and distributed ion pumps.

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