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Vakdyn, a program to calculate time dependent pressure profiles

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Abstract

We describe a program that calculates time dependent pressure profiles in conductance limited vacuum systems where the pump speed and out-gassing can vary as a function of time. In this way pump down or pressure bumps due to temporary leaks or out-gassing can be visualized and analyzed.

Keywords: Vacuum; Pressure; Transients

1. Introduction

In Ref. [1] a method is described to calculate the equilibrium pressure in conductance limited vacuum systems that consist of piecewise constant elements with a definite length, conductance, pump speed, and out-gassing rate. There the differential equation that describes the pressure profile [2]

$$\frac{\mathrm{d}}{\mathrm{d}z}c\frac{\mathrm{d}P}{\mathrm{d}z}-sP=-q \tag{1}$$

is solved by transfer matrices resulting in a graphical display of the equilibrium pressure $P(z)$ as a function of longitudinal position z. Here c, s, and q are the conductance, pump speed, and out-gassing rate per meter, respectively.

In Eq. (1) and the following sections we assume that the temperature T of the system under consideration is controlled externally and can affect the parameters c, s, and q. For example, the conductance c is proportional to the mean free path [3] which in turn depends on the temperature T and the molecular weight M of the gas and is proportional to $\sqrt{T/M}$. The out-gassing rate q may also depend on the temperature of the vacuum vessel depending on the surface processing history of the material.

A notable limitation of the method in Ref. [1] is that only the time-invariant equilibrium condition is described. Transient effects such as pump down or a periodic gas load cannot be described in this framework. In this report we will present the theory and the implementation in a computer program which overcomes these limitations.

2. Dynamic vacuum pressure

In order to calculate transient vacuum effects Eq. (1) needs to be augmented by a term that describes the temporal variation of the pressure. Here we can exploit the fact that the gas in a conduction limited system obeys the natural gas law $PV = NkT$ which relates the pressure P to the number of particles N in a volume V at local temperature T. Here k is the Boltzman constant. Furthermore, we note that the units of Eq. (1) are Torr l/ms which is proportional to the number of particles per second and per meter we can add a term $v\partial P/\partial t$ while keeping the units correct but need to motivate in the following section why this choice is reasonable. The equation for the time dependent pressure then reads

$$v\frac{\partial P}{\partial t}=\frac{\partial}{\partial z}c\frac{\partial P}{\partial z}-sP+q \tag{2}$$

with $C = c/L$, $V = vL$, $S = sL$, and $Q = qL$, where C is the conductance of a pipe of length L and S, Q, and V are the total pump out-gassing rate, and volume of this section of the vacuum system, respectively. Note that in equili-

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brium where the time derivative of the pressure distribution vanishes, the equation for the static distribution as given in Eq. (1) is recovered.

The interpretation of Eq. (2) is straightforward. The left hand side describes the change of number of particles in a longitudinally infinitesimal test volume. The right hand side describes the sources and sinks of these particles. There is out-gassing as described by q, pumping as given by s and a term that describes diffusion along the pipe with specific conductance c.

In an example we ignore conductance and out-gassing and consider a probe volume of length L and volume $V = vL$. We then obtain the equation for the pump down time $v\partial P/\partial t = -sP$ or

$$\frac{\partial P}{\partial t} = -\frac{S}{V}P \tag{3}$$

with the pump down time $\tau = V/S$ for such a very simple system. Our goal, however, is to be able to simulate and calculate the transient behavior of much more complicated systems made of arbitrary sections with out-gassing, pumping, and conductance and describe an algorithm to achieve this, in the following section.

3. The algorithm

We observe that Eq. (2) is a diffusion equation with extra sources and sinks due to pumps (s) and out-gassing (q) where the conductance (c) plays the role of the z-dependent diffusion constant. We can therefore use standard methods to discretize Eq. (2) and solve the partial differential equation. We follow Ref. [4] and choose to use a Crank–Nicholson integrator, because it is unconditionally stable, independent of the discretizing step size in space z or time t.

We discretize the partial differential equation (2) by selecting points on the z-axis labeled by subscript j which runs between 1 and N on which the pressure P_j^n, the pump speed S_j^n, and the out-gassing Q_j^n at time step n are localized where the superscript n denotes the time step. The distance L_j between point j and $j-1$ is denoted by L_j. The volume associated with point j comprises half the volume between point $j-1$ and j and half of that between point $j+1$ and j. The conductance C_j associated with grid point j is given by half that of the section to the left and half of that to the right, added inversely. Using these parameters the discretized version of Eq. (2) reads

$$\begin{aligned} V_j\frac{P_j^{n+1}-P_j^n}{\Delta t} &= \frac{\partial}{\partial z}\left\{L_j^2 C_j \frac{\partial P^n}{\partial z}\right\} - S_j P_j^n + Q_j \\ &= C_j(P_{j+1}^n - P_j^n) - C_{j-1}(P_j^n - P_{j-1}^n) \\ &\quad - S_j P_j^n + Q_j. \end{aligned} \tag{4}$$

Note that we can solve Eq. (4) for P_j^{n+1} which results in only quantities at time step n on the right hand side to appear. This results in the equivalent of a first order forward step algorithm which, however, is stable only for small time steps Δt [4]. The deficiency can be remedied by the Crank–Nicholson trick [4] which suggests the replacement of the right hand side in Eq. (4) by the average of the right hand side at time step n and time step $n+1$ which results in

$$\begin{aligned} P_j^{n+1} - P_j^n = \frac{\Delta t}{2V_j}\{&C_j(P_{j+1}^n - P_j^n) - C_{j-1}(P_j^n - P_{j-1}^n) \\ &- S_j P_j^n + Q_j + C_j(P_{j+1}^{n+1} - P_j^{n+1}) \\ &- C_{j-1}(P_j^{n+1} - P_{j-1}^{n+1}) - S_j P_j^{n+1} + Q_j\}. \end{aligned} \tag{5}$$

After collecting quantities at time step $n+1$ we arrive at the following implicit system of equations for the pressure at time step $n+1$:

$$\begin{aligned} &a_j P_{j-1}^{n+1} + b_j P_j^{n+1} + c_j P_{j+1}^{n+1} \\ &\quad = d_j P_{j-1}^n + e_j P_j^n + f_j P_{j+1}^n + Q_j \Delta t/V_j. \end{aligned} \tag{6}$$

Note that the system of equations is tridiagonal with diagonals given by

$$\begin{aligned} a_j &= -d_j = -\tfrac{1}{2}C_{j-1}\Delta t/V_j, \\ b_j &= 1 + \tfrac{1}{2}(C_j + C_{j-1} + S_j)\Delta t/V_j, \\ c_j &= -f_j = -\tfrac{1}{2}C_j\Delta t/V_j, \\ e_j &= 1 - \tfrac{1}{2}(C_j + C_{j-1} + S_j)\Delta t/V_j \end{aligned} \tag{7}$$

for $j = 2, ..., N-1$. Here a, b, c are the coefficients for the lower, central, and upper diagonal of the left hand side and d, e, f those for the right hand side of Eq. (6). The coefficients at the end points are chosen to have zero gas flow in or out of the system which can be achieved by choosing $P_0 = P_1$ and $P_N = P_{N+1}$ at the virtual grid points 0 and $N+1$. They are given by

$$\begin{aligned} a_1 &= c_N = d_1 = f_N = 0, \\ b_1 &= 1 + \tfrac{1}{2}(C_1 + S_1)\Delta t/V_1, \\ c_1 &= -f_1 = -\tfrac{1}{2}C_1\Delta t/V_1, \\ e_1 &= 1 - \tfrac{1}{2}(C_1 + S_1)\Delta t/V_1, \\ a_N &= -d_N = -\tfrac{1}{2}C_{N-1}\Delta t/V_N, \\ b_N &= 1 + \tfrac{1}{2}(C_{N-1} + S_N)\Delta t/V_N, \\ e_N &= 1 - \tfrac{1}{2}(C_{N-1} + S_N)\Delta t/V_N. \end{aligned} \tag{8}$$

This tridiagonal system of equations can be solved for example with the subroutine tridag from Ref. [4] and yields the pressure profile P_j^{n+1} in terms of the pressure profile at time step P_j^n. The algorithm is very fast, a typical run takes a few seconds on a modern PC, because rather large time steps Δt can be chosen, due to the stability of the Crank–Nicholson method. Moreover, the time of solving a tridiagonal system is only proportional to the number of grid-points N.

4. The program Vakdyn

The algorithm described in the previous section is coded in a program called `vakdyn` that reads a control file in which parameters such as the vacuum structure and the