Calcvac/Vacline

VERSION 2.01

User Manual

(C) 2002-2018 by Markus Hoffmann and Mike Seidel
(xxx@xxx.net)
(see http://xxx.xxx.net/)

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The programs calcvac/vacline can calculate logitudinal one-dimensional pressure profiles in vacuum pipes. The pipes can consist of different sections of different shape and material. Outgasing of several different gas species can be simulated. Also it is possible to install vacuum pumps of different types. Also cryo effects (cold pipes and cryo pumps) are simulated. Finally the pipes can be linked together to form a network.

Calcvac/Vacline

CONTENTS

This document describes the operation and use of the CALCVAC / VACLINE program package by Markus Hoffmann and Mike Seidel, (c) DESY 2002-2018, version 2.01.

1 Introduction

With the proposed method, it is possible to calculate one-dimensional pressure profiles in contiguous vacuum tubes, taking into account the presence of pumps and outgassing elements. The starting points are the tube profiles as well as the materials and pumps used. Cryoeffects are partly taken into account.

For these calculations, the programs `VACLINE` and `CALCVAC` were developed. `VACLINE` is able to produce one-dimensional pressure profiles for a single gas species. `CALCVAC` is an extension to this and allows to calculate a complete mass spectrum of the pressure profile, as well as various events in the vacuum system (e.g. switching on and off of pumps, heating TSPs[1], as well as the desorption of gases by synchrotron light radiation). Both programs are also capable of calculating meshed vacuum systems, such as ring-shaped or star-shaped or arbitrarily linked *Vacuum Lines* and *Vacuum Networks*.

This document will mainly deal with the configuration and operation of the program package. For a detailed description of the underlying concept and the mathematical procedures, please refer to the article [14].

[1] TSP = titanium sublimation pump

2.1 Vacuum

In the so-called high vacuum and ultra-high vacuum ($P < 1 \cdot 10^{-7}$ mbar), the gas concentration is reduced to such an extent that the mean free path of the molecule is so great that collisions of the gas molecules with each other can be neglected[1]. The individual gas particles then interact predominantly with the chamber walls, where they are reflected, adsorbed and desorbed.

The temperature of the chambers also plays a role. For example, in a system of two chambers of different temperature, the equilibrium gas concentration in the colder part will be greater. The important physical parameters describing this state are: mean free path length, the chamber dimension, and the velocity distribution of the molecules.

2.2 Conductivity, suction power and flow

Because of the vanishing viscosity and high velocity of the gas molecules, transport phenomena at pressure differences in thin gases can be compared with the current in an electrical circuit given resistances and voltage differences.

The *flow* Q (or current I) is directly proportional to the potential difference and inversely proportional to the resistance, in direct analogy to Ohm's law ($I = \Delta U / R$) for the flow through a tube with the resistance (or the impedance) Z:

$$Q = (p_1 - p_2)/Z = C\Delta p \quad . \tag{2.1}$$

Where C is the pipe's *conductivity*. Unit: volume/time = [l/s]. The conductivity of a vacuum component is dependent on the geometry of the vaccum chamber, the type of gas and its temperature and, in the case of viscous gas, also on the pressure. From the above context one recognizes the unit for the flow: $[Q] =$ mbar l/s.

Otherwise, you can add the conductivity in a system of vacuum components (parallel connection) and add reciprocally (in series connection).

But for the conductivity C you can also write:

$$C = pvA/\Delta p \quad .$$

[1] so-called *Knudsen Gas*; In contrast to the viscous state, where the gas concentration is so high that collisions of the gas molecules with each other dominate.

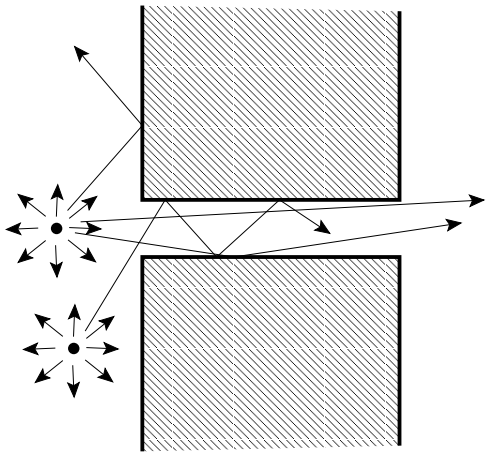

Figure 2.1: To calculate the conductivity C of a pipe between two extended gas tanks.

Since the pressure is a measure of the particle density $n = N/V$, the flow can also be interpreted as the number of molecules N, which pass through a cross-sectional area A of the pipe per unit of time with the flow velocity v.

$$p = nkT/V \quad .$$

$$Q = pC = nk\frac{T}{V} \cdot \frac{V}{t} = nkT/t \sim \frac{N}{Vt} \cdot \frac{A}{A}$$

$$Q \sim NvA = nVvA \quad .$$

This relationship defines the *suction power* S as follows: $N = Avn = Sn$ with the suction power $S = Av$, unit: [S]=l/s.

The suction power determines the rate (volume/time) at which gas is removed from the vacuum system. The throughput of the pump again results from $Q = pS$. The effective pumping capacity of a pump with connection piece therefore results from the reciprocal sum of suction capacity and conductivity of the connection.

2.3 Conductivities

The conductivities of various vacuum components are difficult to calculate. For some simple geometries (infinitely long round tube, infinitely thin aperture) analytical expressions can be found which are provided with correction factors for different lengths. For individual components connected to infinite tanks at both ends, molecular tracker simulations can yield the desired conductivities (e.g., with a program

described in [10]). Here, the passage probability per time for a particle on the one side is calculated for the passage through the tube. However, the assumption of large tanks at both ends is no longer applicable to a multi-element tube system, since the particles no longer have an isotropic velocity distribution after passing through a (thin) tube, because a form of bundling has already occurred.

The following formulas are used for the standard profile types used in accelerators for tubes of length l, usually consisting of a part for the aperture and a part for a tube with length.

- Circular cross-section with diameter d:

$$C_o = \frac{1}{1/C_{\text{ap}} + 1/C_{\text{len}}} \quad ; \quad C_{\text{ap}} = 11.6 \cdot d^2\pi/4 \quad ; \quad C_{\text{len}} = 17.1\frac{d^3}{\sqrt{2}l} \quad .$$

- Elliptical cross-section with diameters a and b:

$$C_e = \frac{1}{1/C_{\text{ap}} + 1/C_{\text{len}}} \quad ; \quad C_{\text{ap}} = 11.6 \cdot ab\pi/4 \quad ; \quad C_{\text{len}} = 17.1\frac{a^2b^2}{l\sqrt{a^2+b^2}} \quad .$$

- Rectangular cross section with side lengths a and b:

$$C_r = \frac{1}{1/C_{\text{ap}} + 1/C_{\text{len}}} \quad ; \quad C_{\text{ap}} = 11.6 \cdot ab \quad ; \quad C_{\text{len}} = 30.9 \cdot f(\min(\frac{a}{b}, \frac{b}{a}))\frac{a^2b^2}{l(a+b)} \quad ,$$

with

$$f(x) = \frac{0.0653947}{x + 0.0591645} + 1.0386 \quad .$$

All other chamber shapes are (roughly) approximated by these basic shapes, for example the octagonal chamber by an ellipse. For the keyhole chamber, the conductance for a rectangle is added to an ellipse. The error that arises because there is no partition in the chamber is reasonably small.

2.4 Temperature and molecular mass

The above values for the conductivities for different tube shapes are valid for air (molecular mass $m = 28$ (mainly nitrogen)) and for room temperature ($T = 300$ K). The higher the temperature and the lighter the gas molecules, the higher the conductivity for the corresponding gas species.

Material	starting	to
Aluminium	$5 \cdot 10^{-14}$	$1 \cdot 10^{-8}$
Stainless steel	$4 \cdot 10^{-12}$	$2 \cdot 10^{-8}$

Table 2.1: Typical total outgassing rates of some materials (from [8]).

They go into the conductivities as follows:

$$C \sim \sqrt{\frac{T}{m}} \quad .$$

2.5 Gas load and equilibrium pressure

In a closed vacuum system, gas is from different sources. These sources can be:

1. Residual gas in the system,
2. Vapor pressure in equilibrium with the condensed matrials (solids),
3. Gases that are produced or incorporated by:
    - Leaks (also virtual leaks of gases trapped in corners),
    - Outgassing (adsorption),
    - Permeation (diffusion of gases through the vacuum chamber).

An equilibrium pressure (or an equilibrium pressure distribution at various internal gas flows) arises from the equilibrium of gas newly produced or incorporated from gas sources and pumping rate (or condensation rate at corresponding temperatures).

$$P = \frac{Q_0}{S_{eff}} \quad . \tag{2.2}$$

The largest unknowns in determining the gas load come from the outgassing mechanisms. Typical outgassing rates are temperature-dependent and also highly dependent on the pretreatment and contamination of the materials. They can fluctuate around several orders of magnitude. Outgassing rates are determined usually as flows per unit area. The unit is thus mbar l/s/cm^2.

2.6 Calculation of longitudinal pressure profiles

Pressure distribution and gas flows should be calculated for any but one-dimensional arrangement of vacuum components. For this one can use a simple differential equation. This is now briefly motivated.

A generalization of the equation (2.1) is

$$Q(x) = -c(x)\frac{dP(x)}{dx} \quad , \tag{2.3}$$

with c: specific conductivity [m l/s].

Furthermore, one can set up a continuity equation (conservation of mass):

$$-\frac{dQ(x)}{dx} + q(x) = P(x)s(x) \quad , \tag{2.4}$$

with x: longitudinal coordinate [m]; P: Pressure [mbar]; Q: Gas flow [mbar l/s]; q: specific outgasing rate [l/s/m].

Combining the equations (2.3) and (2.4) one obtains

$$\frac{d}{dx}\left[c(x)\frac{dP(x)}{dx}\right] - s(x)P(x) = -q(x) \quad . \tag{2.5}$$

It should be recalled that only in the molecular vacuum range are the conductivities independent of pressure.

Assuming that the specific conductivity c, the specific outgassing rate q, and the specific suction power s are each piecewise constant, equation (2.5) is an ordinary second order linear differential equation with (piecewise) constant coefficients[1].

The general solution of the equation (2.5) is then

$$P(x) = C_1 \exp(\alpha x) + C_2 \exp(-\alpha x) + \frac{q}{s} \quad ; \tag{2.6}$$

with $\alpha = \sqrt{s/c}$.

From this it is possible, analogous to particle optics, to develop a matrix formalism from the initial-value problem (compare [5, 1]):

$$\begin{pmatrix} P(x) \\ Q(x) \end{pmatrix} = \mathbf{M} \begin{pmatrix} P_0 \\ Q_0 \end{pmatrix} + \vec{v}$$

[1] This type of differential equation is also found in accelerator physics in the calculation of particle trajectories (Hill's differential equation: $\frac{d^2x(s)}{ds^2} + \left(\frac{1}{\rho^2(s)} - k(s)\right)x(s) = \frac{1}{\rho(s)}\frac{\Delta p}{p}$ bzw. $\frac{d^2z(s)}{ds^2}z(s) + k(s)z(s) = 0$). The solution methods there are quite similar to those presented here, which is the reason for the close relationship between vacuum calculations and accelerator physics.

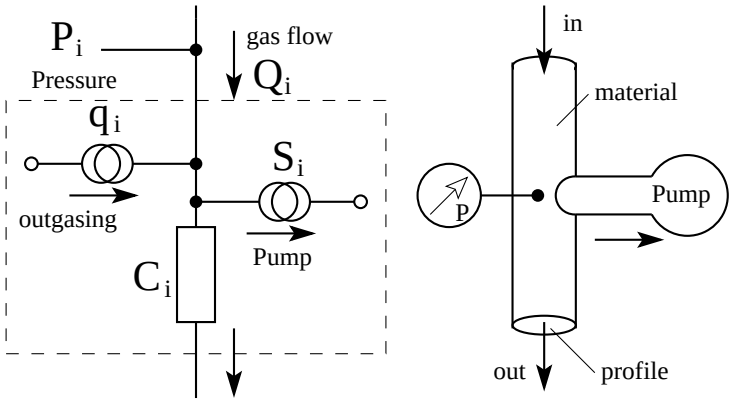

Figure 2.2: Elementary piece of vacuum chamber to illustrate the parameters flow Q, conductivity C, outgassing rate and suction power. On the left: the circuit diagram analogous to an electrical circuit.

with

$$\mathbf{M} = \begin{pmatrix} \cosh(\sqrt{s/c}x) & -\frac{1}{c\sqrt{s/c}}\sinh(\sqrt{s/c}x) \\ -c\sqrt{s/c}\sinh(\sqrt{s/c}x) & \cosh(\sqrt{s/c}x) \end{pmatrix} \tag{2.7}$$

and

$$\vec{v} = \begin{pmatrix} -\frac{q}{s}\left(\cosh(\sqrt{s/c}x) - 1\right) \\ \frac{q}{\sqrt{s/c}}\sinh(\sqrt{s/c}x) \end{pmatrix} \quad .$$

In principle, therefore, one can calculate the entire pressure curve through a vacuum system under given starting conditions by tracking. The constants P_0 and Q_0 must be found from a boundary value problem, for example, if one has periodic boundary conditions, one finds the periodic solution using the 1-turn matrix $\mathbf{M}$ for the entire vacuum line:

$$\begin{pmatrix} P_0 \\ Q_0 \end{pmatrix} = (\mathbf{1} - \mathbf{M})^{-1}\vec{v} \quad .$$

For more general boundary conditions an equation system must be set up and solved.

The problem of calculating a pressure profile is thus reduced to solving a system

of equations, which can be written in the following form:

$$\begin{pmatrix} -m_{11}^1 & -m_{12}^1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ -m_{21}^1 & -m_{22}^1 & 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & -m_{11}^2 & -m_{12}^2 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & -m_{21}^2 & -m_{22}^2 & 0 & 1 & \dots & 0 & 0 \\ & & \vdots & & \ddots & & & & \vdots \\ 0 & 0 & 0 & 0 & \dots & -m_{11}^n & -m_{12}^n & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & -m_{21}^n & -m_{22}^n & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} P_0 \\ Q_0 \\ P_1 \\ Q_1 \\ \vdots \\ P_{n-1} \\ Q_{n-1} \\ P_n \\ Q_n \end{pmatrix} = \begin{pmatrix} v_1^1 \\ v_2^1 \\ v_1^2 \\ v_2^2 \\ \vdots \\ v_1^n \\ v_2^n \end{pmatrix} .$$

The indices on the pressures and gas flows denote the element i, to which the matrix elements m_{ab}^i and v_j^i belong, and on whose Output P_i and Q_i prevail.

As can be seen, the system of equations is underdetermined, since there are $n+1$ pressures and gas flows at only n elements. (Pressure P_0 and Gasflow's Q_0 are added at the input of the first element.)

For this reason, two additional constraints are required: Here, for example, you can specify these parameters at the input of the last element: With $P_0 = b_1$ and $Q_0 = b_2$ the equation system looks like this: (The matrix is now quadratic.)

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ -m_{11}^1 & -m_{12}^1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ -m_{21}^1 & -m_{22}^1 & 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & -m_{11}^2 & -m_{12}^2 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & -m_{21}^2 & -m_{22}^2 & 0 & 1 & \dots & 0 & 0 \\ & & \vdots & & \ddots & & & & \vdots \\ 0 & 0 & 0 & 0 & \dots & -m_{11}^n & -m_{12}^n & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & -m_{21}^n & -m_{22}^n & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} P_0 \\ Q_0 \\ P_1 \\ Q_1 \\ \vdots \\ P_{n-1} \\ Q_{n-1} \\ P_n \\ Q_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ v_1^1 \\ v_2^1 \\ v_1^2 \\ v_2^2 \\ \vdots \\ v_1^n \\ v_2^n \end{pmatrix} .$$

This equation system is band-diagonal and can be solved with appropriately optimized solution algorithms. Of course, one can also specify any other boundary conditions (for any P_i or Q_j or also – which will occur frequently – for start and end flows Q_0 and Q_n). The ones in the first two lines of the matrix are then in the appropriate position (and the matrix is no longer band-diagonal).

If the pressures and fluxes for the inputs of the elements have now been determined by solving this system of equations, it is furthermore easy to determine

the pressures at any point between them by means of the transfer matrices. This method can also be used to reduce the size of the matrix by first combining several elements (where there are no constraints or links). Knowing the initial pressure for this section, the vacuum profile can then be transferred to the other elements by tracking. This, however, reaches its limits at the moment when relatively poorly conducting elements occur (which is relatively common) and the numerical inaccuracies begin to play a role (see below).

2.7 Numerical stability

The difficulty in the vacuum tracking process is the hyperbolic functions that occur in the transfer matrices. As the vacuum tube to be considered becomes longer (and its conductivity becomes smaller and smaller), the arguments of these functions and the functions themselves, which grow exponentially, become larger and larger. So the entries in the matrix will grow very fast[1]. The result is that the matrix becomes more and more singular in terms of numerical accuracy, and the correlation between the pressure and the gas flow at one end is nearly canceled out with those at the other end. According to the basic equation of the vacuum technique (see also equation (2.2) or (2.6)), the pressure inside this part is then only determined by the prevailing suction power and the outgassing rate (see fig. 2.3).

The vacuum system then breaks down on this poorly conducting section into two almost independent parts, which in principle require separate boundary conditions. Unfortunately, these difficulties also arise when you multiply just enough single matricies together for a long vacuum line. The tracking is reaching its limits. To get around these difficulties, a method has already been proposed, the *Finite Differences Method* (see [6]).

`VACLINE` uses a different method to avoid numerical difficulties:

1. To solve the system of equations, the singular value decomposition (SVD) is used, which also provides useful solutions to singular equation systems with possibly additional boundary conditions.
2. For elementary transfer matrices, a modified model is used for those where numerical difficulties are to be expected ($l\sqrt{\frac{s}{c}} > \log(1 \cdot 10^{13})$). In this case, it is assumed that the pressure profile approaches a constant value exponentially with a sufficiently long element from the ends, and the net flux in

[1] In particle optics, these difficulties do not occur because there occur trigonometric instead of the hyperbolic functions whose range of values is limited.

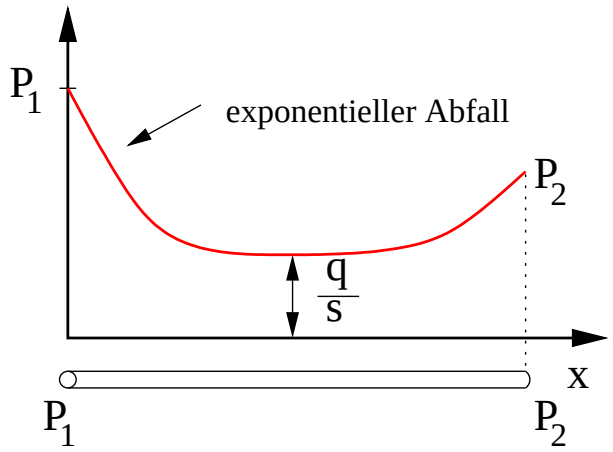

Figure 2.3: A long piece of vacuum chamber with pump power decouples the vacuum system, since the pressure conditions inside are no longer determined by those at the entrance. This problem causes almost singular transfer matrices, which leads to numerical instability due to the finite computational precision of $l\sqrt{\frac{s}{c}} > \log(1 \cdot 10^{13})$.

equilibrium disappears correspondingly:

$$P(x) = C_1 \cdot \exp(-\alpha x) + \frac{q}{s}$$
$$Q(x) = \alpha c C_1 \cdot \exp(-\alpha x)$$

with $C_1 = (P(0) - \frac{q}{s})$ and $\alpha = \sqrt{s/c}$.
The same applies to the other end of the vacuum tube (see also Fig 2.3). Thus, a boundary condition for the ratio of pressure to flow for $x = 0$ arises for both ends:

$$P(x \to 0) = \frac{1}{\alpha c} Q(x \to 0) + \frac{q}{s} \tag{2.8}$$

and for $x = l$ from

$$P(x) = C_1 \cdot \exp(-\alpha(l - x)) + \frac{q}{s}$$
$$Q(x) = -\alpha c C_1 \cdot \exp(-\alpha(l - x))$$

accordingly

$$P(x \to l) = -\frac{1}{\alpha c} Q(x \to l) + \frac{q}{s} \quad . \tag{2.9}$$

Instead of the matrices (2.7), the following can then be used for vacuum tracking (although here the pressure and the flow at the other end must be known):

$$\begin{pmatrix} P(x) \\ Q(x) \end{pmatrix} = \begin{pmatrix} \Pi & 0 & \Gamma & 0 \\ 0 & \Pi & 0 & \Gamma \end{pmatrix} \begin{pmatrix} P_0 \\ Q_0 \\ P_1 \\ Q_1 \end{pmatrix} + \begin{pmatrix} \frac{q}{s}(1 - \Pi - \Gamma) \\ 0 \end{pmatrix} \quad , \tag{2.10}$$

with $\Pi := \exp(-\alpha x)$ and $\Gamma := \exp(-\alpha(l-x))$.
This takes into account the fact that the flow through the vacuum element practically disappears. The system of equations practically decays into two parts at this element, using two new boundary conditions (according to equations (2.8) and (2.9))

$$P_i = \frac{1}{\alpha c} Q_i + \frac{q}{s} \quad \text{und} \quad P_{i+1} = -\frac{1}{\alpha c} Q_{i+1} + \frac{q}{s} \quad ,$$

in the large matrix instead:

$$\begin{pmatrix} & \vdots & & & \vdots & \\ \dots & 1 & -1/\sqrt{s_i c_i} & 0 & 0 & \dots \\ \dots & 0 & 0 & 1 & 1/\sqrt{s_i c_i} & \dots \\ & \vdots & & & \vdots & \end{pmatrix} \cdot \begin{pmatrix} \vdots \\ P_i \\ Q_i \\ P_{i+1} \\ Q_{i+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ q_i/s_i \\ q_i/s_i \\ \vdots \end{pmatrix} \quad .$$

2.8 Mesh networking of vacuum systems

With the method presented here, only one-dimensional pressure profiles can be calculated in a one-dimensional topology of the vacuum system. For more complicated three-dimensional structures, this algorithm is usually not well suited. Such structures are then treated by molecular tracking techniques (see [10]). Accelerator Vacuum systems are, however, usually sufficiently one-dimensional.

At HERA however, one of the largest electron proton colliders of its time, the two accelerator vacuum systems were interconnected in the interaction zones. There have been also special design features, such as the photon beam absorption beamlines at the interaction zones. Similar situations arise in synchrotron radiation sources, where many tubes of the vacuum system branch off from the actual ring. Also some pumps are provided with a longer connection tubes and can be treated similarly.

In the following a method is presented how such networks of several one-dimensional vacuum systems can easily be considered in the algorithm presented here.

With a special instruction, the inputs of various elements of the vacuum line can be additionally interconnected. For example, you can reconnect the end of a line to

its beginning and thus get periodic boundary conditions, or several parts of the line, (which are possibly loosely connected by a (closed) valve or a poorly conductive section) can be linked.

Mathematically speaking, such a connection represents a channel with infinitely high conductivity. The equation system thus has a boundary condition for the pressure (which must be the same at both ends of the connection) and another unknown, namely the flow through this channel (see Fig. 2.4).

The equation system looks like this, with the rank of the matrix increasing by one:

$$\begin{pmatrix}
1 & 0 & m & m & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & 0 \\
0 & 1 & m & m & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & 0 \\
 & & \vdots & & \ddots & & & & & & & & & \vdots \\
0 & 0 & 0 & 0 & \dots & & & \dots & & & \dots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \dots & & & \dots & & & \dots & 0 & 0 & 1 \\
 & & \vdots & & & & & & & & & & & \vdots \\
0 & 0 & 0 & 0 & \dots & & & \dots & & & \dots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \dots & & & \dots & & & \dots & 0 & 0 & -1 \\
 & & \vdots & & & & & & & & \ddots & & & \vdots \\
0 & 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & m & m & 0 \\
0 & 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & m & m & 0 \\
 & & & \dots & 1 & \dots & & & & & & & & 0 \\
 & & & \dots & & & \dots & 1 & \dots & & & & & 0 \\
0 & 0 & 0 & 0 & \dots & 1 & 0 & \dots & -1 & 0 & \dots & 0 & 0 & 0
\end{pmatrix}
\cdot
\begin{pmatrix}
P_0 \\ Q_0 \\ P_1 \\ Q_1 \\ \vdots \\ P_i \\ Q_i \\ \vdots \\ P_j \\ Q_j \\ \vdots \\ P_{n-1} \\ Q_{n-1} \\ P_n \\ Q_n \\ Q_{\mathrm{AB}}
\end{pmatrix}
=
\begin{pmatrix}
v_0^1 \\ v_0^2 \\ v_1^1 \\ v_1^2 \\ \vdots \\ v_i^1 \\ v_i^2 \\ \vdots \\ v_j^1 \\ v_j^2 \\ \vdots \\ v_{n-1}^1 \\ v_{n-1}^2 \\ b_1 \\ b_2 \\ 0
\end{pmatrix}.$$

2.9 Solvers

Although one can apply elimination algorithms to a quadratic system of equations (e.g., Gauss-Jordan elimination), the solutions are often not numerically stable. This always happens when two parts of the vacuum line are connected by a poorly conductive element. The solution then suddenly becomes extremely sensitive to the boundary conditions, and often the solution diverges. This problem can be circumvented by defining more additional boundary conditions for vacuum systems

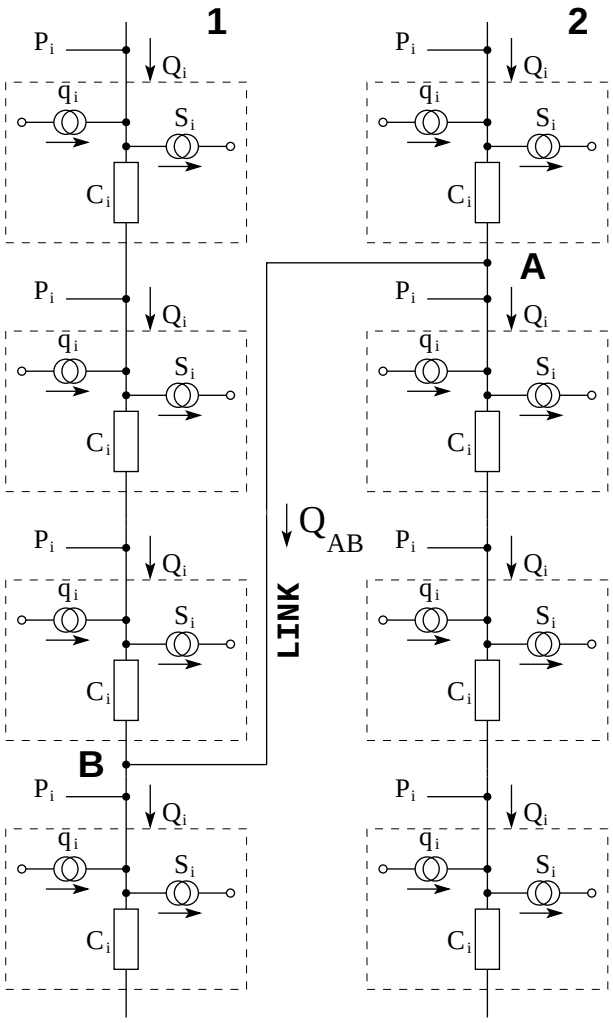

Figure 2.4: Principle of linking two vacuum systems. (It may also be two places in the same vacuum system.) The connection creates an additional (virtual) channel through which gas can flow. So there is one more unknown Q_{AB} in the equation system per link. But also a new condition comes into play, namely that the pressure at the two points **A** and **B** must be the same.

that are divided in this way. And only approximatively solve the overdetermined system of equations. The pressure profiles then fit better locally to "their" boundary condition.

With the help of the singular value decomposition (SVD) there is a good instrument here. So it does not matter if the equation system is over- or underdetermined. The solution from the solution space is always chosen (or a solution found nearby) that minimizes the amount $|M\vec{p} - \vec{b}| \longrightarrow 0$. It turns out that this almost always provides a realistic pressure profile, interestingly, even without specifying any boundary conditions at all.[1] Maybe because pressure distortions are intrinsically damped away and thus have only local effects.

[1] In the rare case that the system of equations has a too big kernel or too many singular values are too largely distribute or too small, `VACLINE` will issue a warning. In this case, the result is most likely not a realistic pressure profile. This can be recognized by jumps in pressure at the element boundaries. In practice, however, this means that the vacuum system is poorly designed because there are gas traps, that is, areas that are not pumped off in a controlled manner, virtual leaks, and the like. This should be avoided anyway.

3 AN EXAMPLE: THE HERA VACUUM SYSTEM

HERA[1] has long been the largest hadron electron collider in Europe with a circumference of 6336 m. Located in Hamburg (germany) it was put into operation in 1992 and shut down in 2007. The facility consisted of two accelerators: A proton accelerator accelerated protons up to energies of 920 GeV. The electron accelerator accelerated electrons or positrons to 27.5 GeV. At two interaction points (surrounded by the detectors ZEUS and H1) the accelerated particle beams were collided.

In order to bring the two particle beam to collision, the vacuum system of the two accelerators in the collision points of the two beams (interaction zones) had to be connected to each other.

The interaction zone also had other special features: HERA-p was an accelerator with superconducting magnets and also the solenoids of the detectors were partially realized with superconducting coils. The superconducting material must be cooled with liquid helium. As a consequence, the vacuum chamber inside thouse magnets was also cold.

Finally, when the electron beam is deflected, synchrotron light is produced in the form of high-energy radiation. Upon impact of this light from the inside on the vacuum chamber, this can heat up considerably. To prevent this, specially cooled so-called absorber chambers were installed in order to intercept the synchrotron light at defined locations and to dissipate the heat. In addition, in an additional vacuum chamber, a light bundle of this radiation is first conducted away from the collision point and then absorbed further back. In this way, the sensitive particle detector was kept free of the synchrotron radiation and the secondary particles that may occur in the absorber.

All this led to a particularly challenging vacuum chamber design with linked tubes.

The accelerator vacuum system typically used different types of pumps: NEG pumps, ion getter pumps, and titanium sublimation pumps. In superconducting magnets, the 40 K cold vacuum chamber acts as a cryo-pump for some gas species. Varian's IGP-type pump used at HERA has a nominal suction capacity of 60 l/s at the connection flange.

NEG pumps are often integrated into the vacuum chamber of some magnets. IGP and TSP pumps are usually found in combination, with some ports not al-

[1] HERA=**H**adron-**E**lektron-**R**ing-**A**nlage

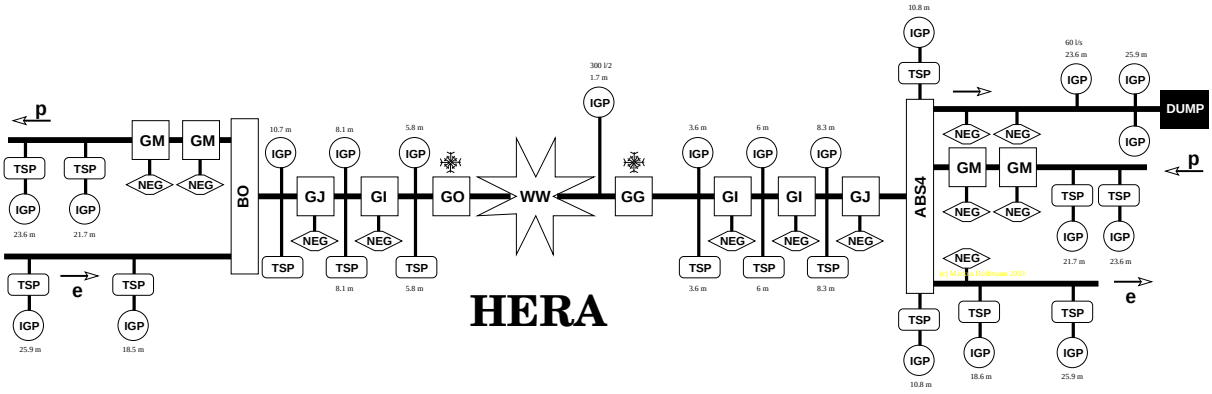

Figure 3.1: The vacuum system at HERA near the interaction zones.

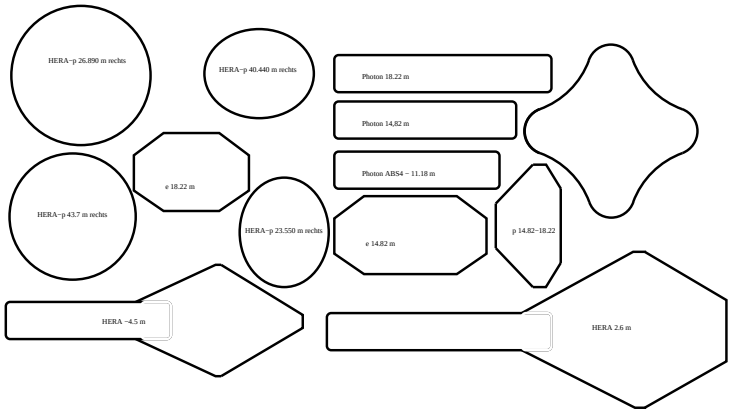

Figure 3.2: Tube profiles used at HERA.

lowing both pumps to be connected directly to the vacuum chamber. Here the pumps are connected in series. The pressure can be measured on each IGP pump. The structure of the vacuum system at the interaction zones at HERA is shown in Fig. 3.1.

The vacuum chambers used had different, sometimes quite complicated cross-sections. Very common were circular and elliptical profiles, also rectangular ones, keyhole and butterfly shapes. Also octagons, heptagons and various tapered transitions could be found (see Fig. 3.2).

The vacuum components consisted mainly of stainless steel, copper, aluminum and an AlBe (aluminum and beryllium) alloy. Tungsten was used in the beam collimators. Unfortunately, on the bellows of the cold magnets, brass studs have been installed which strongly outgas zinc at elevated temperatures.

The topology of the vacuum system consists of several interconnected vacuum chambers. The electron and proton tubes unite on the left side and on the right

side the chamber divides into three tubes: electron tube, proton tube and a tube for the synchrotron radiation, at the end of which there is an absorber (see Fig. 3.1).

This vacuum chamber topology will be used below as an example configuration for the VACLINE and CALCVAC programs.

4 VACLINE AND CALCVAC

The command line utility (VACLINE) was originally developed by Mike Seidel and relied on M. Sullivan's method described in [6, 7]. The version 2 of the program was improved by a more stable solution algorithm (the singular value decomposition), and supplemented by the possibilities to define any number of additional boundary conditions (see below: BOUNDARY) (e.g. valves can be so realized), as well as networks (see below): LINK) between parts of the vacuum systems. Furthermore, minor extensions have been made in the syntax, so that more complex expressions can be used to calculate values.

By principle, VACLINE can only calculate one pressure profile for one gas species given the geometry and topology of the vacuum system. The specific outgassing rates, conductivities and pumping capacities of vacuum tubes of given shape and material must be calculated separately, if necessary by hand, and are required by VACLINE as input parameters.

In order to integrate these calculations and also to calculate several partial pressures of different gas species, the extension CALCVAC was created. CALCVAC does not require the outgassing rates, conductivities and specific pumping capacities of individual pipe sections as input parameters, but rather the material, pump type and geometry of the vacuum chamber. Corresponding formulas as mentioned in chapters above on conductivities, suction power and outgassing rates, temperature and molecular masses are incorporated.

CALCVAC takes care of the accounting for calculating mass spectra, partial pressure distributions and dynamic effects (events), e.g. the heating of TSP's or the deactivation of pumps. CALCVAC also generates the graphical representation of the profiles (where available together with gnuplot) and can also display measurements or adapt pressure profiles to given measurements, such as: to determine the pumping power of pumps. In addition, the pressure response matrix (see Appendix) can be calculated.

The port of CALCVAC for Android also provides a graphical user interface, so that you no longer have to work from the command line. In addition, a calculator for conductances is integrated.

In their original form, CALCVAC and VACLINE each read a configuration file, which must be created by the user. Internally, the Android version also works with configuration files, even if this is created via a more user-friendly interface and the user can put together his vacuum line interactively. The resulting file can still be

copied from the smartphone and can then be used in the command line version of CALCVAC on another computer.

4.1 The VACLINE configuration

A typical call to `VACLINE` looks like this:

```
vacline HERA.inf
```

The file `HERA.inf` contains the instructions. e.g.:

Example: HERA.inf

```
! first test file for vacuum calculations
TITLE, "HERA little example"
! common constants
! Outgasing rate for steel
 q0:=5.0e-12
! Outgasing rate for Cu
 q1:=2.0e-11
! pumping speeds
pabs0:=65.
! Now lattice definition
 Begin:   START, S0=-18.12, BOUNDARY(Q=0)
 End:     END, BOUNDARY(Q=0)

 !zusammengesetzt GM1L
 GM1L_s:   SECTION, L=0.30875, q=q0, W=8.5, A=1600
 GM1L_p:   SECTION, L=0.15,    q=q0, W=33,  A=1600, Ps=24/0.15
 GM1L:     LINE= (GM1L_s,GM1L_p,GM1L_s,GM1L_p,GM1L_s,GM1L_p,GM1L_s,GM1L_p,&
        GM1L_s,GM1L_p,GM1L_s,GM1L_p,GM1L_s,GM1L_p,GM1L_s)

Abs0:    SECTION, L=0.55, q=q0, W=15, A=1900, Ps=pabs0/Abs0.L
 GO:     SECTION, L=3.5,  q=q1, W=45, A=2300, Ps=pabs0/9
 MyLine:   LINE= (Begin, GM1L, Abs0,GO, GM1L, End)

USE, MyLine
```

The essential parts of the syntax are briefly described here:

4.1.1 Comments

Comments are marked by a ! or a # at the beginning of a line. Lines that have a & or a backslash as the last character are considered as one line along with the

following line.

4.1.2 Statements

Statements are comma separated lists, where the first part is the keyword and all following parts are parameters. Statements can be TITLE, USE or LINK.

4.1.3 TITLE

With TITLE a title for the project can be assigned. It appears in the graphical output and all files that are generated.

4.1.4 USE

With USE you tell VACLINE what vacuum system should be calculated. You can specify the name of the vacuum line (which you have defined somewhere in the configuration file). Only for this vacuum line calculations are made.

4.1.5 Lattice Definitions

Definitions have the form:

```
Name: keyword, parameters with more keywords
```

Each statement defines a typ of vacuum chamber. The Lattice definitions are used to build the vacuum line.

Keywords can be START, END, SECTION, MARKER or LINE=.

- SECTION –> Parameters: L,q,W,A[,Ps, Keyword: BOUNDARY()]
- LINE=(List)
- START –> Parameter S0[, Keyword BOUNDARY()]
- END [, BOUNDARY()]
- MARKER

START defines only the starting position for calculation of the pressure profile (in meters) and optionally a boundary condition for the start of the vacuum line.

SECTION defines an elementary part of the vacuum line with the following meanings:

- L – Length of the piece in meters [m],
- q – Area-specific outgassing rate of the material [mbar l/s /cm^2],
- W – Specific conductivity [l/s*m],
- A – Specific inner surface [cm^2/m] e.g. A=3400 means that if the pipe would be a tube with circular crosssection and a length of 1 m the diameter would be approximately 10 cm. ($\pi \cdot 10$ cm*1m/1m=3100cm^2/m).
- Ps – optional – specific pumping rate in l/s per meter.

The specific conductivities are strongly dependent on the geometry of the piece and can only be approximated. This must be done externally (and will be done later by tt CALCVAC).

`LINE` The LINE Statement defines a list of vaccum components addressed by their names. The list must be comma separated and surrounded by parenthesis.

`BOUNDARY` defines a boundary condition for the beginning of an element. A boundary condition for the pressure (P =) or for the gas flow (Q=) or both can be given.

`MARKER` defines only a marker and no real physical part of the vacuum line. It is often used to to address the end of an element, since the starting position of the element is addressed by default with the assigned names. E.g.:

```
Element: SECTION, L=3, q=..., W=..., A=..., BOUNDARY(Q=0)
Endflange: MARKER, BOUNDARY(P=1e-8)
SmallLine: LINE=(Element, Endflange)
```

Thus, a boundary condition can be defined at both ends of an element.

`END` is just a special marker and marks the end of the vacuum line.

4.1.6 Symbol assignments and expressions

A line can also contain a symbol assignment. In this case the line has the format:

```
Symbolname := expression
```

Symbol names once defined, can be used everywhere, where a regular expression can be used. They can be used to calculate more complicated values and may be used as macros to manage changes in parameter values.

:= assigns an expression to a symbolic variable that may use additional symbolic variables and numbers as well as the basic arithmetic operations.

These variables can then be used anywhere instead of numerical values. Furthermore, the following mathematical functions with their usual meaning are available (functions must be written in capital letters):

ABS(), ACOS(), ACOSH(), ASIN(), ASINH(), ATAN(), ATAN2(), ATANH(), ATN(), CBRT(), CEIL(), COS(), COSH(), EXP(), EXPM1(), FLOOR(), HYPOT(), LN(), LOG(), LOG10(), LOG1P(), LOGB(), MOD(), SIN(), SINH(), SQR(), SQRT(), TAN(), TANH().

4.1.7 Boundary conditions

The directive `BOUNDARY` defines a boundary condition for the beginning of an element. Here, a boundary condition for the pressure (`BOUNDARY(P=...)`) or for the gas flow (`BOUNDARY(Q=...)`) or for both (`BOUNDARY(P=...,Q=...)`) can be specified.

In the equation system, which calculates the starting pressures and gas flows at the inputs of the elements, one line is added per boundary condition.

This looks like this:

$$\begin{pmatrix} & \vdots & \\ 0 \ \dots & 1 & \dots \ 0 \\ & \vdots & \end{pmatrix} \cdot \vec{P} = \begin{pmatrix} \vdots \\ b \\ \vdots \end{pmatrix} \quad .$$

For a coherent vacuum line 2 boundary conditions are necessary. If the vacuum line breaks down into two (for example because a poorly conductive element has been installed), more boundary conditions are needed. If a ring system is built with the LINK command, no further boundary conditions are required as a periodic system is created. If too many constraints are specified, `VACLINE` tries to find a solution that comes closest to the boundary conditions. If too few boundary conditions are specified, the solution is the one with the lowest local gas flows.

4.1.8 Meshed networks

With the special LINK command, the inputs of various elements of the vacuum line can be additionally interconnected. For example, you can reconnect the end of a line to its beginning and thus get periodic boundary conditions, or you can link several parts of the same line, (which are maybe separated by a valve or a poorly conductive or deliberately non-conductive section).

An example:

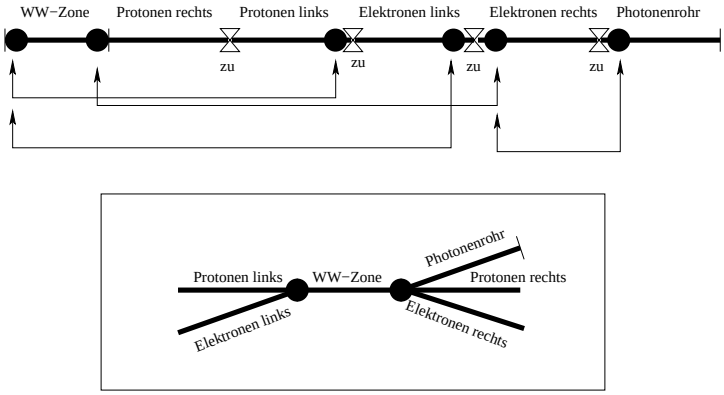

Figure 4.1: Topology of the HERA vacuum chambers in the interaction regions and how it can be realized as a linear vacuum line with closed valves and additional links to form a star shaped network.

```
! VALVE defines a poorly conducting element
VALVE: SECTION, L=0.05, q=0, W=0.0001, A=3100, BOUNDARY(Q=0)
ELine:   LINE=(...)
PhotonLine: LINE=(...)
PLine:   LINE= (Begin, ... ,GJR,Abs4,GM1,GM2,PM0,VALVE,ELine,VALVE, \
               PhotonLine,End)
LINK, Abs4, PhotonLine
LINK, Abs4, ELineR
USE, PLine
```

The `ELine` and the `PhotonLine` are integrated into the `P-Line` but separated by the element `VALVE`, thus decoupled from each other. Then the pieces are all connected with each other at the element `Abs4`. The result is a star-shaped topology (see Fig. 4.1).

4.1.9 Subtleties of the syntax

Multiplicities in line Not to mention the possibility to easily build vacuumlines from many identical pieces. There is the possibility to use multiplies in the definition of a LINE:

```
a: SECTION, L=2,   q=q0, W=99, A=2600
b: SECTION, L=0.2, q=q0, W=99, A=2600, Ps=200
c: SECTION, L=2,   q=q0, W=99, A=2600

MyLine:   LINE= (Begin,a,10*b,c,End)
```

In the above example, MyLine is composed of one piece a, ten pieces b and one piece c. This should produce the same result as if at b instead of 0.2 m we would define 2 m. This may be useful if you need intermediate values for pressure or medium pressure in the Twiss files.

Hints for Syntax

- USE must be capitalized (as well as TITLE).

increment There are two command line options to set the step size for the calculations:

- `-r 0.01` would set 1 cm as the smallest increment. or:
- `-n 1000` subdivides the vacuum line into at most 1000 points.

By the way, the program calculates the step size as

$$\Delta_z = \max(r, \frac{z_{\text{end}} - z_0}{n-1}) \quad .$$

If you specify nothing, 0.001 is used as -r and 2048 as -n, ie at most 2048 points and not finer than 1mm.

Hints for the Structure of the configuration

- Boundary conditions apply to the end of an element, LINK refers to the beginning of the two linked elements.
- The message "Too many boundary conditions" is not an error message, but only an indication that the system is over-determined. Here it is worthwhile to take a look at the value that appears under acuracy. If this is too low you should be mistrusting the calculation. Especially in underdetermined systems, the value decreases, or if the equation system has a larger core.
- There can be only one START element and only one END element. The specification of a second starting position is impossible. If you want to calculate a branch, you have to put the three parts (A, B.C, A branched in B and C) in a row

  ```
  START -  A -a- B -b- C - END
  ```

  Between B and C then set a closed valve and set a link from a to b.
  You can then set the boundary conditions (presumably Q=0) for START, END and the valve. It is important that the link always starts at the front of the element and the boundary condition at the back.

4.1.10 Output files with results

VACLINE produces a .dat file with the results (pressure profile) and optionally another, so-called twiss file (with all individual components and their properties).

The .dat output file contains a table in ASCII format, with columns separated by white space.

From the starting position of the USE-specified vacuum line to its final position, up to 3072 lines[1] with the following information in the columns are produced:

1. Position in meters,
2. Pressure in mbar,
3. Gas flow in mbar l/s,
4. Conductivity in l m/s,
5. specific outgasing rate in mbar l/s m, and
6. specific suction power in l s/m.

The file format is designed to be easily transformed into a graphical form with `gnuplot`.

4.1.11 Command line parameters

VACLINE can be called with some parameters from the shell.

-h or `--help` prints out a brief description of the possible Command line parameters.

-v be more verbose (provides additional information about the program flow, mainly useful for troubleshooting).

-q be more quiet: Apart from error messages, nothing is output to the console.

-o <filename> place output into file: The output of the print data is output to the file <filename>. If this is not specified, the default file name is output.dat.

–twiss <filename> place twiss output into file: Returns additional information about the used elements in the form of a list in the specified file.

-n or `--nplot <number>` specify maximum number of output points. default: 3074

-r or `--resolution <number>` specify resolution in meters. default: 0.001 m

[1] The finest position resolution here is 1 mm, but can be changed with commandline parameters to VACLINE.

4.1.12 Twiss files

The Twiss files have the following structure:

A table in ASCII format, with columns separated by white space. For each element of the USE-specified vacuum line, one row each with the following information is output in the columns:

1. Name of the elements,
2. Starting position of the element in meters,
3. Length of the element in meters,
4. Pressure at the end of the element in mbar,
5. Gas flow at the end of the element in mbar l/s,
6. Conductivity of the element in l m/s,
7. Outgasing rate of the element in mbar l/s m,
8. Suction power of the pump in l s/m,
9. Average Pressure inside the element in mbar, and
10. Inner surface of the element in cm^2.

4.2 The CALCVAC configuration

`CALCVAC` is an extension for `VACLINE` with the following main features:

- Calculation of outgassing rates, specific Conductivities and inner surfaces for rectangular, circular and elliptical chambers (and for HERA especially for the keyhole chamber) from simple geometry values such as diameter or side lengths and the material type;
- consideration of different gas species,
- consideration of different chamber temperatures,
- graphical output of profiles and gas spectra,
- various comparative calculations are possible.

CALCVAC is available both in a command line version for Linux and WINDOWS, as well as with a graphical user interface for the operating system Android. In all cases, CALCVAC also reads the configuration from an input file. Users of the Android version of CALCVAC do not necessarily get to see them. The CALCVAC configuration files have the extension .vac to distinguish them from those for VACLINE.

The typical call from the console (command line) looks like this:

```
calcvac --use ZEUS input.vac
```

With `--use ZEUS` it is determined that the profile is calculated and output only for the interaction zone in the south of HERA. With the `--use` command line parameter, the command USE can be overwritten from the configuration file. It is therefore a bit more flexible. However, the use of command line parameters is not necessary. All settings and commands can be specified in the configuration file. Since the command line parameters also differ in the different versions of CALCVAC, their use is generally discouraged and therefore will not be discussed further.

The structure of `input.vac` is a bit more complicated than the `VACLINE` configuration file.

4.2.1 Comments

Comments are initiated with # at the beginning of a line.

4.2.2 Sections

The file consists of the 7 sections:

- `[general]`
- `[pumping]`
- `[outgasing]`
- `[lattice]`
- `[events]`
- `[plot]` and
- `[measurements]`.

Only the section `[lattice]` is mandatory. But without the sections `[pumping]` and/or `[outgasing]` the functionallity of CALCVAC reduces to thouse of VACLINE.

`[general]` In this section general parameters are defined. So far, you can only specify the title of the project here. It also appears as a headline in the graphical outputs of CALCVAC. (And since version 2.01, you can also specify the molecule mass numbers of the gas types that you want to calculate. So far, these are only the gases H2, CH4, and CO.)

```
# HERA.VAC    Settings for vacline and calcvac (c) Mike Seidel + Markus Hoffmann
#
# last modified: 18.03.2003   MH
#
[general]

#
# This is the overal HERA-Interaction Vacuum Geometry file
#
#

TITLE="Events taken on Nov.28 2002"
```

Note that the lines have sligtly different format to thouse used in VACLINE.

`[pumping]` In this section, the pumping rates of different pumps are defined in a kind of table. For example:

```
[pumping]
# specific pumpung speeds (l/s/m) or
# relative pumping speeds compared to nitrogen-equivalent

cold: 0(default)   0(2)  20(16) 30(28)
tsp:  0(default)   1(2)   0(16)  1(28)
neg:  0(default) 1.6(2)   0(16)  1(28)
igp:  0(default)   2(2) 0.6(16)  1(28)
```

Each type of pump gets a name followed by a colon. Then follows a space-separated list of values which have the form `value(molecular mass)`. In parentheses without spaces directly behind the value the molecular weight. The values denote the specific pumping capacity in l/s/m or merely a relative factor related to the pumping rate which is defined with the parameter `SPEED` (see below).

The molecular masses can be specified using only positive integers. The molecular mass 0 or `default` indicates the value taken if no specific pumping rate has been defined for one gas type, i.e. for all other gas species not specified here.

`[outgasing]` In this section the outgassing rates of different materials are defined. In addition, the exhaust spectrum for the actions for e.g. pump heating and synchrotron light heating can be defined here. For example:

```
# Material specific  outgasing rates for calcvac
[outgasing]
# Unit: mbar l/s /cm^2

steel:   0(default)  1.0e-12(2)        0(16)   5e-13(28)
wolfram: 0(default)  1.0e-12(2)        0(16)   5e-13(28)
Cu:      0(default)  1.0e-12(2)        0(16)   1e-12(28)
Al:      0(default)  2.0e-12(2)   1e-13(16)  20e-12(28)
AlBe:    0(default)  2.0e-12(2)   1e-13(16)  20e-12(28)
cold:    0(default)  1.0e-13(2)        0(16)        0(28)
neg:     0(default)         0(2)   8e-14(16)        0(28)
tspheat: 0(default) 5800e-11(2) 5.8e-11(16) 5.8e-11(28)
heating: 0(default)    4e-11(2) 0.7e-11(16)   6e-11(28)
syli:    0(default)    1e-11(2) 0.8e-11(16)   8e-11(28)
```

The unit for the outgassing rates is mbar l/s/cm^2 and the format of the lines is the same as described above for the pumping rates.

`[lattice]` In the `[lattice]` section very similarly to the configuration file for VACLINE the individual components of the vacuum lines are defined and assembled.
Like for VACLINE, definitions have the form:

```
Name: keyword, parameters with more keywords
```

Each statement defines a typ of vacuum chamber. The Lattice definitions are used to build the vacuum line.
Keywords can be START, END, SECTION, MARKER or LINE=, same as in VACLINE, but the syntax for CALCVAC is extended by a few types and key words: Keywords in CALCVAC can in addition be: TUBE and PUMP.

- `SECTION` –> Parameters: L,q,W,A[,Ps, Keyword: `BOUNDARY()`]
- `TUBE` –> Parameters: L,Mat,Form[,T,Keyword: `BOUNDARY()`]
- `PUMP` –> Parameters: L,Mat,Form,Ptyp,Speed[,T,Keyword: `BOUNDARY()`]
- `LINE=(`List`)`
- `START` –> Parameter S0[, Keyword `BOUNDARY()`]
- `END` [, `BOUNDARY()`]
- `MARKER`

`START` defines only the starting position for calculation of the pressure profile (in meters) and optionally a boundary condition for the start of the vacuum line.

`TUBE` defines a vacuum tube with the following parameters:

- L – Length of the piece in meters [m],
- Mat – specifies the material as defined in the outgasing section,
- Form – specifies the geometry of the tube. Form specifies the form of the crossection and can be:
  - square
  - rect
  - circ
  - ellipt
  - schluesselloch .

  square takes a parameter a in meters for the side length of the sqare cross section, rect takes two parameters a and b as lengths in meter for each of the sides, circ takes a parameter d for the (inner) diameter in meters, ellipt takes parameters a and b for both of the diameters in meters, schluesselloch takes parameters a,b,c and d.
- T – Temperature of the chamber in [K],

`PUMP` defines a vacuum tube with integrated vacuum pump with the following parameters:

- L – Length of the piece in meters [m],
- Mat – specifies the material as defined in the outgasing section,
- Form – specifies the geometry of the tube. Form specifies the form of the crossection and can be square, rect, circ, ellipt and schluesselloch, defined with the same parameters as already desscribed for the TUBE section.
- Ptyp – specifies the pump type as defined in the pumping section,
- Speed – defines the (specific) pumping speed either in l/s/m or as a factor.
- T – Temperature of the chamber in [K],

`SECTION` defines an elementary part of the vacuum line with the following meanings:

- L – Length of the piece in meters [m],
- q – Area-specific outgassing rate of the material [mbar l/s /cm^2],
- W – Specific conductivity [l/s*m],
- A – Specific inner surface [cm^2/m] e.g. A=3400 means that if the pipe would be a tube with circular crosssection and a length of 1 m the diameter would be approximately 10 cm. ($\pi \cdot 10$ cm*1m/1m=3100cm^2/m).
- Ps – optional – specific pumping rate in l/s per meter.

`LINE` The LINE Statement defines a list of vaccum components addressed by their names. The list must be comma separated and surrounded by parenthesis.

`BOUNDARY` defines a boundary condition for the beginning of an element. A boundary condition for the pressure (P =) or for the gas flow (Q=) or both can be given.

`MARKER` defines only a marker and no real physical part of the vacuum line. It is often used to to address the end of an element, since the starting position of the element is addressed by default with the assigned names.

`END` is just a special marker and marks the end of the vacuum line.

`[events]` The `|[events]|`section is optional and has a special function if it exists.
In each line an event can be defined. The structure of the lines is again:

```
Name: action=, comment=""
```

For the action parameter, none, heat(x), syli(x) or off can be specified. Where:

none no action,

heat(x) heating out a pump whereby the outgas rate of the affected elements is increased by a factor of x.

syli(x) Irradiate a vacuum tube. The outgas rate of the affected elements is increased by a factor of x.

off switching off a pump. The pumping power of the affected elements is set to 0.

Optionally, you can enter a comment after each action, which is used as a caption in the corresponding plot.

`[plot]` In this section additional gnuplot commands can be inserted to modify the graphical output. The most useful application of this is to specify a range for the plot:

```
[plot]
# Plot kommandos (passed to gnuplot)
set grid
set xrange [-10:30]
```

`[measurements]` In this section pressure measurement values can be stored to which a fit calculation can be performed.

4.2.3 Boundary conditions

Boundary conditions work the same as already described for the VACLINE configuration file format.

4.2.4 Meshed networks

Meshed networks work the same as already described for the VACLINE configuration file format. The only difference is the syntax of the LINK command: there is no comma used after LINK.

4.2.5 Symbol assignments and expressions

You can use symbols and mathematical expressions in exacly the same way as for VACLINE.

4.2.6 USE

USE works the same as for `VACLINE`. The only difference is the syntax of the USE command: there is no comma used after USE.

4.2.7 Output files

The produced output .dat files habe exactly the same format as the VACLINE files. The only difference is that multiple files are produced, for each gas species one. The molecular mass is then part of the file name.

4.2.8 An example: Calculation of the pressure in the arcs of HERA-e

The FODO unit cell of HERA-e in the arcs is quite simple:

Corrector magnet, quadrupole, short sextupole, dipole, correction magnet, correction magnet, quadrupole, long sextupol, IGP pump, dipole. The vacuum chamber consists entirely of the octagonal standard profile. NEG pumps are integrated in the vacuum chamber of the dipoles. Although there is an integrated getter pump in the quadrupole and sextupole common chamber, it is not connected. Varian's IGP pump has a suction capacity of 60 l/s with a 100 mm diameter connection.

The complete configuration file for CALCVAC then would looks like this:

```
# Zum Berechnen des Drucks im HERA-e Bogen
# Last modified: 10.05.2003   MH
#
[general]

#
# This is the overal HERA-Interaction Vacuum Geometry file
#
# Specify a title:

TITLE="HERA-e Bogen"

# Specify the list of gas species to calculate for:

SPECIES=(2,16,28)

[pumping]
# specific pumpung speeds (l/s/m) or
# relative pumping speeds compared to nitrogen-equivalent

cold: 0(default)   0(2)  20(16) 30(28)
tsp:  0(default)   1(2)   0(16)  1(28)
neg:  0(default) 1.6(2)   0(16)  1(28)
igp:  0(default)   2(2) 0.6(16)  1(28)


# Materialspezifische Ausgasraten fuer calcvac
[outgasing]
# Unit: mbar l/s /cm^2

steel:     0(default) 1.0e-12(2)  0(16)   5e-13(28)
wolfram:    0(default) 1.0e-12(2)  0(16)   5e-13(28)
Cu:     0(default) 1.0e-12(2)  0(16)   1e-12(28)
Al:     0(default) 2.0e-12(2)  1e-13(16)   20e-12(28)
AlBe:     0(default) 2.0e-12(2)  1e-13(16)   20e-12(28)
cold:     0(default) 1.0e-13(2)  0(16)       0(28)
neg:     0(default)       0(2)   8e-14(16)       0(28)
tspheat:    0(default)   5800e-11(2)   5.8e-11(16)   5.8e-11(28)
heating:    0(default)   4e-11(2) 0.7e-11(16)   6e-11(28)
syli:     0(default)   1e-11(2) 0.8e-11(16)   8e-11(28)

##############################################################################
# lattice section. Here the lattice of all beamlines are defined
#
[lattice]
#
```

```
# Here all components are defined
#
# PUMP:   L,MAT,FORM,TYP,SPEED= [, T=temperature in K]
# TUBE:   L,MAT,FORM [, T=temperature in K]
# FORM=circ   d=diameter
# FORM=ellipt a,b=diameters
# FORM=square a=side length
# FORM=rect   a,b=side lengths
# FORM=schluesselloch  a,b=central diameter, c,d=side lengths of the photon tube

Begin:   START, S0=0

# This will be used to separate Vacuum systems

VENTIL: SECTION, L=0.03, q=0, W=0.0001, A=3100, BOUNDARY(Q=0)

# definitions for corrector vaccum chambers
ks1:   TUBE, L=0.600, mat=Cu, form=ellipt, a=0.1, b=0.05
ks2:   TUBE, L=1.100, mat=Cu, form=ellipt, a=0.1, b=0.05
# for quadrupoles and sextupoles
QS1:   TUBE, L=1.500, mat=Cu, form=ellipt, a=0.1, b=0.05
QS2:   TUBE, L=2.000, mat=Cu, form=ellipt, a=0.1, b=0.05
# Dipol
DIP_A: TUBE, L=0.0925, mat=Cu, form=ellipt, a=0.1, b=0.05
DIP_P: PUMP, L=9.000, mat=Cu, form=ellipt, a=0.1, b=0.05, typ=neg, speed=495
DIP:   LINE=(DIP_A,DIP_P,DIP_A)

VARIAN: PUMP, L=0.1, mat=steel, form=circ, d=0.1, typ=igp, speed=60

End:  END

LINK, Begin, VENTIL

Bogenline: LINE= (Begin,KS1,QS1,DIP,KS2,QS2,VARIAN,DIP,VENTIL,End)

USE Bogenline

#########################################################################
[events]
#
# Define Events
# action can be: none,heat,syli,off
# In parenthesis the strength of the action
#
Z0:  action=none,        comment="normal"
Z1:  action=heat(1.8),   comment="TSP heated"

[plot]
```

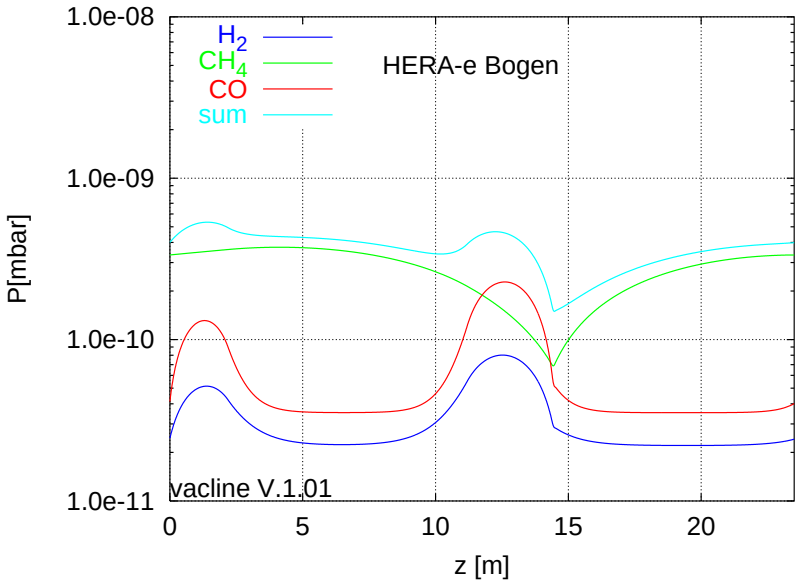

Figure 4.2: Pressure curve for different gas species in a unit cell of the arcs in HERA-e. This piece was calculated with periodic boundary conditions.

```
# Plot commands (passed to gnuplot)
set grid
set xrange [0:23]

[measurements]
# to be added to the plot
% Pos      H0         H1       H2       H3  Event 3    Event 5 Base 2
 -5.8   6.91e-11 6.91e-11 6.91e-11 2.84e-9  6.91e-11    8.1e-10 6.91e-11
```

The calculated results are ploted with gnuplot resulting in fig. 4.2.

5 Calcvac for Android

Because the code is still occasionally used to design vacuum configurations on new beamlines and to simulate pressure profiles where no measurement is available, it was ported to an up-to-date computing platform: Android phones and tablets. This aims to make the usage more easy and user friendly. The original commandline interface as used on ancient UNIX workstations, Linux and also the WINDOWS version of Calcvac, was kept for compatibility reasons, but in addition an interective user interface was added, where the vacuum line designer can build his pumping concept on the fly.

5.1 Installation

The Android version of Calcvac comes as a regular app and can be dowloaded from the app store or from the Calcvac homepage. You will get an .apk file, which can be installed on the Android device.

Files and data are stored on the devoce in a folder called calcvac. You can access this folder with any file explorer on the device. There you will find the output data from the pressure calculations. You can copy or send them to other computers for further processing if you wish.

Also if you have .inf or .vac files already you want to process, just copy them into the calcvac folder and the Calcvac app will find them.

5.2 Usage

After having started the app, you are supposed to select a file (or choose "New" in the menu), and run the pressure calculation (with "Run" in the menu).

The pressure profile is then immedeately shown in the plot in the middle and potential errors and warnings will be shown, if there are any as in fig. 5.1.

The results are now already stored in the formerly mentioned calcvac folder.

But the app offers several possibilities to look at them: With menu –> "plotting tool" you can have a closer look at the details of the plot. You can move around and zoom in and out to see the details of the pressure profile and gas flows.

If you want to have a look at the twiss parameters of the elements, select the "table tool" from the menu.

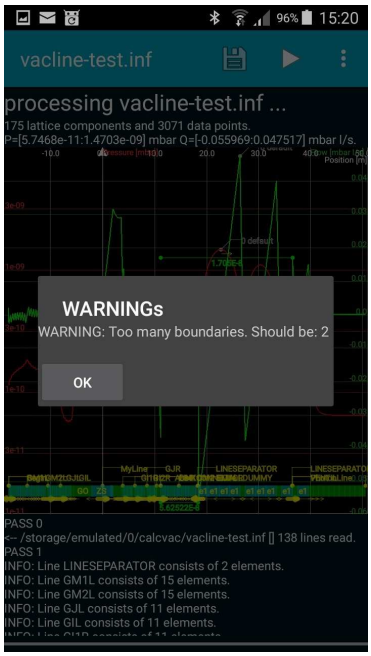

Figure 5.1: After calculation of a vacuum configuration.

Now, you probably want to change the configuration or start from scratch (Menu –> New) to design you own vaccum system.

After having selected "New" from the menu, (if not already exists) a new file is created called "new.vac". In this newly created file, three pump types and three materials are already predefined, as well as two vacuum sections. But starting from this you can edit and change everything.

The whole menu structure looks like this:

1. Load file ...
2. Run calculation
3. About
4. Info/settings
5. component editor ...
   (a) Help
   (b) add component ...
   (c) file editor
   (d) add marker ...
   (e) add symbol ...
   (f) add vakuum line ...
   (g) Pumps
      i. Help

   ii. add new pump type ...
   iii. select from database
   iv. define molecule spectrum
(h) Material
   i. Help
   ii. add new material ...
   iii. select from database
   iv. define molecule spectrum
(i) Links ...
   i. Help
   ii. add Link ...
   iii. exit link editor
(j) File info...
(k) exit component editor

6. File editor
7. New
8. Help...
9. Plot tool ...
10. Table tool ...
11. Statistics
12. Conductivity calculator ...
13. Quit programm

All program parts should be reasonably self-explanatory. Mostly there is also a built-in help page or information that can be displayed.

6 Conclusion

Although originally developed for HERA, the program package CALCVAC/VACLINE described here has also proven itself for other projects. In a relatively simple manner, a useful pressure profile can be calculated in elongate vacuum systems. The accuracy is sufficient to calculate and design common vacuum systems. The number of required pumps, their type and distance can be optimized.

The newly ported version for Android shows that it is possible to revive older programs for the calculation and simulation of accelerator physical issues.

With the possibilities of the user-friendly Platform Android, a new group of users may possibly be addressed. Instead of the command-line-oriented operation and the ASCII file-oriented configuration, the resulting App for Android allows a user-friendly graphical operation with finger gestures and the use of the smartphone on the go.

A INTERESTING CONCEPTS

The calculation of one-dimensional pressure profiles in long tube systems uses methods that are common and practical in electrical engineering or accelerator physics. Many concepts in these areas can thus be transferred in a completely analogous way, for example, those of the optical functions.

For example, for a one-dimensional periodic system, the periodic solution of the homogeneous part of the equation (2.5) can be constructed using a Greens function (see [2]).

In an analogous way, even a beta function $\beta(x)$ can be defined.

A.1 The Pressure Response Matrix

By analogy with the orbit-response matrix customary in accelerator physics, a *Pressure Response Matrix* (PRM) can be set up in a similar way with enough pressure gauges in the vacuum system. Among other things, the matrix can be measured directly on the real vacuum system, and thus one obtains a direct comparison to the design model.

Suppose there are n gauges in the vacuum system that show the pressures P_i. And suppose there were m possible sources of gas load, which can be represented by the outgassing rates Q_j.

The pressure increases $\delta\vec{P}$ at all measuring points, caused by a change in the outgassing rates $\Delta\vec{Q}$, can then be determined using the PRM:

$$\Delta\vec{P} = M\Delta\vec{Q} \quad .$$

The definition of the *Pressure Response Matrix (PRM)* is generally:

$$M = \begin{pmatrix} \frac{dP_1}{dQ_1} & \frac{dP_1}{dQ_2} & \cdots & \frac{dP_1}{dQ_m} \\ \frac{dP_2}{dQ_1} & \frac{dP_2}{dQ_2} & \cdots & \frac{dP_2}{dQ_m} \\ \vdots & & \ddots & \vdots \\ \frac{dP_n}{dQ_1} & \frac{dP_n}{dQ_2} & \cdots & \frac{dP_n}{dQ_m} \end{pmatrix}$$

It is not necessarily square.

If the PRM were quadratic (and not singular), one could infer with its inverse also from (possibly measured) pressure increases on possibly existing additional gas loads (eg leaks or synchrotron light desorption).

$$\Delta\vec{Q} = M^{-1}\Delta\vec{P} \quad .$$

However, in most cases the PRM is highly non-square, since there are many more sites with potential outgassing than pressure gauges.

In the case of non-square and / or singular matrices, the singular value decomposition (SVD) can be used for meaningful inversion of the matrix. $M^{-1}\Delta\vec{P}$ then gives the vector of outgassing rates from all possible solutions of the multidimensional solution space, which assumes that the rates are distributed as evenly as possible over many locations.

The eigenvalue spectrum of the PRM

When properly set up, the PRM incorporates all the measurable features of the vacuum system. It can be easily measure with the help of e.g. pump heating experiments or even be calculated using the vacuum model and the programs for pressure profile calculation.

Some features are not immediately obvious. Suppose we find a vector $\Delta\vec{Q}$ for which:

$$\Delta\vec{P} = M\Delta\vec{Q} = \lambda\Delta\vec{Q} \quad .$$

Let us first consider the case $\lambda = 0$. If we have found a vector $\Delta\vec{Q}$ that is different from $\vec{0}$, it is probable that its components are partly positive and partly negative. Negative outgasing rates can only be realized by pumping. This vector now states that there are certain places where gas can outgas, which can be compensated for with certain additional pumping powers at other locations without seeing a difference in pressure at the measuring points. (Of course, the pressure at the unobserved sites may well change.)

If there are other eigenvalues $\lambda \neq 0$ (which, if present, should all be positive), this may give an indication that the vacuum system is falling apart into several independent parts.

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