Pressure Profile Calculations by the Finite Element Method

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§1. The Method

For a complicated vacuum system such as one like CESR, it is very difficult, if possible, to calculate the pressure profile analytically. The finite element method is therefore widely adopted to calculate the pressure distributions in large complicated vacuum systems. In this method, the CESR vacuum system is divided to n elements. The length of each element is small enough that the pressure can be consider uniform in the element. At equilibrium condition, the net mass flow for all elements should be zero. At equilibrium condition, as explained by figure 1, one can easily write the pressure equations as :

$$C_i(P_{i-1} - P_i) + C_{i+1}(P_{i+1} - P_i) + Q_i = S_i P_i \qquad \text{(i=1, 2, ... ,n)} \qquad (1)$$

where C_i and C_{i+1} are the gas conductance between element *i* and *i-1* and between element *i* and *i+1*, respectively; Q_i is the gas load (thermal or/and SR-induced desorption, etc.) of element *i*, and S_i is the pumping speed of element *i*. Molecular flow condition is also assumed throughout this note.

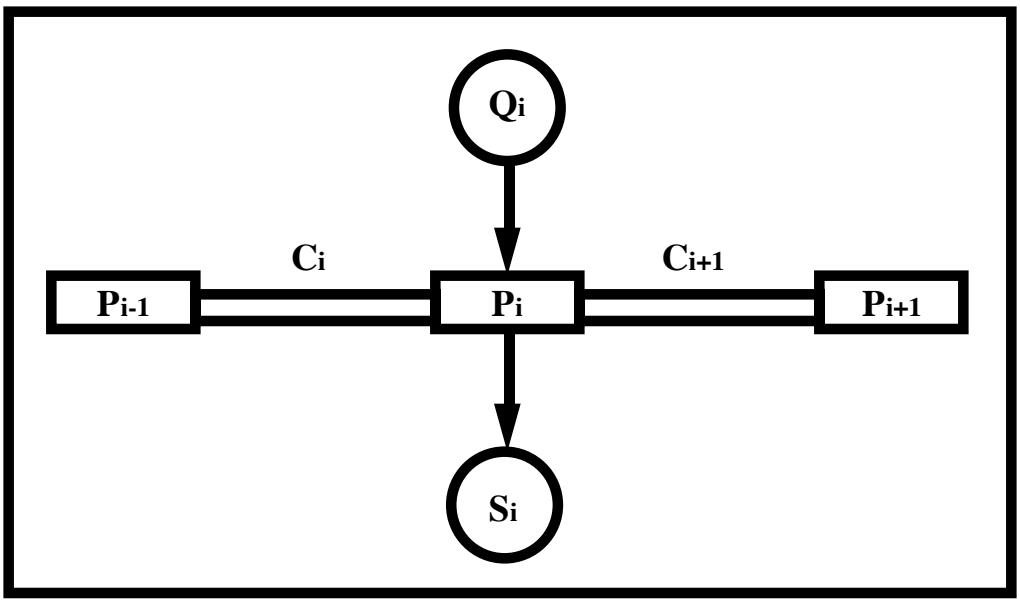

Figure 1 Finite-element method

The pressure profile of the whole vacuum system can be obtained by solving the equations (1) with proper boundary conditions.

§2. Boundary Conditions

Certain boundary conditions should be defined, by the physical situation, in order to solve the pressure equations (1). Three kinds of boundary conditions are given below.

§2.1 Periodic boundary condition

$$P_0 = P_n \tag{2a}$$

$$P_{n+1} = P_1 \tag{2b}$$

Substituting eqs.(2) into eqs. (1), eqs.(1) become

$$C_1(P_n - P_1) + C_2(P_2 - P_1) + Q_1 = S_1 P_1 \tag{3a}$$

$$C_i(P_{i-1} - P_i) + C_{i+1}(P_{i+1} - P_i) + Q_i = S_i P_i \qquad (i=2,3, \ldots, n-1) \tag{3b}$$

$$C_n(P_{n-1} - P_n) + C_1(P_1 - P_n) + Q_n = S_n P_n \tag{3c}$$

§2.2 Smooth boundary condition

$$P_0 = P_1 \tag{4a}$$

$$P_{n+1} = P_n \tag{4b}$$

Substituting eqs.(4) into eqs. (1), eqs.(1) become

$$C_2(P_2 - P_1) + Q_1 = S_1 P_1 \tag{5a}$$

$$C_i(P_{i-1} - P_i) + C_{i+1}(P_{i+1} - P_i) + Q_i = S_i P_i \qquad (i=2,3, \ldots, n-1) \tag{5b}$$

$$C_n(P_{n-1} - P_n) + Q_n = S_n P_n \tag{5c}$$

§2.3 Fixed boundary condition

Set the pressures of the elements at both ends of the system to known values. Eqs.(1) become

$$-C_1 P_1 + C_2(P_2 - P_1) + (Q_1 + C_1 P_0) = S_1 P_1 \tag{6a}$$

$$C_i(P_{i-1} - P_i) + C_{i+1}(P_{i+1} - P_i) + Q_i = S_i P_i \qquad (i=2,3, \ldots, n-1) \tag{6b}$$

$$C_n(P_{n-1} - P_n) - C_{n+1} P_n + (Q_n + C_{n+1} P_{n+1}) = S_n P_n \tag{6c}$$

The periodic boundary condition should be used when (1) the vacuum system under consideration consists of periodic structures and eqs.(1) describes one of the base unit of the periodic system, or (2) eqs.(1) describes a closed vacuum system such as the entire CESR vacuum system.

The fixed boundary condition applies when the pressures at the ends (i.e. P_0 and P_{n+1}) of the system under consideration can be directly measured.

When the vacuum system under consideration does not meet the above two situations, the smooth boundary condition can be used as an approximation. The smooth boundary condition

works best when the pressure changes smoothly at the ends of the system, or the size of the elements is very small.

§3. Calculation of the Pressure Profile by Iteration Method

Eqs. (3), (5), and (6) can be rewritten as followings.

§3.1 The periodic boundary condition

$$P_1 = \frac{1}{C_1 + C_2 + S_1}(C_1 P_n + C_2 P_2 + Q_1) \tag{7a}$$

$$P_i = \frac{1}{C_i + C_{i+1} + S_i}(C_i P_{i-1} + C_{i+1} P_{i+1} + Q_i) \tag{7b}$$

$$P_n = \frac{1}{C_1 + C_n + S_n}(C_1 P_1 + C_n P_{n-1} + Q_n) \tag{7c}$$

§3.2 The smooth boundary condition

$$P_1 = \frac{1}{C_2 + S_1}(C_2 P_2 + Q_1) \tag{8a}$$

$$P_i = \frac{1}{C_i + C_{i+1} + S_i}(C_i P_{i-1} + C_{i+1} P_{i+1} + Q_i) \tag{8b}$$

$$P_n = \frac{1}{C_n + S_n}(C_n P_{n-1} + Q_n) \tag{8c}$$

§3.3 The fixed boundary condition

$$P_1 = \frac{1}{C_1 + C_2 + S_1}(C_2 P_2 + (Q_1 + C_1 P_0)) \tag{9a}$$

$$P_i = \frac{1}{C_i + C_{i+1} + S_i}(C_i P_{i-1} + C_{i+1} P_{i+1} + Q_i) \tag{9b}$$

$$P_n = \frac{1}{C_1 + C_n + S_n}(C_n P_{n-1} + (Q_n + C_1 P_{n+1})) \tag{9c}$$

In the iteration method, one can compute a new set of pressures, P_i^{new} (i=1,2,...,n), using eqs. (7), or (8), or (9) with an old set of pressure, P_i^{old}(i=1,2,...,n) on the right side of the equations. Then the newly calculated values are used to calculate another set of pressures. The procedure is repeated until the P_i^{new} (i=1,2,...,n) converge to P_i^{old} (i=1,2,...,n) with the required accuracy.

§4. Calculation of the Pressure Profile by Solving Linear Equations

§4.1 Smooth and fixed boundary conditions

For the cases of smooth and fixed boundary conditions, the pressure equations can rewritten as,

$$P_1 + b_1 P_2 = d_1 \tag{10-1}$$
$$a_2 P_1 + P_2 + b_2 P_3 = d_2 \tag{10-2}$$
$$a_3 P_2 + P_3 + b_3 P_4 = d_3 \tag{10-3}$$
... ...
$$a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \tag{10-i}$$
... ...
$$a_{n-1} P_{n-2} + P_{n-1} + b_{n-1} P_n = d_{n-1} \tag{10-(n-1)}$$
$$a_n P_{n-1} + P_n = d_n \tag{10-n}$$

where

$$\begin{cases} a_i = -C_i/(C_i + C_{i+1} + S_i) \\ b_i = -C_{i+1}/(C_i + C_{i+1} + S_i) \\ d_i = Q_i/(C_i + C_{i+1} + S_i) \end{cases} \quad \text{(i=2,3,...,n-1)} \tag{11}$$

and for the smooth boundary condition

$$\begin{cases} a_1 = 0 \\ b_1 = -C_2/(C_2 + S_1) \\ d_1 = Q_1/(C_2 + S_1) \end{cases} \tag{12a}$$

$$\begin{cases} a_n = -C_n/(C_n + S_n) \\ b_n = 0 \\ d_n = Q_n/(C_n + S_n) \end{cases} \tag{12b}$$

or for the fixed boundary condition

$$\begin{cases} a_1 = 0 \\ b_1 = -C_2/(C_1 + C_2 + S_1) \\ d_1 = (Q_1 + C_1 P_0)/(C_1 + C_2 + S_1) \end{cases} \tag{13a}$$

$$\begin{cases} a_n = -C_n/(C_n + C_{n+1} + S_n) \\ b_n = 0 \\ d_n = (Q_n + C_{n+1} P_{n+1})/(C_n + C_{n+1} + S_n) \end{cases} \tag{13b}$$

Solving P_1 in eq.(10-1), and substituting P_1 to eq.(10-2), then solving P_2 in resulted eq.(10-2) and substituting P_2 to eq.(10-3), ..., and so on, it is easy to prove that eqs.(11) can be re-written as,

$$P_i = d_i' - b_i' P_{i+1} \qquad \text{(i=1, 2, ... , n-1)} \tag{14a}$$
$$P_n = d_n' \tag{14b}$$

where

$$\begin{cases} b_1^{'} = b_1 \\ d_1^{'} = d_1 \end{cases} \tag{15a}$$

$$\begin{cases} b_i^{'} = b_i / (1 - a_i b_{i-1}^{'}) \\ d_i^{'} = (d_i - a_i d_{i-1}^{'}) / (1 - a_i b_{i-1}^{'}) \end{cases} \quad \text{(i=2, 3, ..., n-1)} \tag{15b}$$

$$d_n^{'} = (d_n - a_n d_{n-1}^{'}) / (1 - a_n b_{n-1}^{'}) \tag{15c}$$

Now, the pressure profile can be easily calculated with eqs.(14) by so-called chasing-back method, i.e. calculating P_n, then substituting P_n to the (n-1)th equation to calculate P_{n-1}, and then to calculate P_{n-2}, P_{n-3}, ..., P_2, P_1.

§4.2 Periodic boundary conditions

For the periodic boundary condition, equations (3) can be rewritten as

$$\begin{cases} a_1 P_n + P_1 + b_1 P_2 = d_1 \\ a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \\ a_n P_{n-1} + P_n + b_n P_1 = d_n \end{cases} \quad \text{(i=2, 3, ..., n-1)} \tag{16}$$

where,

$$\begin{cases} a_i = -C_i / (C_i + C_{i+1} + S_i) \\ b_i = -C_{i+1} / (C_i + C_{i+1} + S_i) \\ d_i = Q_i / (C_i + C_{i+1} + S_i) \end{cases} \quad \text{(i=1, 2, ..., n-1)} \tag{17a}$$

and

$$\begin{cases} a_n = -C_n / (C_n + C_1 + S_n) \\ b_n = -C_1 / (C_n + C_1 + S_n) \\ d_n = Q_n / (C_n + C_1 + S_n) \end{cases} \tag{17b}$$

It is easy to prove that eqs. (16) can be rewritten as

$$P_i = d_i^{'} - b_i^{'} P_{i+1} + a_i^{'} P_n \quad \text{(i=1, 2, ..., n-1)} \tag{18a}$$

and

$$P_n = d_n^{'} - b_n^{'} P_1 \tag{18b}$$

and

$$P_1 = d_n^{'} / b_n^{'} - P_n / b_n^{'} \tag{18c}$$

where

$$\begin{cases} a_1^{'} = -a_1 \\ b_1^{'} = b_1 \\ d_1^{'} = d_1 \end{cases} \tag{19a}$$

$$\begin{cases} a_i^{'} = -a_{i-1}^{'} a_i / (1 - a_i b_{i-1}^{'}) \\ b_1^{'} = b_i / (1 - a_i b_{i-1}^{'}) \\ d_1^{'} = (d_i - a_i d_{i-1}^{'}) / (1 - a_i b_{i-1}^{'}) \end{cases} \quad \text{(i=2, 3, ..., n-1)} \tag{19b}$$

and

$$\begin{cases} d_n^{'} = (d_n - a_n d_{n-1}^{'}) / (1 + a_n (a_{n-1}^{'} - b_{n-1}^{'})) \\ b_n^{'} = b_n / (1 + a_n (a_{n-1}^{'} - b_{n-1}^{'})) \end{cases} \tag{19c}$$

Substitute eq.(18c) into eq.(16a), and eq.(18b) into eq.(16c), eqs.(16) becomes

$$P_1 + b_1^{"} P_2 = d_1^{"} \tag{20-1}$$

$$a_2 P_1 + P_2 + b_2 P_3 = d_2 \tag{20-2}$$

$$a_3 P_2 + P_3 + b_3 P_4 = d_3 \tag{20-3}$$

... ...

$$a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \tag{20-i}$$

... ...

$$a_{n-1} P_{n-2} + P_{n-1} + b_{n-1} P_n = d_{n-1} \tag{20-(n-1)}$$

$$a_n^{"} P_{n-1} + P_n = d_n^{"} \tag{20-n}$$

where

$$\begin{cases} b_1^{"} = b_1 / (1 - a_1 b_n^{'}) \\ d_1^{"} = (d_1 - a_1 d_n^{'}) / (1 - a_1 b_n^{'}) \end{cases} \tag{21a}$$

$$\begin{cases} a_n^{"} = a_n / (1 - b_n / b_n^{'}) \\ d_n^{"} = (d_n - d_n^{'} * b_n / b_n^{'}) / (1 - b_n / b_n^{'}) \end{cases} \tag{21b}$$

Eqs.(20) has the same form as that of eqs.(10). So one can solve eqs.(20) to get the pressure profile at the periodic boundary condition by using the same method (i.e. the so-called chasing-back method) as described in the case of the smooth and the fixed boundary conditions.

§5. Program Block Diagrams

§5.1 Iteration method

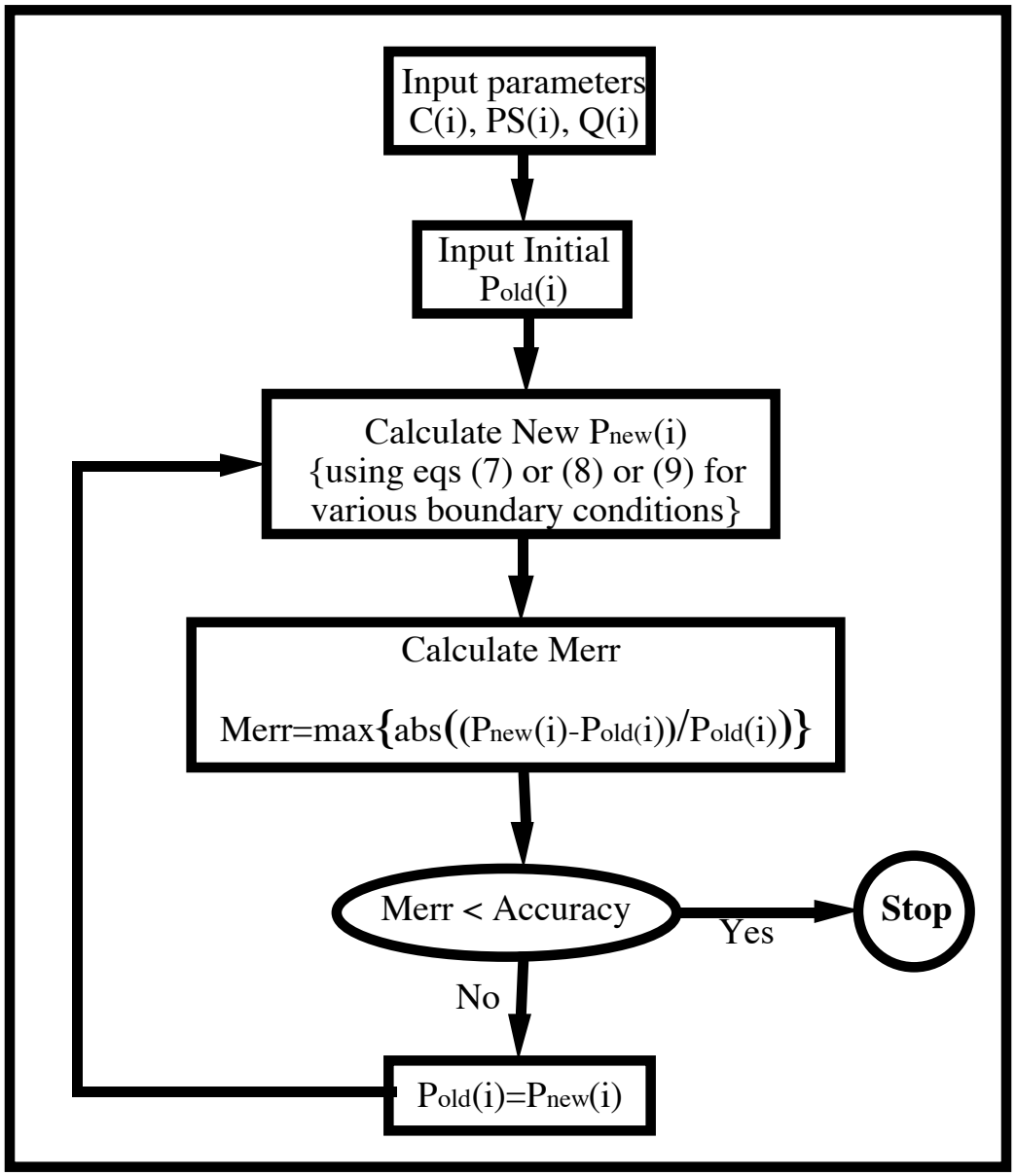

Figure 2. Flow diagram for the iteration method

§5.2 Solving equations method

§5.2.1 Smooth boundary and fixed boundary conditions

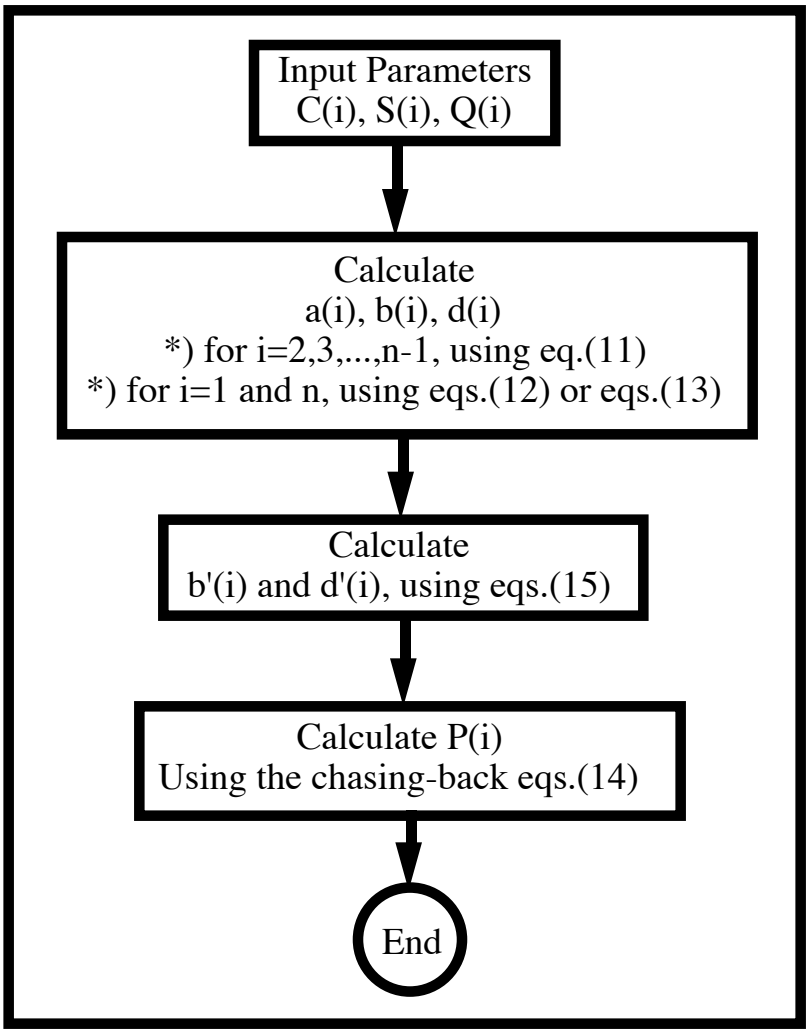

Figure 3. Flow diagram for the solving equation method

§5.2.2. Periodic boundary condition

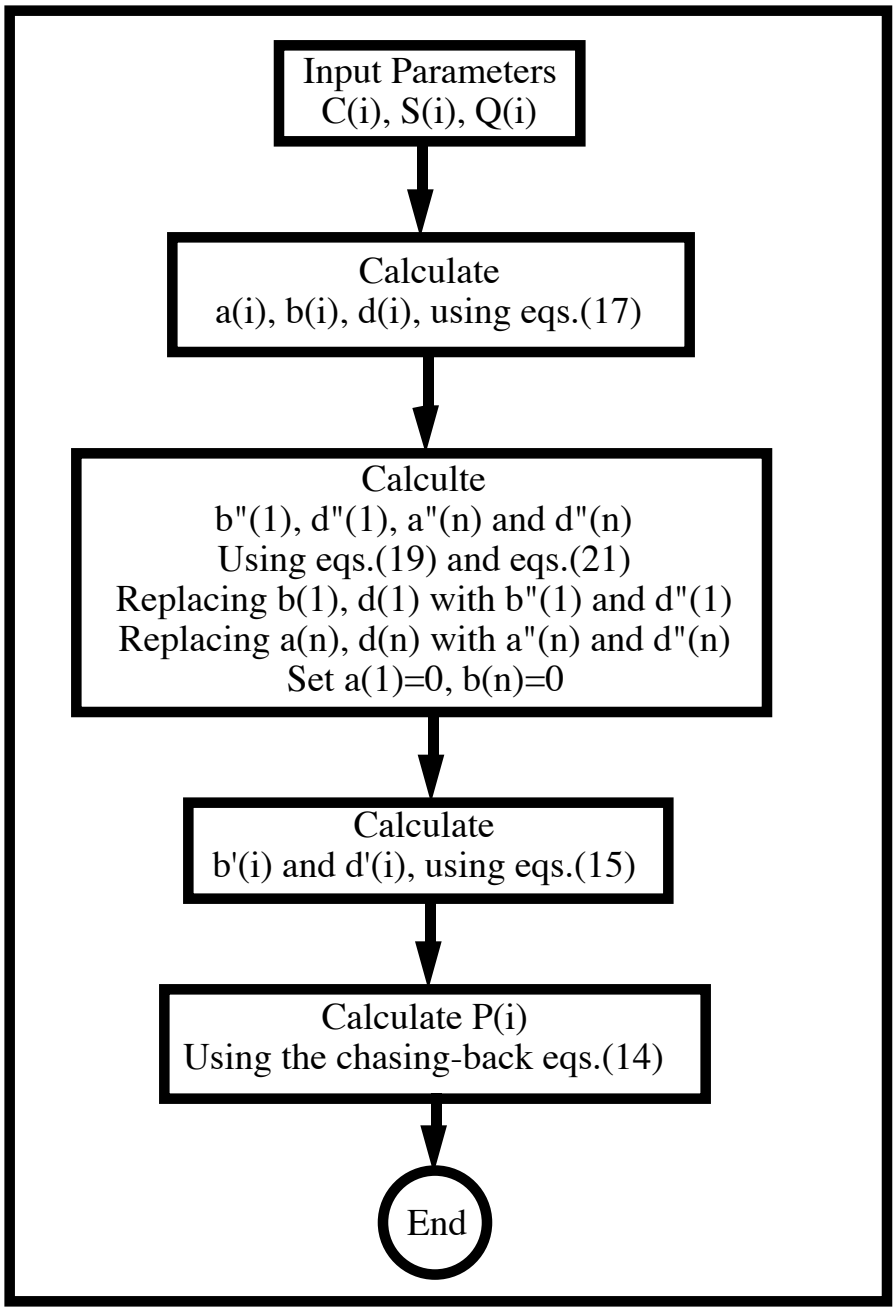

Figure 4. Flow diagram for the solving equation method

§6. Implantation

The finite element method has been implanted in the application program Igor Pro® (WaveMetrics, Inc.) on a Macintosh computer. Testing runs has been carried out for both the iteration method and the solving equation method at both the smooth boundary condition and the periodic condition. As expected, both methods yield same results. The testing runs results are

plotted figure with testing conditions (i.e. the conductance, pumping speed and gas load profiles). The programs are also attached with the test results. The testing runs indicates that the solving equation method is much more faster than the iteration method. But the iteration method can be used as a verification for the programming of the solving equation method, since the iteration method is easier to program then the solving equation method and the numerical truncation error for the iteration method is also smaller than the solving equation method.