## ELECTRICAL CALCULATIONS SOFTWARE

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These programmes are designed to calculate the dielectric constant of a microwave resonator from its geometry, the geometry of the test cavity, the dielectric constants of the surroundings, and the resonant frequency. There are essentially two geometries accounted for in this software, that of Hakki-Coleman and that of Itoh-Rudokas.

## HakCol.EXE

The Hakki-Coleman geometry, sometimes called the post-resonator method, is the simpler (and more mathematically precise) of the two configurations. In this, a cylindrical resonator is sandwiched between two conducting plates (typically of copper) of mathematically infinite proportions (this means that they must be sufficiently larger than the resonator so there is no field beyond them). Two probes are then inserted on either side of the resonator between the plates. These probes are hooked horizontally at the testing end to set up a magnetic field with force lines in the vertical plane. This magnetic field then couples with the test piece to induce the TE<sub>01</sub> resonant mode. If the piece is of very high dielectric constant, most of its electrical field will remain in the piece (DUT) (it is efficiently reflected into the piece at the solid-air interface) so the probes must be placed close enough to couple (always, of course, without over-coupling occurring). In this way, frequencies are scanned, and a network analyser is able to distinguish the frequency of maximum transmission, which is the resonant frequency. If the test jig is not of the correct proportions for the piece, one or more resonant peeks belonging solely to the jig may appear and must be distinguished from the TE 01 frequency. Once this frequency is known, the dielectric constant can be calculated with the additional information of resonator diameter and thickness. The main equations which are involved were first derived by Hakki and Coleman in 1970 and are transcendental in nature (they must be solved by an iterative method which would be very time-consuming without computer help).

If one assumes the resonator is isotropic, has a dielectric constant of  $\varepsilon_r$ , permeability of  $\mu_o$ , thickness *t*, and diameter *d*, then for a TE<sub>0nl</sub> mode:

$$\frac{\alpha J_0(\alpha)}{J_1(\alpha)} = \frac{-\beta K_0(\beta)}{K_1(\beta)}$$
(1)

where  $J_0(\alpha)$  and  $J_1(\alpha)$  are Bessel functions of the first kind of orders 0 and 1, respectively.  $K_0(\beta)$  and  $K_1(\beta)$  are modified Bessel functions of the third kind (also called modified Hankel functions) of order 0 and 1, respectively. The values of  $\alpha$  and  $\beta$  are dependent upon geometry, free-space resonant wavelength ( $\lambda$ ), and the dielectric constant of the resonator ( $\epsilon_r$ ), as shown below:

$$\alpha = \frac{\pi d}{\lambda} \sqrt{\varepsilon_{\rm r} - (c/\nu_{\rm p})^2}$$
(2)  
$$\beta = \frac{\pi d}{\lambda} \sqrt{(c/\nu_{\rm p})^2 - 1}$$
(3)

where *d* is the diameter of the resonator, *c* is the speed of light, and  $v_p$  is the phase velocity in the structure so that

$$\frac{c}{v_{\rm p}} = \left(\frac{l\lambda}{2t}\right)_{\rm (4)}$$

and l is the number of longitudinal variations of the field along the axis. Combining (2) and (4), we obtain:

$$\varepsilon_{\gamma} = \left(\frac{\alpha\lambda}{\pi d}\right)^2 + \left(\frac{l\lambda}{2t}\right)^2$$

Then, for the  $TE_{01\delta}$  mode (n = 1, l = 1), (3) can be re-written as:

$$\beta = \frac{\pi d}{\lambda} \sqrt{\left(\frac{\lambda}{2t}\right)^2 - 1}$$
(5)

The characteristic equation of (1) is therefore clearly transcendental and requires a graphical or iterative approach.

Hakki and Coleman provided several graphs which related  $\alpha$  to  $\beta$ . A simple curve fit to their data is sufficient as a starting point for the iteration. In fact, a ninth-order polynomial fit is used to calculate  $\varepsilon_r$  to a good approximation. First  $\beta$  is calculated from (5), that value is then plugged into (2) along with the approximate  $\varepsilon_r$  to calculate  $\alpha$ . Both  $\alpha$  and  $\beta$  are then checked by (1). If the equation is invalid with those values,  $\varepsilon_r$  is adjusted accordingly,  $\alpha$  is re-calculated, and the process is repeated until (1) is satisfied. It is worth noting here that there is a slight error in Hakki and Coleman's paper in that  $K_0$  and  $K_1$  are called Bessel functions of the second kind. They are, in fact, modified Bessel functions of the third kind, as stated above.

## ErCalc.EXE

The algorithm developed to solve the Itoh-Rudokas equations is long and complicated. First, a mathematical construct is used to numerically solve for the eigenvalues. In software currently available, a curve-fit is used to estimate the *ratio* of Bessel functions and modified Hankel functions, leading to a small but measurable error. The chief advantage of this programme is that all of the various Bessel functions are numerically calculated individually for an improved accuracy.

Once the eigenvalues are known, the dielectric constant can be calculated, and a new resonant frequency obtained from the variational method. The dielectric constant is then adjusted appropriately until the calculated frequency is equal to the experimental frequency.

Values of  $\varepsilon_r$  were calculated from the resonant frequency and the dimensions of the sample and cavity using the appropriate system of transcendental equations published by Itoh and Rudokas. No account is taken of the conductivity of the cavity walls which are assumed to be very distant from the resonator; nevertheless, the calculation is not trivial. The software developed here is based on the model suggested





Schematic model of the resonant cavity. The side walls have been omitted, as they are of no mathematical significance. Region 6 is the resonator; region 1 is the support, and the remaining regions are typically air-filled.

For a high- $\varepsilon$ r material, most of the electrical field is contained within the resonator itself (region 6), and very little exists in regions 1 and 2, and even less in regions 3 and 5. To a fair first approximation, then, the fields in regions 3 and 5 can be ignored (this approximation is compensated for later on). For the TE <sub>018</sub> modes the requirement for continuity of fields leads to two simultaneous eigenvalue equations:

$$-i\beta \overline{E}_{\rho} - \frac{\delta \overline{E}_{z}}{\delta \rho} = -i\omega\mu \overline{H}_{\phi}$$
(6)
$$\beta \overline{L} = \frac{\beta_{1}}{2} + \frac{\beta_{2}}{2} + \ell \pi \ell = 0, 1, 2, 3 \dots (7)$$

In (6),  $J_0$  and  $J_1$  represent Bessel functions (sometimes called cylindrical functions, hence their appropriateness in this cylindrically-symmetrical model) of the first kind of order zero and one, respectively; and  $K_0$  and  $K_1$  are the modified Hankel functions (sometimes called modified Bessel functions of the third kind) of the zeroth and first order.

The radius of the resonator is *a*, as defined in the figure below. The symbol *k* represents the radial propagation constants in the different regions of the model, which are functions of both frequency and dielectric constant; and  $\rho$  is the radial distance from the geometric centre. The arguments of the various Bessel functions are the eigenvalues of the system, where  $k_{\rho l}a$  is called the eigenvalue of the TE<sub>0n</sub> mode, and  $k_{\rho 2}$  is given by:

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$$k_{p2} = \sqrt{k_0^2 (\varepsilon_{76} - \varepsilon_{74}) - k_{p1}^2}$$
(8)

where  $k_0$  is called variously the *propagation constant*, *wavenumber*, or *phase constant* of free space, and has units of m<sup>-1</sup>:

$$k_0 = \omega_0 \sqrt{z_0 \mu_0}$$

In (7),  $\beta$  is the propagation constant of the resonator, and  $\ell$  is part of the resonant mode description (see appendix). For the TE <sub>01  $\delta$ </sub> mode,  $\ell = 0$ .

$$\mathcal{S} = \sqrt{k_o^2 \mathcal{S}_{r6} - k_{o1}^2}$$
(9)

The symbols  $\phi_1$  and  $\phi_2$  are called the *phase angles* and are complex hyperbolic functions of the cavity geometry and the propagation constant of the resonator:

$$\begin{split} p_1' &= 2 \tan^{-1} \left( \frac{\alpha_1}{\mathcal{I}} \coth \alpha_1 L_1 \right) \\ p_2' &= 2 \tan^{-1} \left( \frac{\alpha_2}{\mathcal{I}} \coth \alpha_2 L_2 \right) \end{split}$$

Here,  $\alpha_1$  and  $\alpha_2$  are called the *attenuation constants* above and below the resonator. These constants can be calculated directly from the frequency and radius, thus:

$$\alpha_1 = \sqrt{k_{\rho 1}^2 - k_{\rho}^2 \, \varepsilon_{\gamma 1}}$$
$$\alpha_2 = \sqrt{k_{\rho 1}^2 - k_{\rho}^2 \, \varepsilon_{\gamma 2}}$$

In these equations,  $\varepsilon_{r1}$  and  $\varepsilon_{r2}$  are the dielectric constants of the material below (the support) and above (air) the resonator. Of course,  $\varepsilon_{r2} = 1$ ; but  $\varepsilon_{r1}$  is more difficult to define as, for instance, a fused quartz support has  $\varepsilon_r ~ 4$  but may be only  $~ 1/_5$  the diameter of the simple shape shown in the figure. As an approximation,  $\varepsilon_{r1}$  is generally set equal to unity. The errors this introduces are very small, generally only manifest in the hundredths place of the dielectric constant  $\varepsilon_{r6}$ .

The solution of these simultaneous equations is obtained using an algorithm based on that published by Kajfez and Guillon. Dielectric constants calculated in this way have a typical error of  $\sim +14.8\%$ .

An improvement to the model can be made by accounting for the fields in regions 3 and 5. So far the model assumes the fields to be zero here, creating a discontinuity in the field distribution on the boundaries of these regions. If one chooses instead appropriate electric fields for these regions, a continuous distribution can be restored; but the equations necessary do not satisfy the Helmholz wave equation, making it impossible to construct a self-consistent *magnetic* field in these regions. In this case, the magnetic fields are simply left to be zero. To compensate for this case, artificial surface electric

currents are introduced on the boundaries of regions 3 and 5, as shown in the figure. This technique is called a variational method, and the net effect is to lower the dielectric constant for a given resonant frequency. Again, in order to establish the correct dielectric constant, an iterative algorithm must be invoked which adjusts  $\varepsilon_{r6}$  until the calculated resonant frequency matches the experimentally measured one. The solution is shown as the figure in red at the bottom of the screen. Errors are typically brought down to ~ -5.7% in this way.

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