Configuration of COMSOL Multiphysics for simulating axisymmetric dielectric resonators: explicit weak-form expressions axisymmetric electromagnetic resonators

Mark Oxborrow

Appendix I

It is here explained, in some detail, how to set up a dielectric-resonator simulation in COMSOL Multiphysics [1] -from scratch. These explanations should also be helpful to anyone wishing to modify one of the author's existing models -as incarnated in an .MPH file. At least in the first instance, it is recommended that the following instructions be meticulously adhered to -lest one stray from a tried-and-tested path. And it is suggested that the reader work through them with COMSOL Multiphysics open and running on his/her desktop. All menu items, expression names and variables associated with the program are displayed in typed text font. A good deal of supplementary information can be found in the documentation supplied with COMSOL Multiphysics itself; the author found the following chapters therein to be the most useful/relevant: 'PDE Modes for Equation-Based Modeling', 'The Weak Form', and 'COMSOL Multiphysics Scripting'. Upon reading these chapters, one might be left with the impression that COMSOL is simply not sufficiently flexible to embrace the task in hand (i.e. to implement sections II through IV of this article explicitly); the following instructions demonstrate how COMSOL Multiphysics can, despite these first impressions, and most straight-forwardly, be so configured to implement the 2D simulation of isotropic dielectric resonators. From the beginning then:

A. Setting up –fundamentals

Get COMSOL Multiphysics up and running. Access the Model Navigator panel via File \Rightarrow New ... and select the New tab if not already selected.

(a) Select '2D' from the Space dimension: drop-down menu [note: do *not* choose 'Axial symmetric (2D)'].

(b) Browse to and select 'COMSOL Multiphysics \Rightarrow PDE Modes \Rightarrow Weak Form, Subdomain' from the Application Mode navigator.

(c) Type (verbatim) 'Hrad Hazi Haxi' into the Dependent variables: text field. These three variables are the radial, azimuthal and axial components of the magnetic field strength, respectively; all three are dependent on (*i.e.* are functions of) the Cartesian coordinates for the COMSOL

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simulation's 2D space, namely x (horizontal on the screen) and y (vertical) –both in units of metres [m]. The coordinate names 'x' and 'y' are already fixed by COMSOL (*i.e.* they are reserved symbols) and need not be explicitly entered (in COMSOL terminology, x and y are 'geometric variables').

(d) For the Application mode name: (default u) one can type in anything one likes.

(e) Select 'Lagrange - Quadratic' from the Element: drop-down menu. [This choice is proven to work.]

B. Constants

All of the various constants (*i.e.* independent of x or y) included within the weak-form expressions given below are defined and described in TABLE I. The equivalent of this table needs to be typed (or loaded) into COMSOL's Options \Rightarrow Constants Each Expression thus Value therein [except those for e0, eperp0, epara0 –which define the (unit) relative permittivity of free-space], can be user-varied. But every Name should be entered verbatim; *i.e.*, each constant must be named exactly as it appears in the expressions that subsequently include it.

C. Expressions (for Postprocessing)

The post-processing of the calculated magnetic-field strength (as a function of position) for each solved eigenfunction is facilitated through the various definitions presented here.

1) Scalar expressions: The equivalent of TABLE II (or some subset thereof) needs to be typed into COMSOL's Options \Rightarrow Expression ... \Rightarrow Scalar expressions

2) Subdomain expressions: The functionality of Subdomain expressions is required for generating post-processed fields, like the electric field strength \mathbf{E} —as per the 6th, 7th and 8th entries in TABLE II. Those constants associated with each such field's definitions, like (in the case of \mathbf{E}) the relative permittivities epara and eperp, *vary* from one subdomain within the medial half place to another. The variation of these subdomain-dependent 'constants' is represented through Options \Rightarrow Expressions \Rightarrow Subdomain expressions; therein, the Name of each such variable is the same in each and every Subdomain

(as identified by an integer), but its Expression reflects the variable value in the selected Subdomain. Thus, the Expression for epara in a Subdomain corresponding to (cryogenic and axisymmetrically oriented) sapphire would be eparal, with eparal defined (globally) as 11.3486 (or whatever) through TABLE I, whereas in a Subdomain corresponding to free space, the Expression for epara should be set to 1. Similarly (and more simply), the single Subdomain-dependent variable erel can be used to represent the variation of relative permittivity within an axisymmetric resonator containing solely isotropic dielectrics (incl. free space).

D. Weak-form expressions

The simulation's defining weak-form expressions are set up through the Physics \Rightarrow Subdomain Settings ... control panel. On the left of this panel, first select the Groups tab. A New Group must be named and defined for each dielectric within the resonator being simulated. The author chose to name these dielectric Groups 'dielectric O:vacuum', 'dielectric_1', ..., 'dielectric_n', For each dielectric Group, (in general) dielectric n say, corresponding weak-form expressions need to be entered into the weak terms (i.e. three slots or text fields), for expressions involving spatial derivatives, and also into the dweak terms, for expressions involving temporal derivatives; these slots are accessed through the weak and dweak tabs, respectively, located on the right of the Subdomain Settings ... control panel. These terms govern the electromagnetic field in regions filled with the n-th dielectric, as specified in the Constants ... table introduced above. No other fields on the right of Subdomain Settings ... need(/should) be touched; in particularly, don't monkey with the contr-tabbed sub-panel. Note that it is imperative that the Name of each constant entered into Options \Rightarrow Constants ... above match (verbatim) its appearances within the expressions (below) that are entered into the weak and dweak text fields here. For each dielectric Group, two weak and one dweak terms are required: (i) a 'Laplacian' term (corresponding to the left most term on the left-hand side of equation 6 in the main paper and (ii) a 'penalty' term, included to suppress spurious modes, corresponding to the middle term of the same.

1) Laplacian term [first weak-term slot]: The form of the Laplacian weak term, $(\nabla \times \tilde{\mathbf{H}}^*)_{\epsilon}^{\perp} (\nabla \times \mathbf{H})$, here given for the

1st axisymmetric dielectric, is¹

```
((eperpl*(test(Hazi)*Hazi
-M*(test(Hazi)*Hrad
+Hazi*test(Hrad))
+M^2*test(Hrad)*Hrad)
+eparal*M^2*test(Haxi)*Haxi)/x
+eperpl*(test(Hazix)*(Hazi-M*Hrad)
+Hazix*(test(Hazi)-M*test(Hrad)))
-eparal*M*(test(Haxi)*Haziy
+Haxi*test(Haziy))
+x*(eperpl*test(Hazix)*Hazix
+eparal*((test(Haxix))
-test(Hrady))*(Haxix-Hrady)
+Haziy*test(Haziy)))
)/(eparal*eperpl)
```

where Hazix denotes the partial derivative of Hazix with respect to the coordinate x, Hrady the partial derivative of Hazi with respect to y, etc.; test(Hazi) denotes the 'test function' of Hazi, *etc.* Its equivalent for the 2nd axisymetric dielectric is obtained by replacing eperp1 by eperp2 and epara1 by epara2, and so forth for all other axisymetric dielectrics (should more be required). The above expression can be significantly simplified for the (subdomain) Groups corresponding to isotropic dielectrics or free space (*viz.* dielectric_0); for computational efficiency, it is recommended that these simplifications be implemented wherever possible. The required form of the Laplacian weak term, $[(\nabla \times \tilde{\mathbf{H}}^*) \cdot (\nabla \times \mathbf{H})]/\epsilon_1$, for the 1st isotropic dielectric is given explicitly as

```
((test(Hazi)*Hazi
-M*(test(Hazi)*Hrad
+Hazi*test(Hrad))
+M^2*(test(Hrad)*Hrad
+test(Haxi)*Haxi))/x
+(test(Hazix)*(Hazi-M*Hrad)
+Hazix*(test(Hazi)-M*test(Hrad)))) (I.2)
-M*(test(Haxi)*Haziy
+Haxi*test(Haziy))
+x*(test(Hazix)*Hazix
+((test(Haxix))*Hazix
+((test(Haxix)))))/e1,
```

where el is the material's dielectric constant (as appearing in TABLE I). The Laplacian weak term for the vacuum is the same with $\epsilon_1 \rightarrow 1$, and those for other isotropic dielectrics are similarly obtained by swopping ϵ_1 with ϵ_2 , ϵ_3 , and so forth.

2) Penalty (divergence-suppressing) term [second weakterm slot]: The form of the penalty weak term, $\alpha(\nabla \cdot$

¹Note that, when typing (or 'cutting-and-pasting') this and the following (d)weak-form expressions into their slots, *all spaces and new lines* must be eliminated from the whole expression within each slot –otherwise COMSOL will reject the expression.

 $\tilde{\mathbf{H}}^*$) · (∇ · \mathbf{H}), the same for each subdomain Group, is

here, the coefficient alpha (whose value is determined through COMSOL's equivalent of TABLE I) controls the aggressiveness of the divergence suppression induced by this term. The remaining, 3rd slot, should be zero-filled. [As a general rule, unused weak-form slots should always be filled with zeroes -this applies to the the dweak term slots below.]

3) Frequency term [first dweak-term slot]: The form of the temporal-derivative/frequency (so-called 'dweak') term $\tilde{\mathbf{H}}^* \cdot \partial^2 \mathbf{H}/\partial^2 t$, common to all subdomain Groups, is entered into the first slot within the dweak-tabbed panel of Physics \Rightarrow Subdomain Settings ..., and is given as

where Haxitt denotes the double partial derivative of Haxi with respect to time, *etc.* The remaining 2nd and 3rd slots of the dweak-tabbed panel should be zero-filled.

E. Boundary conditions

Here the constraints stated in subsection II.C of the main paper are expressed in COMSOL-ready forms. The model resonator's boundary conditions are defined through the Physics \Rightarrow Boundary Settings ... control panel. On the left of this panel, select the Groups tab. Each named boundary Group here corresponds to a particular electromagnetic boundary condition, the most essential of which are described here. These different e.m. boundary conditions are specified by the expressions that populate the three slots within their respective contr-tabbed sub-panels, located on the right-hand side of Boundary Settings ...; 'contr' here stands for 'constraint'. [The neighboring weak-tabbed and dweak-tabbed panels within the Boundary Settings ... need not be touched (and left zero-filled).]

1) Electric wall (for a bounded isotropic dielectric):

-Haxix+Hrady; (I.6)

here nx and ny are, as 'geometric variables' within COMSOL (in 2D), the components of the (outward) unit normal vector on the boundary of a subdomain.

2) Magnetic wall (for a bounded isotropic dielectric):

3) Radiation match (in free-space): As has already been discussed in subsection II.C of the main paper, the constraints appropriate to implementing a radiation match, can be regarded (complex) linear combinations or 'mixings' of pure electric- and magnetic- wall constraints. The first constraint mixes the magnetic-wall constraint 23 in the main paper, *i.e.* I.9 above, with the electric-wall constraint 20 in the main paper, *i.e.* I.7 above:

note that 'i' here is the square root of minus one. And the second constraint mixes the electric-wall constraint 18 in the main paper, *i.e.* I.6 above, with the magnetic-wall constraint 22 in the main paper, *i.e.* I.8 above:

Here, the pair of constants {CMW and CEW}, are defined through TABLE I. When they are set to their standard (default) values of { $1/\sqrt{2}$, $1/\sqrt{2}$ }, equations I.11 and I.12 impose a radiation match on tangential field components at the impedance of plane e.m. waves in free-space. Here also, cbar= $\bar{c} \equiv 2\pi/c$; and mf is the mode's (center) frequency; both need to be defined within Options \Rightarrow Constants-as per their corresponding rows in TABLE I;

The final (optional) constraint mixes the electric wall constraint 17 in the main paper, *i.e.* I.8 with the magnetic wall constraint 21 in the main paper, *i.e.* I.10:

Here; the constants tngM and tngE, are also defined through TABLE I and thereupon Options \Rightarrow Constants Setting {tngM, tngE} = {1,0}({1,0}) constrains the magnetic (electric) field to be wholly tangential on the impedancematching plane as is characteristic of electromagnetic traveling waves. The default setting for this third constraint was (arbitrarily) {tngM, tngE} = {1,0}). [It is remarked here that the author sought to implement the radiation-matching constraints more directly and elegantly with time derivatives, *i.e.*, replacing 2*pi*mf*Hazi by Hazit, and similarly for Hrad and Haxi. But COMSOL did not generate the intended frequency factor when interpreting them. He thus resorted to entering the expressions as stated in equations I.11 through I.13, requiring mf to be set, by hand, for each mode.]

F. Geometry

Each resonator's geometry needs to be either constructed within or imported into COMSOL. COMSOL's manual provides instructions on how to implement both. Though simple geometries (*e.g.* a cylinder of solid dielectric material inside a cylindrical metal can) can be quickly constructed by hand within COMSOL, the author found it advantageous to define the sets of quadrilateral subdomains into which many axisymmetric dielectric resonators can be readily decomposed using MATLAB scripts, where the script was run to generate the resonator's medial cross-section. The key lines in these scripts were those of the form

```
q1 = poly2vert([[x1,y1];
[x2,y2];[x3,y3];[x4,y4]]);
```

this particular line defines a quadrilateral, named q1, whose vertices have the x-y coordinates: [x1,y1], ... [x4,y4]. These quadrilaterals could then be imported into COMSOL by entering a list comprising their names into File \Rightarrow Import \Rightarrow Geometry Objects. Each complete MATLAB script (also available from the author upon request) included, where known/relevant, the cryogenic shrinkages of the resonator's constituent materials.

G. Meshing

If constructed out of quadrilaterals, the resonator's geometry can be meshed either into sub-quadrilaterals using Mesh \Rightarrow Map Mesh. Else, the geometry can always be meshed into (psuedo-random) triangles using Mesh \Rightarrow Initial Mesh with (recommended) mesh refinement over selected areas (covering the bright spots of WG modes). Note that, for the geometry to be Map Mesh-able, the vertices of its internal quadrilaterals should generally all meet at 'cross-roads', where, at each, four vertices belonging to four separate quadrilaterals all meet at a point, as opposed to 'T-junctions', where, at each, two vertices belonging to two separate quadrilaterals meet at a point along the boundary edge of a third quadrilateral. The reader is advised to consult the COMSOL manual (chapter 'Meshing', section 'Generating Meshes', subsection 'Creating Mapped Meshes in 2D') for a fuller (though a still not wholly satisfactory) explanation of this rather quirky requirement. The meshing density can be controlled by, for selected edges, activating and entering an appropriate integer in the 'Contrained edge element distribution' field within of the Boundary tab of the Map Mesh control panel. With regard to both Map Mesh-ability and control over meshing density, it can be advantageous (or plain necessary) to divide odd-shaped subdomains (e.g. an 'L'-shaped region covered throughout by a single spatially uniform dielectric material) into several, more simply shaped adjoining subdomains (e.g., in the case of dividing up the L-shaped subdomain, two or even three rectangular subdomains). Note that the geometry will not mesh if the allocations of elements along too many edges are (inconsistently) specified; in other words, the edge element distribution must not be over constrained.

H. Assignments

1) Interiors of subdomains: The (either hand-made or imported) quadrilaterals composing the resonator's cross-sectional geometry are assigned to one of the defined dielectric Groups via the Subdomain Settings ... \Rightarrow Subdomains tab. Activating (*i.e.* ticking) the Select by group option here aids the verification of assignments.

2) Edges of subdomains: The external edges of quadrilaterals should be set be obey one of the three abovedescribed Group boundary conditions via the Physics \Rightarrow Subdomain Settings ... \Rightarrow Subdomains tab. COMSOL appears to be smart enough to recognize those edges that are external on its own accord and automatically 'ghosts' (grays) internal edges; the latter should not be assigned to any boundary Group condition. Thus, with the Select by group feature activated, all the appropriate edges can be assigned to the appropriate (usually electric-wall) boundary condition in a single selection of the Groups dropdown menu.

I. Solution

In Solve \Rightarrow Solve Parameters:

(a) set the selected Solver: to 'Eigenvalue:';

and, with the General tab selected,

(b) set the Desired number of eigenvalues: to '10' -or whatever ones desires;

(c) set Search for eigenvalue around: to '0' -or whatever;

(d) set Linear system solver: to 'Direct (SPOOLES) (this is at least the author's starting recommendation);

(e) set Matrix symmetry: to Symmetric'.

Having implemented all of the above, one should now be able to Solve \Rightarrow Solve Problem.

J. Postprocessing

COMSOL Multiphysics' standard documentation explains how to configure and use of the Postprocessing \Rightarrow Plot Parameters control panel. Only a few specific pointers are supplied here:

[1] The center frequencies of solved resonances can be viewed through the Solution to use \Rightarrow Eigenvalue: drop-down menu in the General-tabbed sub-panel of the Plot Parameters control panel.

[2] To display the morphology and features of the solved eigenmodes, the Expression: slot within the Surface-tabbed sub-panel of the same is filled with either (i) some function of the solved field variables {Hrad, Hazi, Haxi } or (ii) one of those expressions (*e.g.* ElecMagSqrd) pre-defined in Options \Rightarrow Expressions Scalar Expressions as COMSOL's equivalent of TABLE II, or (iii) some function/combination thereof. For example,

$$log10(AbsMagEnDens+10^{(-10)})$$
 (I.14)

can be inserted to view the magnetic energy density on a logarithmic scale. To view (as a diagnostic) the divergence

of the magnetic field strength, which should be zero, one inserts $DivH \equiv (Hrad-Hazi*M+(Haxiy+Hradx)*x)/x$ instead.

[3] Determinations of an electromagnetic mode's volume, filling factor(s), and length (Λ), as per equations 24 , 25 , and 27 , respectively, in the main paper, all make use of the Postprocessing \Rightarrow Domain Integration panel. For example, the numerator $\int \int \int_{h.-s.} \epsilon |\mathbf{E}|^2 dV$ on the right-hand-side of equation 24 in the main paper can be evaluated by inserting ElecEnDens \equiv Erad*Drad+Eazi*Dazi+Eaxi*Daxi into this panel's Expression: slot, with those entries selected in the Subdomain selection list on the left-hand side of the same panel covering all significant parts of the mode's bright spot.

[4] With regards to determining filling factors, the numerator on the right-hand side of equation 25 in the main paper can be evaluated by selecting only those subdomains filled with the relevant dielectric (as opposed to free-space).

determine resistive-wall-loss [5] То the integral ∫ |**n** × $\mathbf{H}|^2 dS$ (forming the denominator of equation 27 in the main paper), one uses the Postprocessing \Rightarrow Boundary Integration panel with 2*pi*x*(abs(Hazi)^2 +abs((Haxi*nx -Hrad*ny))^2) inserted into the Expression: slot within the Expression to integrate box therein, and where entries selected with Boundary selection correspond to the resonator's enclosing (metallic and lossy) surfaces.

[6] The maximum/minimum of a field variable, as required to evaluate the denominator on the right-hand side of equation 24 in the main paper, can be determined through the Postprocessing \Rightarrow Plot parameters \Rightarrow Max/Min, wherein the Expression: slot is filled with the field variable's expression (*viz.* ElecEnDens for evaluating said denominator).

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TABLE I

COMSOL CONSTANTS -INCLUDED IN WEAK-FORM EXPRESSIONS

Name	Expression	Description [unit]
	(= value)	
С	299792458	speed of light (exact) [m/s]
cbar	2*pi/c	frequency constant [s/m]
	(=2.095845e-8)	
cbar2	4*pi^2/c^2	frequency constant [s ² /m ²]
	(=4.392566e-16)	
alpha	1.0	penalty-term coefficient
M	9	azimuthal mode order
e0	1.0	relative permittivity
o1	n_AlGaAs^2	of free-space
el	(= 11.2896)	relative permittivity of isotropic_dielectric_1
e2	1.0	same but of
22	1.0	isotropic dielec2
e3	1.0	etc.
eperp0	1.0	relative permittivity
		of free-space
		in directions transverse
		to cylindrical axis
epara0	1.0	same but in direction
		parallel to cylindrical axis
eperpl	9.2725	relative permittivity of
		uniaxial_dielectric_1
		in directions transverse
	11 2496	to cylindrical axis same but in direction
eparal	11.3486	parallel to cylindrical axis
epara2	1.0	relative permittivity of
eparaz	1.0	uniaxial_dielectric_2
		transverse to cyl. axis
eperp2	1.0	same but parallel to
- <u>-</u> - <u>-</u> -		cylindrical axis
eperp3	1.0	etc.
epara3	1.0	etc.
e_293K_alumina	9.8	relative permittivity of
		alumina at room temperature
epe_4K_sap_UWA	9.2725	UWA values for cryogenic
		HEMEX sapphire
epa_4K_sap_UWA	11.3486	• •
epe_293K_sap	9.407	nominal room temperature
ana 2027 gan	11.62	values for same
epa_293K_sap epe_4K_sap_NPL	11.62 9.2848	Values fitted to
cpc_m_bap_mb	7.2040	NPL Cs-fountain
		HEMEX resonator
epa_4K_sap_NPL	11.3660	
n_silica	1.4457	refractive index of
		thermally grown
		silica (Fig B.2, p. 172 of
		ref. [2])
n_AlGaAs	3.36	average refractive index of
		GaAs and AlGaAs layers
-		(p. 172 of ref. [3])
mf	2.374616e14	match frequency
ttgH	1	toggle
ttgE mix ang	0 45	toggle
mix_ang	-J.	electric-magnetic mixing angle (in degrees)
cMW	sin(mix_ang	angle (in degrees)
0	* pi /180)	magnetic-walled-ness
	(= 0.707107)	
CEW	cos(mix_ang	
	* pi /180)	electric-walled-ness
	(= 0.707107)	
tngM	1	
tngE	0	

 TABLE II

 COMSOL Scalar Expressions –for postprocessing

Name	Expression		
	(Description)		
DivH	(Hrad-Hazi*M+(Haxiy+Hradx)*x)/x		
	(divergence of magnetic field –should be zero!)		
MagEnDens	Hrad*Hrad+Hazi*Hazi+Haxi*Haxi		
	(magnetic energy density)		
Drad	(Haxi*M-Haziy*x)/x		
	(radial component of electric displacement)		
Dazi	-Haxix+Hrady		
	(azimuthal component of electric displacement)		
Daxi	(Hazi-Hrad*M+Hazix*x)/x		
	(axial component of electric displacement)		
Erad	Drad/eperp		
	(radial component of electric field strength)		
Eazi	Dazi/eperp		
	(azimuthal component of electric field strength)		
Eaxi	Daxi/epara		
	(axial component of electric field strength)		
ElecMagSqrd	Erad*Erad+Eazi*Eazi+Eaxi*Eaxi		
	(electric field strength magnitude squared)		
ElecEnDens	Erad*Drad+Eazi*Dazi+Eaxi*Daxi		
	(electric energy density)		
AbsMagEnDens	abs(Hrad)^2+abs(Hazi)^2		
	+abs(Haxi)^2		
	(absolute magnitude energy density)		
MagNrmlHSqrd	2*pi*x*abs(Haxi*ny		
	+Hrad*nx)^2		
	(magnitude normal mag. field strength squared)		
MagTngHSqrd	2*pi*x*(1*abs(Hazi)^2		
	+1*abs(Haxi*nx-Hrad*ny)^2)		
	(magnitude tangential magnetic field squared)		
AbsElecSqrd	abs(Erad)^2+abs(Eazi)^2		
	+abs(Eaxi)^2		
	(absolute electric field squared)		