Fast and Rigorous BoR FDTD Algorithm for the Modelling of Coupled EM-Thermal Processes in Axisymmetrical Devices

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Outline

1. Motivation and background
2. Coupled electromagnetic and thermal simulation of axisymmetrical microwave process
3. Extension to a nonlinear microwave process in axisymmetrical resonators
4. Conclusions and future work

Motivation and background

1. **Improving computational efficiency by changing from 3D microwave heating to Bodies-of-Revolution in axisymmetric problems.**
2. **From NanoBat Project to I4Bags**:

In our H2020 NanoBat project, the specific interest was on the modelling of electromagnetic (EM) heating in batteries, many of which are in practice cylindrical. This has stimulated our work to couple the Bodies-of-Revolution (BoR) formulation of the FDTD method for Maxwell equations with an analogous BoR FDTD for heat flow equations. Let us note that this requires casting the equations into the cylindrical coordinate system. While the operation appears in principle straightforward, its practical implementation it requires solving specific mathematical problems due to e.g. on-axis singularities, which influence stability and efficiency of the algorithm.

Background:

Heat transfer refers to the exchange of energy in the form of heat between bodies or environments that are at different temperatures. This transfer can occur through conduction, convection, or radiation. The second laws of thermodynamics dictate that over time, temperature differences within a closed system will become more uniform as heat is transferred from hotter areas to cooler ones. This homogenisation process is accompanied by the movement of heat flux from high-temperature areas to low-temperature areas, with the rate of heat flux increasing as the temperature difference between the two points becomes larger. Using heat transfer theory, the differential equation for heat transfer shows how temperature is distributed continuously with respect to both spatial and time coordinates, allowing for the solution of heat conduction problems.

Coupled electromagnetic and thermal simulation of axisymmetrical microwave process – **Battery model**

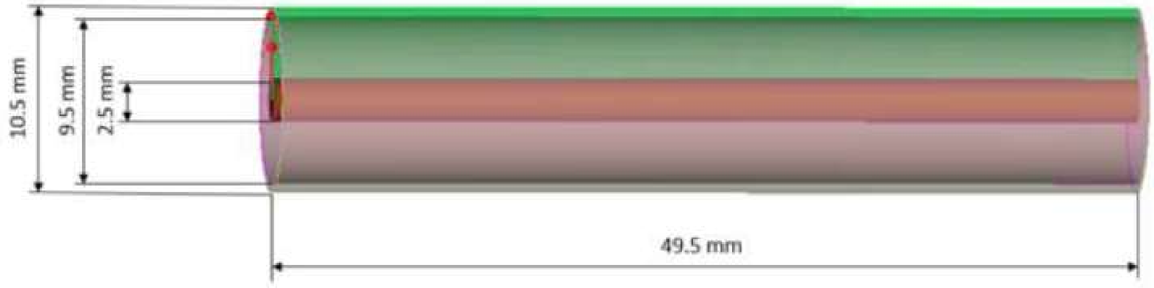


Fig. 1. Dimensions of the considered model of the popular AAA battery.

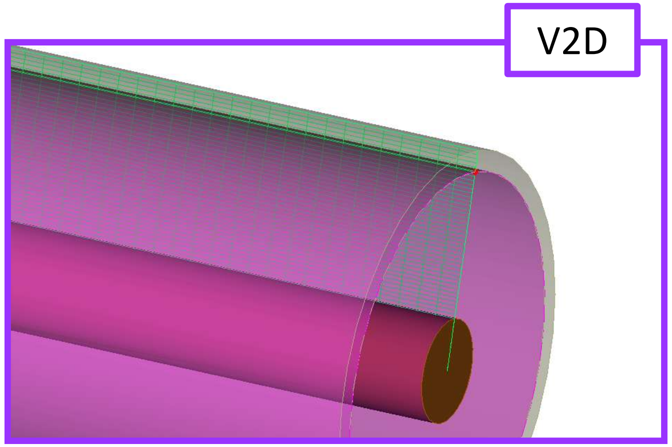
A common electrolyte is chosen as the loss material;
Lithium hexafluorophosphate (LiPF6) salt with a concentration of **0.5 mol/kg** dissolved in dimethyl carbonate (DMC). At this concentration, as shown in Tab. 1 conductivity hardly increases with temperature. For this reason, it has been assumed that it is constant over temperature and its value has been set to **0.2 S/m**.

Tab. 1. LiPF6 (electrolyte) parameters

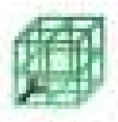
Temperature [°C]	LiPF6 concentration* [mol/kg] **0.5**	**1.5**	Specific Heat capacity** [J/g°C]	Density* [g/cm³]	Dielectric Constant*
	Conductivity* [S/m]				
0	0.2	0.58	1.704	1.063	3.1075
10		0.65			
20		0.82			
30		1.04			
40		1.52			

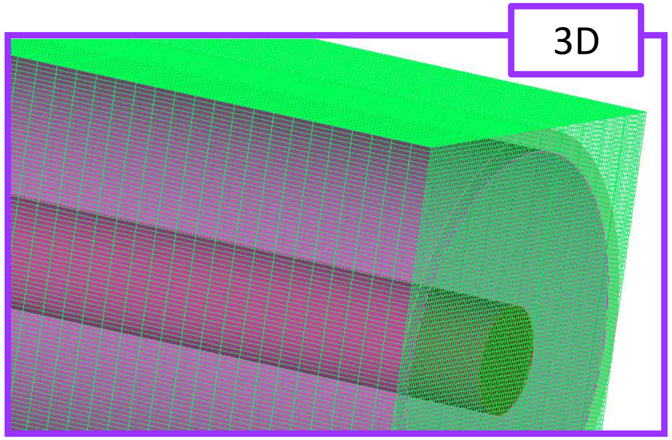
*E. R. Logan *et al* 2018 *J. Electrochem. Soc.* **165** A705
** Zhou, Y. , Wu, J. and Lemmon, E. (2011), Thermodynamic Properties of Dimethyl Carbonate, J. Phys. & Chem. Ref. Data (JPCRD), National Institute of Standards and Technology, Gaithersburg

Coupled electromagnetic and thermal simulation of axisymmetrical microwave process – **QuickWave model**



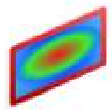
Cell size:
X: 0.5 mm
Y: 0.1 mm
Number of Cells: 11 948
RAM used:~**1 MB**





Cell size:
X: 0.5 mm
Y: 0.1 mm
Z: 0.1 mm
Number of Cells: 1 212 516
RAM used:~**117 MB**

Two models are considered, for which accuracy and efficiency will be compared: classical full 3D and BoR developed in this work. In both models, the meshing in the axial direction is set to 0.5 mm while 0.1 mm is used in the cross-section (of which only the radial direction is discretised in the BoR model). To generate a steady state, the models are bounded by a source and a load and excited by a sinusoidal TEM field. Here, the frequency of 2.45 GHz is used for compatibility with ISM microwave applications and in the range of GHz technologies explored in for battery materials' testing.



Transmission Line excited by sinusoidal TEM field with frequency of **2.45 GHz**

Total heating time: **10 sec**.
with a <u>single</u> heating step

Coupled electromagnetic and thermal simulation of axisymmetrical microwave process – **Simulation parameters**

Tab 2. The final parameters of the electromagnetic and heat flow simulation procedure performed for the battery model.

Calculations method	BoR FDTD			3D		
	Simulation time (min:sec)	Iterations	Number of cells	Simulation time (min:sec)	Iterations	Number of cells
EM	0:04	17647	11948	0:54	20504	1212516
HFM	0:08	1764		1:36	2050	

Tab 3. Simulation times obtained after the heating procedure with the heat flow module for different electrolyte thicknesses of the BoR FDTD and 3D model with adiabatic boundary conditions.

Thickness of electrolyte [mm]	BoR FDTD	3D
	Simulation time (min:sec)	Simulation time (min:sec)
1	0:08	0:59
10	0:10	1:06
20	0:10	1:39
30	0:11	2:03
40	0:12	2:21

Coupled electromagnetic and thermal simulation of axisymmetrical microwave proces - **Results**

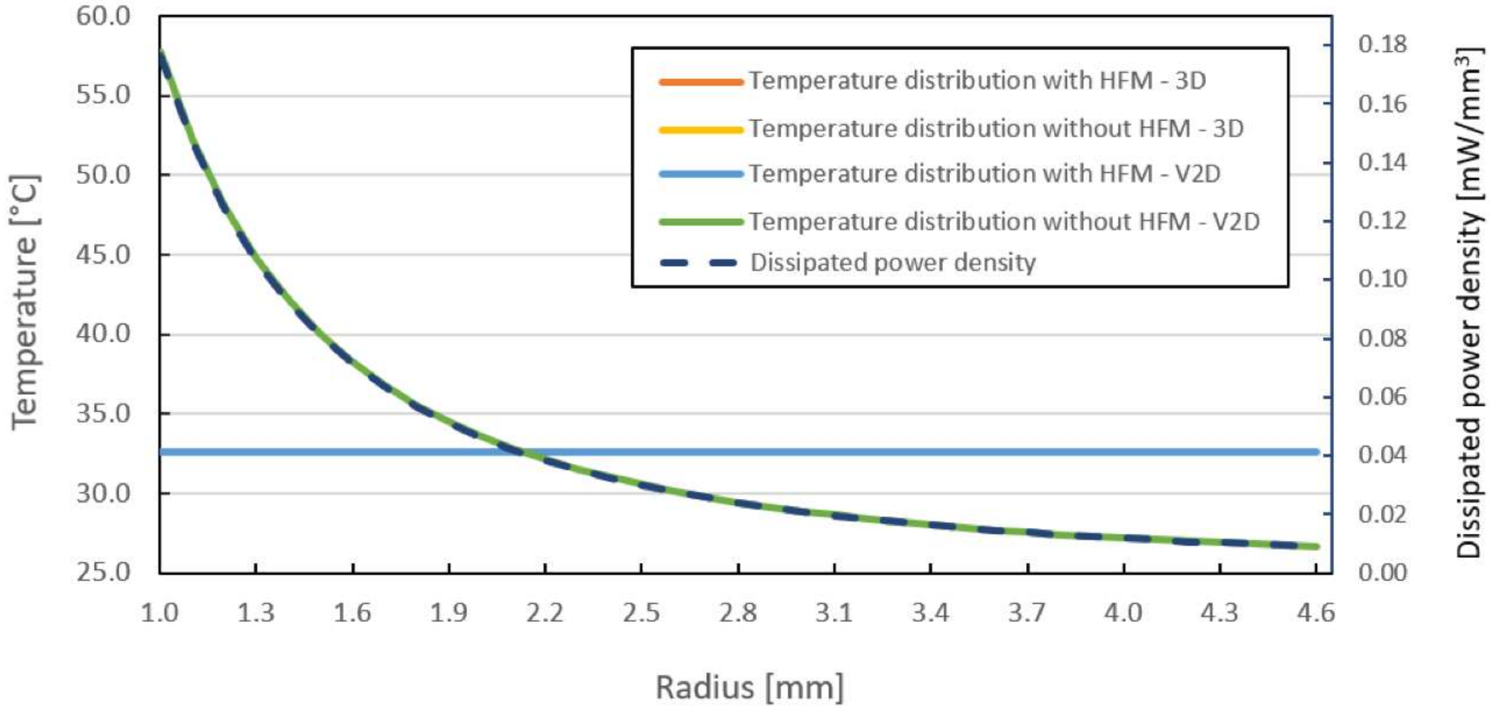


Fig. 2. Temperature distribution for heating simulations without and with flow with adiabatic boundary conditions in the radial direction (on the inner and outer conducting electrode) at an initial temperature of 25 °C – BoR and 3D results overlap.

Extension to a nonlinear microwave process in axisymmetrical resonators – **Microwave heating device**

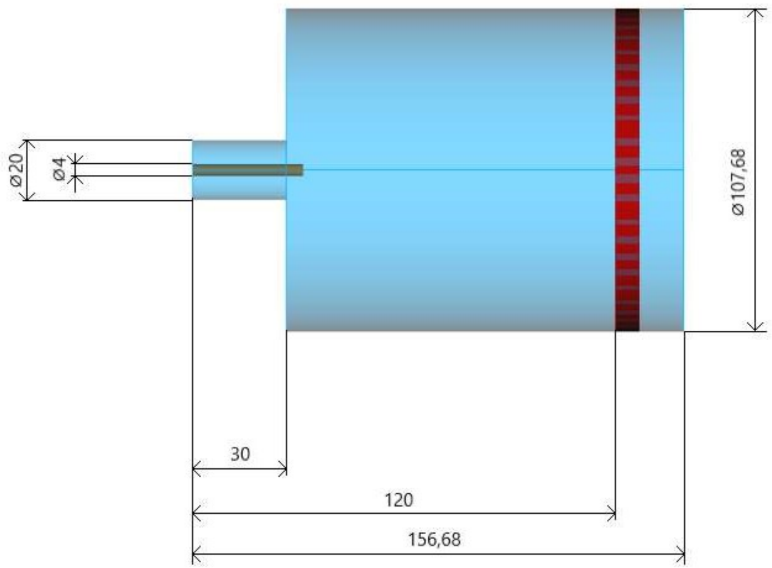


Fig. 3. Considered microwave applicator, it's dimensions after Per O. Risman, United States Patent

The previous BoR FDTD algorithm with a heat flow module will be extended with an algorithm for automatic updating of material parameters as a function of temperature. The device itself is designed to produce TM_{011} wave patterns, TM_{010} wave patterns, or a combination of the two, depending on the object's dielectric constant. The applicator's dimensions are carefully selected to meet two conditions: to create cylindrical TM_{011}.

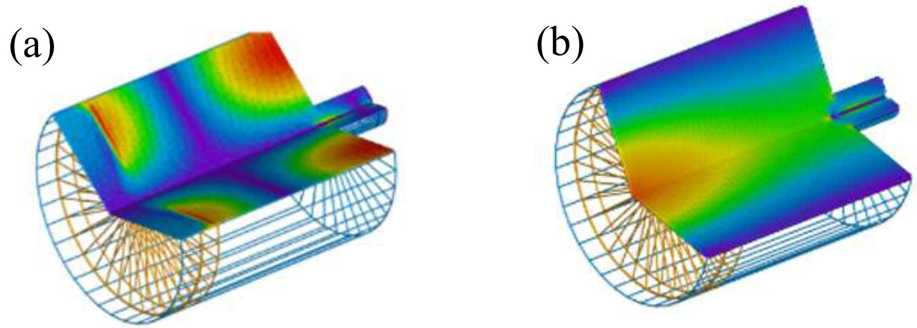


Fig. 4. Distribution of the (a) magnetic field and (b) electric field of the TM_{011} mode, in a 270 degree view of the cylinder.

Extension to a nonlinear microwave process in axisymmetrical resonators – **Eigenvalue problem**

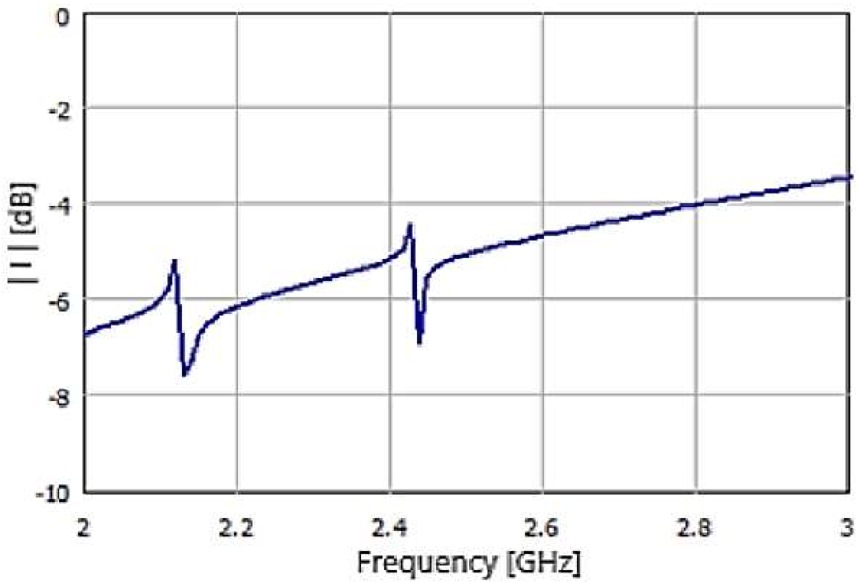


Fig. 5. Fourier transform of current flowing between the virtual point source and the resonator.

From equation below for the obtained radius, the frequencies for TM_{010} and TM_{011} modes are analytically calculated as **2.13 GHz** and **2.44 GHz**.

$$f_{c,TMmn} = \frac{c}{2\pi}\frac{\chi_{m,n}}{r},$$

where **fc** is the cutoff frequency [Hz], **c** is the speed of light in vacuum [m/s], **r** is the radius of the waveguide [mm] and χ**m,n** is n-th root of m-th Bessel function.

We first create a pure EM model and simulate it with BoR FDTD. We aim to solve an eigenvalue problem in the cylindrical applicator, confirming the analytically pre-calculated eigenfrequencies. To this end, we eliminate the feeding structure and simulate only the cylindrical. Since FDTD is in itself a deterministic method, we need to approximate the eigenvalue problem by a resonant deterministic problem. We do so by inserting a **virtual point source** connected to a longitudinal E-field node close to the axis of rotation.

Extension to a nonlinear microwave process in axisymmetrical resonators – **Bread case**

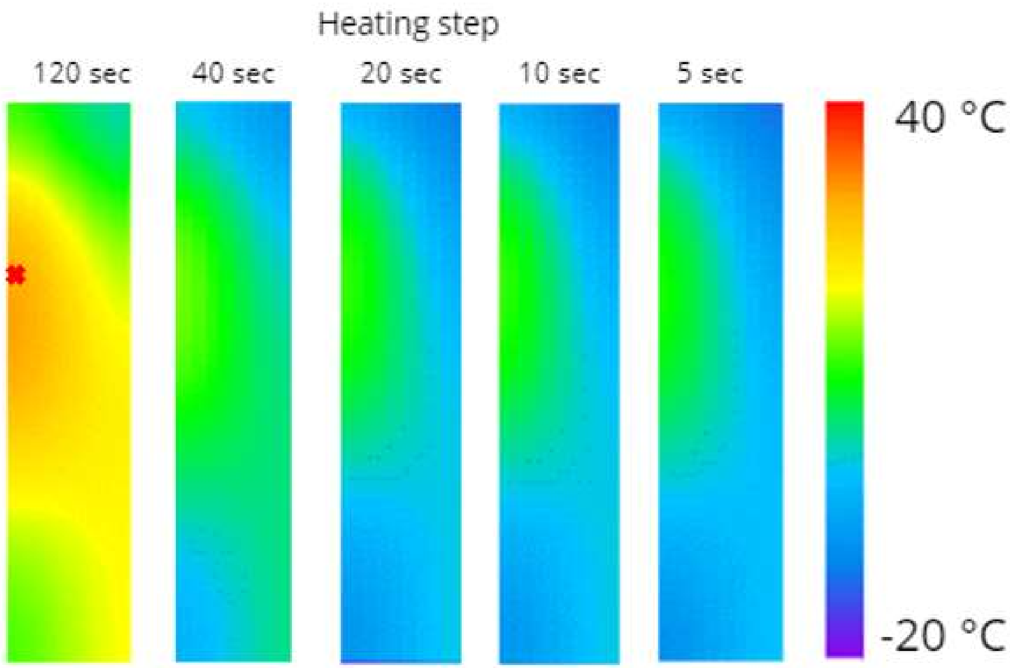
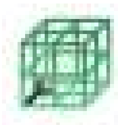
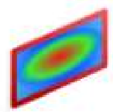


Fig. 6. Distribution of final temperature in bread after heating for 120 sec, including heat flow phenomenon – parameterised simulations using different heating steps. Red spot means hot spot in bread.

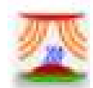
One of the heated objects is bread, whose parameters are defined as temperature-independent constants. It will serve as a test of the algorithm and a comparison with temperature-dependent material. The electrical conductivity of bread is equal **0.221 S/m** and the effective permittivity is **4.17**. The simulation assumes an initial temperature of **-20 °C**.



The meshing is uniform in both directions and is **1 mm**.



Transmission Line excited by sinusoidal TEM field with frequency of **2.13 GHz**



Total heating time: **120 sec**.
with steps; 5, 10, 20, 40, 120 sec.

Extension to a nonlinear microwave process in axisymmetrical resonators – **Bread case**

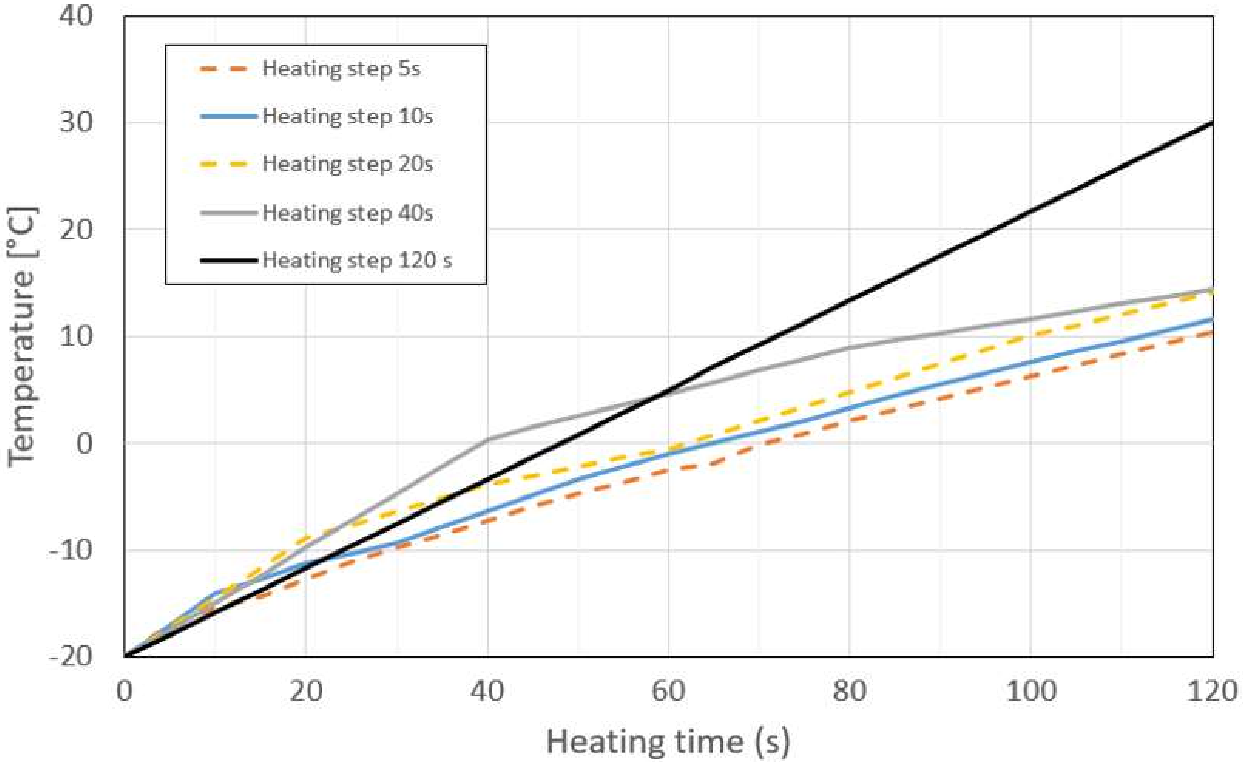
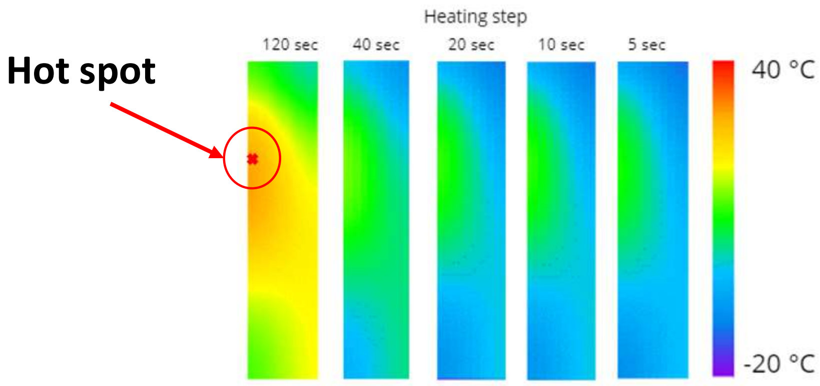


Fig. 7. Comparison of temperature evolution in simulated bread **hot spot** in heating simulations including heat flow.



What it can be notice at Fig. 7 is that when we increase the number of steps during heating the bread including the heat flow module, the temperature doesn't go up so quickly. This happens because we are splitting the total power delivered over 120 seconds into smaller parts. That means there are more instances of heat flow during the simulation.

Extension to a nonlinear microwave process in axisymmetrical resonators – **Beef case**

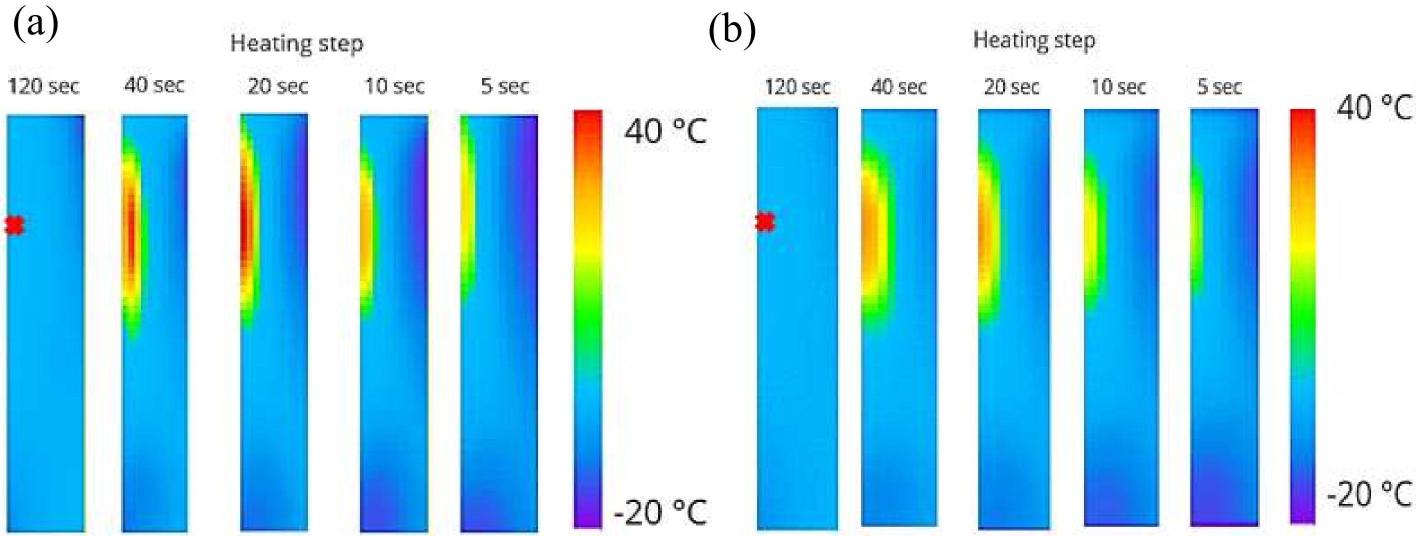
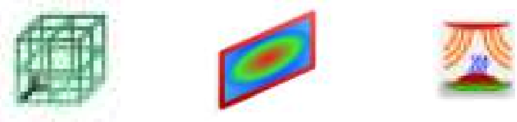


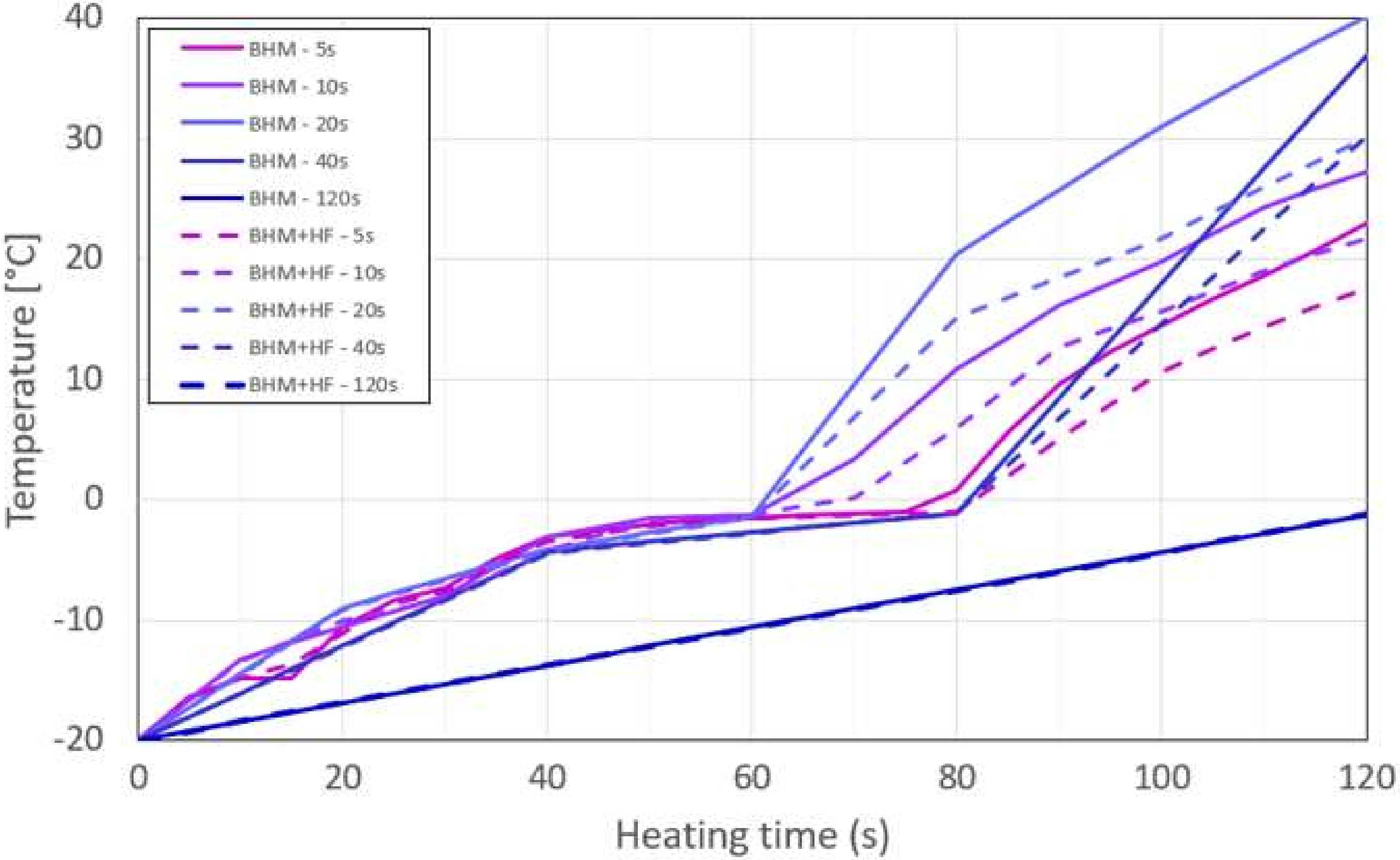
Fig. 8. Distribution of final temperature in beef after heating for 120 seconds (a) heat flow neglected (b) including heat flow phenomenon. Parameterised simulations using different heating steps. Red spot means hot spot in beef.

The second material considered is beef whose parameters depend significantly on temperature. Parameters are also as in [17]. The relative permittivity changes from **4.9** to **41.7** in the temperature range from **-20** to **80 °C**. In the same range, its conductivity changes from **0.064** to **2.426 S/m** maximum conductivity, which occurs in the **-1 °C**.



Simulation parameters are the same as in bread case.

Extension to a nonlinear microwave process in axisymmetrical resonators – **Beef case**



When beef gets to around -1 °C its properties start changing significantly. It is important to mention that Fig. 8 shows that after 120 seconds, the values for BHM and BHM+HF are a bit different by 0.02 °C.

Fig. 9. Comparison of temperature evolution in simulated beef hot spot in with and without considering heat flow with different simulation time step.

Conclusions and future work…

1. **Extension of Bodies-of-Revolution FDTD Algorithm**:
    1. The Bodies-of-Revolution FDTD algorithm has been extended to address coupled nonlinear electromagnetic-thermal problems, including heat flow phenomena and temperature-dependent material parameters.
2. **Improved Simulation Efficiency**:
    1. Comparative analysis with 3D modeling demonstrates significantly reduced simulation times using the BoR approach.
    2. This efficiency gain is expected to be even more pronounced in more complex models.
3. **Application to Cylindrical Microwave Heating:**
    1. The algorithm was applied to a cylindrical microwave heating applicator, initially treating it as an electromagnetic eigenvalue and deterministic problem. Subsequently, it was expanded to a multiphysics problem to account for thermal effects.
4. **Ongoing Work on Charge Transport Mechanisms:**
    1. Current research efforts are directed towards incorporating charge transport mechanisms into the multiphysics problem.
    2. This is especially significant for the battery industry to enhance the accuracy of characterizing energy materials, such as those used in Li-ion batteries.
    3. The developed solvers, along with representative examples, are accessible through the Open Platform of **NanoBat** and **I4Bags** projects.

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...And thank you for your attention!