# Modeling of large microwave cavities for industrial and scientific applications

The cavities of microwave heating devices need to be carefully designed in order to ensure safe, efficient operation and homogeneous field distributions. The size, the number of modes and the resonant nature of a cavity can pose difficulties for their simulation. This paper discusses the modeling of microwave cavities and demonstrates how a system for heating test samples was optimized using electromagnetic simulation.

Microwave heating is increasingly used in industrial processes for drying and curing products, since it has a number of advantages over electrical heating – chief among them being energy efficiency. Many products can be thoroughly penetrated by microwaves, resulting in simultaneous inner and outer heating of the material. Furthermore, microwave heating takes place even below the skin depth, albeit with a much smaller amount of energy than above the skin depth. The surface of the heated material radiates heat to the environment and is therefore cooled, while the interior cannot lose heat and so may actually be hotter than the surface. This results in a temperature profile inverse to the one obtained by conventional heating and yields heating and drying times much shorter than those obtained by conventional methods – another major advantage of microwave heating. With properly designed microwave heating equipment, an even temperature profile can often be obtained inside the material, with a nearly uniform temperature distribution.

Applications of industrial microwave heating include pre-drying of fabrics, drying of wood and fiberglass, eradication of pests in food crops after harvest, pasteurization of pasta, curing of synthetic fibers and composite materials, and post-curing of fiber-optic and optoelectronic adhesives. In the most common arrangement, products are exposed to microwave radiation for a duration of time as they are continuously moved by a conveyor. Microwave energy is contained in a cavity providing for the entrance, passage and exit of products. The cavity tends to be electrically large, in order to accommodate processing the largest product volumes possible to maximize the efficiency of the industrial process.

In scientific applications of microwave heating or excitation, a test sample is typically exposed to time-varying electromagnetic fields of a desired intensity and polarization, and the sample's response to the fields as a function of time is observed. In order to measure the sample's responses, the microwave cavity needs to be large enough to accommodate a suite of sensors in addition to the sample itself. As a result, microwave cavities for scientific experiments also tend to be electrically large.

The main goal of microwave cavity and feeding system design for industrial applications is to maximize the delivery of microwave power to a predetermined volume of space. The secondary goal, whenever design constraints allow, is to control the power distribution within the volume to facilitate uniform heating. In scientific applications, instead of uniformity of heating, requirements typically call for well-defined distributions of E-field and/or B-field. Often, field deviations and inhomogeneity within the test sample space need to be minimized. In addition, engineers usually need specific polarization properties of the fields. This paper will show how the high-frequency electromagnetic simulation tool CST STUDIO SUITE® can be successfully used in optimization of these properties.

## Simulation considerations
### Choice of solver

Being electrically large, the cavities of microwave heating apparatuses are overmoded microwave resonators. Household microwave ovens – some of the smallest microwave heating devices in use – employ cavities ranging in size typically from 20 to 60 cubic wavelengths at the frequency of operation (2.45 GHz), but industrial cavities can be hundreds or thousands of cubic wavelengths in size. The cavity size alone presents a computational domain of appreciable volume and handling it can be a non-trivial task in numerical calculations.

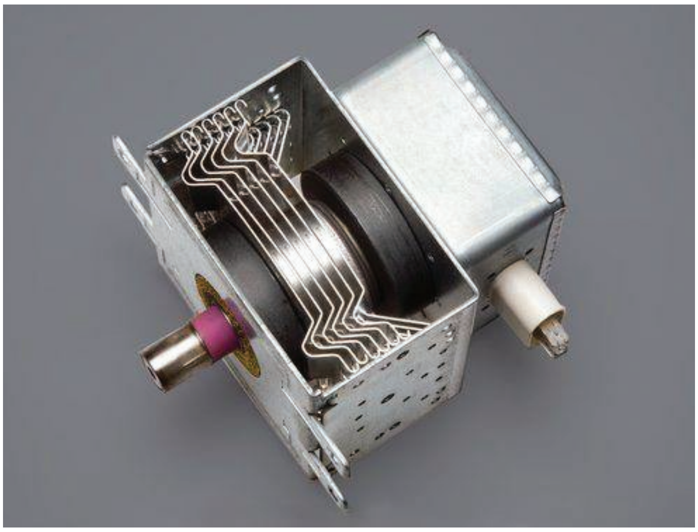

**Figure 1** 700W magnetron of typical household microwave oven.

Moreover, any meaningful electromagnetic analysis of the cavity also has to include the system that couples microwave energy to the cavity. This could be the probe of a magnetron (**Figure 1**) directly inserted into the cavity or the end section of the waveguide that conveys energy from a microwave source to the cavity. The simulation of the sources themselves is beyond the scope of this article – for more information on magnetron simulation, please see the CST whitepaper "A Multiphysics Approach to Magnetron and Microwave Oven Design".

Increasing the complexity further, some microwave heating devices use rotating field stirrers to counteract the two primary limitations of most microwave ovens: electrically hot and cold regions in the microwave cavity, and arcing to metal objects such as utensils and aluminum foil. In order to properly assess the effects of a field stirrer, electromagnetic fields within the cavity have to be modeled several times, corresponding to the critical angular positions of the stirrer over a rotation cycle. When a numerical optimization by repeated analyses of such a problem is called for, high-performance computing methods such as GPU processing and distributed computing are invaluable for carrying out the calculations in a reasonable time.

Both time and frequency-domain computational electromagnetics modeling techniques have their place in the analysis of microwave heating systems. Since time-domain solutions can cover a wide frequency range with a single simulation, these are particularly suitable for the first, quick-look assessment of impedance match, which provides valuable information about the amount of coupling of individual electromagnetic field modes into the microwave cavity. If a particular mode is not coupled to the desired degree, this can be rectified by adjusting the cavity dimensions, if this is allowed by the product requirements, or relocating or redesigning the cavity feeding system.

On the other hand, time-domain techniques are generally poorly suited for the analysis of systems with a high quality factor, such as empty microwave cavities, since the techniques require very long simulation times to allow the energy in the system to dissipate to sufficiently low levels; frequency-domain solvers are much better suited for this type of analysis. Electromagnetic simulations of empty, unloaded resonant microwave cavities are important for determining parameters such as the maximum electric current flowing through the probe of the feeding magnetron. If the current density is too high, it can cause the magnetron probe to wear prematurely or even fail destructively.

## Meshing and model detail

Both time and frequency-domain techniques require that the entire computational domain be meshed. In order for the simulation to be meaningful, the mesh spatial discretization must be sufficiently fine to resolve the smallest electromagnetic wavelength in the model. The usual rules of thumb additionally require the grid spatial discretization to resolve also the smallest geometrical feature in the model. While this is justified in general, analyzing the problem this way is not always feasible or necessary. A manageable way of analyzing large microwave cavities rests in judicious application of subgridding techniques [1] to mesh the computational domain.

For example, in many practical applications, the modeling of the cavity walls in full detail becomes less important the electrically larger the cavity is. A number of structural features such as indentations and ribs increasing the mechanical stiffness of the cavity walls can be neglected without affecting the accuracy of the simulation significantly. At the same time, features that are crucial for the particular purpose of the electromagnetic simulation must be modeled precisely. For example, if investigating the effectiveness of the microwave seal, it must be modeled in the utmost detail and without approximations. This approach, using CST STUDIO SUITE, was utilized to successfully design an electromagnetic bandgap seal for a microwave oven, described in [2].

## Practical example
### Background

One widespread example of a scientific application for microwave cavities is the multi-sample dissolution dynamic nuclear polarization (DNP) system for magnetic resonance imaging purposes operating in cryogenic conditions at 94 GHz described in detail in [3]. Dynamic nuclear polarization is a technique to transfer spin polarization from electrons to nuclei by continuous microwave irradiation of the electron spins in a static external magnetic field. The method is mostly used to generate small molecules with high spin polarization that are subsequently dissolved by superheated water. The molecules can then be used in medical diagnostics to follow metabolic pathways using magnetic-resonance imaging techniques [4]. The polarization transfer by DNP requires continuous microwave irradiation at a frequency close to the resonance frequency of the electron paramagnetic resonance (EPR). Consequently a facility for microwave irradiation of the test sample is needed. In the built DNP system, a resonant microwave cavity is used to increase the DNP efficiency at low incident microwave power while also minimizing dielectric heating of the sample during microwave irradiation. For monitoring the nuclear polarization during DNP experiments as well as for investigation of the DNP process itself, nuclear magnetic resonance (NMR) and EPR capabilities are included in the polarizer, allowing NMR and EPR measurements to be carried out on the sample at the location of the cavity.

The DNP system accommodates up to six samples in a revolver-style sample changer that allows the changing of samples at liquid-helium temperature down to 1.4 K and at pressures ranging from ambient down to 1 mbar. In the system, six identical metallic cups, each capable of forming the bottom part of the microwave cavity, can in turn be coupled with one shared top part of the cavity to form a resonant microwave structure. This construction allows the microwave cavity, built from non-magnetic brass as shown in Figure 2, to be opened to change the samples. To ensure correct closing of the cavity, the metallic cups are mounted on sapphire beads acting as spherical bearings. Correct functioning of the closing mechanism is checked by means of a vertical lift monitor.

The shared top part of the cavity also contains an NMR coil to determine the nuclear polarization levels of the test sample. The coil, built to be compatible with the revolver mechanism, is of the saddle type with two effective windings, and allows NMR experiments at all operating temperatures. For monitoring of the EPR spectrum under DNP conditions, a solenoid EPR coil enabling longitudinal detection of EPR is wound on the outer surface of the shared top part of the cavity. The coil's axis is aligned with that of the cavity. The EPR detection utilizes modulation frequencies in the range of 1 kHz. In the area of the EPR coil, the brass wall of the cavity was chosen to be only 400 µm thick, below 10% of the skin depth of brass at the frequency of 1 kHz. The EPR coil consists of 380 turns of a 100 µm diameter copper wire. The EPR detection circuit is non-resonant and well insulated from ground to minimize cross talk with the power-modulation signal.

The DNP system is inserted in a cryostat. Liquid helium is dragged into the sample space by evacuating the cryostat with two vacuum pumps. Through a capillary, liquid helium is guided to the bottom of the cryostat and enters the sample space. As the liquid helium bath inside the cavity boils, the exhaust gas leaves the cavity through a set of microholes drilled into the cavity lid. Temperatures down to 1.4 K in the sample space are achieved.

The frozen samples under test sit in sample cups made of PCTFE, as shown in Figure 2. Each cup is closed by a perforated lid permitting the dissolution medium to penetrate during dissolution. The lid prevents frozen sample beads from being jolted out of the cup during movement of the revolver or due to boiling helium. The lower sections of the sample cups are hollow.

## Simulation

The microwave cavity measures 218 cubic wavelengths in internal volume and is designed to yield a high quality factor, so as to efficiently use the available microwave power, allowing for cost-effective sources; to focus the excited microwave magnetic field within the sample volume, and to minimize the electric field at the sample location, so as to avoid dielectric heating of the sample. Oversized (overmoded) cavities generally offer enough flexibility to achieve the abovementioned goals to some extent. The designed cavity and its feeding system (Figure 2a) have been optimized, using CST STUDIO SUITE, to maximize and homogenize the transverse component of the magnetic fields within the sample volume (Figure 2b). For this purpose, eight metallic rods, acting as a mode filter, are placed inside the cavity. The four located in the bottom part of the cavity also facilitate accurate positioning of the sample cup, guiding the cup to the correct position as the cup is lowered by a grabber (not shown in Figure 2) into the bottom part of the cavity. The metallic rods, by enforcing zero tangential *E*-field components on the rod surfaces, reduce the *B*-field magnitudes in the upper and lower sections of the cavity. This can be seen in Figure 3, which shows the computed *B*-field magnitude in the cavity with only the test sample present.

Performance tests of the microwave system have demonstrated that the microwave magnetic field is effectively concentrated at the sample location, requiring only 10–20 mW of microwave power measured at the microwave source for reaching maximum DNP enhancements [3]. Due to the low power requirements achieved in the cavity, lower temperatures can be reached and, therefore, higher polarization levels can be achieved than in comparable designs.

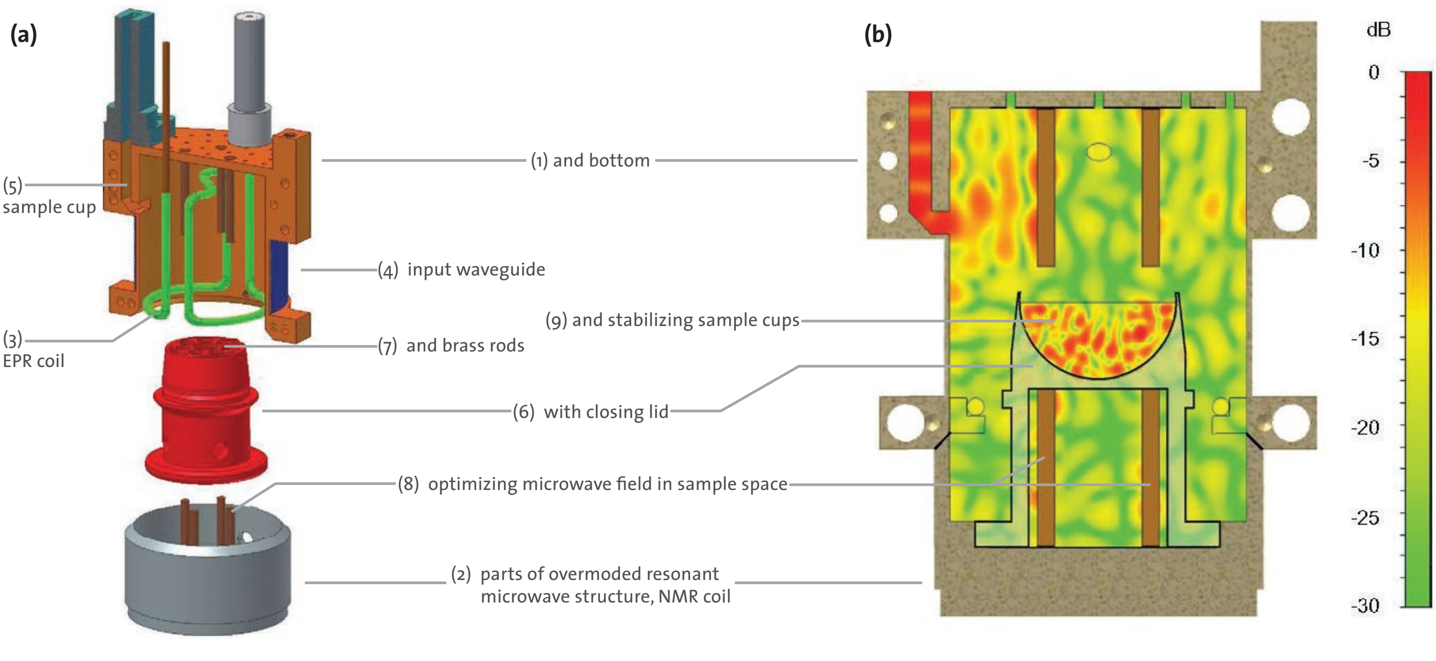


**Figure 2**

**(a)** Microwave cavity of DNP system at 94 GHz. Top (1) and bottom (2) parts of overmoded resonant microwave structure, NMR coil (3), EPR coil (4), input waveguide (5), sample cup (6) with closing lid (7) and brass rods (8) optimizing microwave field in sample space (9) and stabilizing sample cups. **(b)** Longitudinal cross-section of microwave cavity. Overlaid is computed normal component of B-field, plotted in dB with respect to maximum B field found in input waveguide. (Reproduced with permission from [3].)

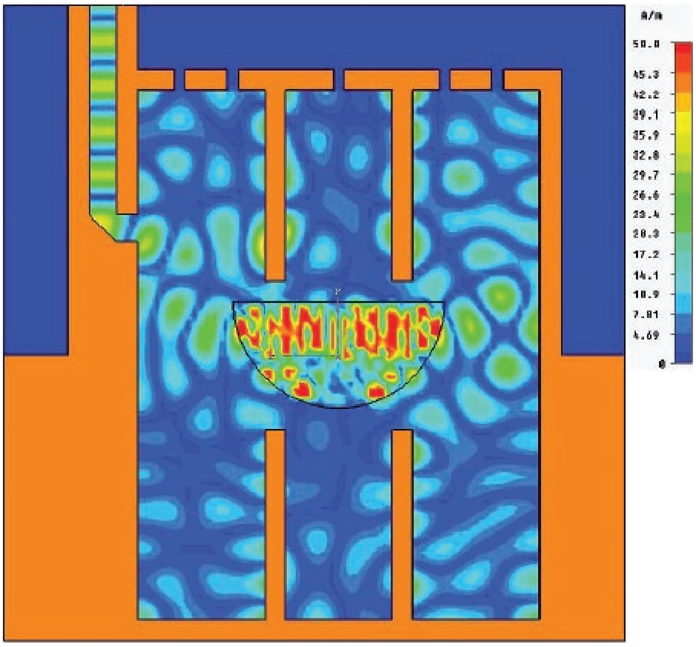


**Figure 3** Computed H-field magnitude in microwave cavity with only test sample present at 94 GHz.

## Conclusion

EM simulation offers great potential for designing and optimizing microwave heating and excitation cavities. Different solver types are needed for different classes of problem: time-domain techniques are well suited to broadband analysis, such as identifying different cavity modes, but struggle with very resonant cavities. For investigating high Q-factor cavities, frequency-domain techniques are far more suitable.

The use of simulation was demonstrated using a real-world example of a dynamic nuclear polarization system. This device includes a microwave cavity for irradiating samples, with brass rods used to adjust the E and B-fields inside the cavity. The lengths of these rods were optimized to give a large, homogeneous field over the region of interest, improving the efficiency and accuracy of the device.

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[4] K. Golman *et al.*, "Molecular imaging with endogenous substances," *Proceedings of the National Academy of Sciences of the United States of America*, 100 (2003), pp. 10435–10439.

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