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Simulative Approach for Predicting the Heating Behavior of Elastomers in the Solid-State Microwave Heating Process

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Simulative Approach for Predicting the Heating Behavior of Elastomers in the Solid-State Microwave Heating Process

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Abstract: The increasing demand for energy efficient vulcanization of rubber extrusions requires the optimization and further development of existing processes. Microwave vulcanization allows the energy required for this process to be coupled directly into the material via dielectric losses. Microwave heating requires the polarity of the rubber so that the electromagnetic wave can cause the polar components of the material to vibrate. These vibrations cause internal friction, resulting in an increase in the temperature of the rubber compound. In this research project, microwaves were used to heat a rubber strand placed in a specially prepared waveguide. This method offers advantages over conventional methods, such as hot air vulcanization. A key advantage is that the energy is coupled directly into the material, resulting in low losses. In contrast to hot air vulcanization, where the air must first be heated, the heating of the material also takes place within the product to be heated. This results in a significant increase in energy efficiency, reaching up to 90 %. In addition, internal heating provides a more homogeneous heat distribution in the rubber strand compared to external heating by hot air vulcanization. To predict the heating behavior of rubber in the microwave process, a simulative model is created in the multiphysics simulation environment CST Studio Suite®. The model describes the microwave heating behavior of rubbers based on the thermodynamic and electromagnetic material data of the rubber compound. This simulation is known as a bi-directional simulation, so that temperature-dependent variables such as dielectric loss and thermal conductivity can be considered. The model is used to analyze parameter variations of the electromagnetic wave frequency, waveguide geometry, and strand orientation in the waveguide. Finally, optimized settings for the real process are recommended.

Keywords: Microwave Heating, Solid-State, Rubber, Simulation, CST Studio Suite, Dielectric Loss, Efficiency, Optimization, Waveguide, Microwave, Heating, Vulcanization

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Introduction

In rubber extrusion processes, it is important to achieve homogenous crosslinking throughout the material's cross-section to ensure consistent properties in the final product [1-3]. Achieving high energy efficiency is also crucial for the vulcanization process from an economic point of view, as it allows for high throughput in a short time while minimizing energy consumption [3-5]. In conventional vulcanization processes like hot-air vulcanization, heat is conducted from the outside to the inside of the material. Thus, the heat capacity, thermal conductivity, and heat transfer between the elastomer and the intermediate medium play significant roles in the vulcanization process. Elastomers generally have low thermal conductivity, which can result in thermal damage in the edges of thick-walled profiles while the core remains insufficiently heated and in a plastic state. With good insulation and a vulcanization energy requirement of 0.1 kWh/kg, the total system energy requirement is approximately 0.3 kWh/kg. This results in a relatively low efficiency of 33 % [6].

To ensure a higher efficiency of energy input, a uniform temperature distribution, and consistent vulcanization across the cross-section, dissipative heat input is necessary within the extrudate. Microwave irradiation provides an effective means of achieving this internal heat input. The heating process primarily occurs through the electrical component of the electromagnetic wave. As the wave penetrates the material, a phase shift occurs between the electric field and the polarization of the polar components within the material [7]. This reorientation of dipoles generates internal friction, which leads to a heating of the elastomer. This phenomenon is known as dielectric loss. To describe this process, the materials loss angle is required [8], equation 1.

$$tan\delta = \frac{\epsilon_r''}{\epsilon_r'} \tag{1}$$

In the given equation, the loss angle is denoted as δ, the imaginary part of the permittivity as ϵ_r'', and the real part as ϵ_r'. The loss angle represents a material-specific parameter that exhibits an increase with greater polarity. Furthermore, the value of the loss angle is contingent on both the material's temperature and the frequency of the electromagnetic field. By employing the loss angle, the energy P_V imparted into the material volume can be determined through the utilization of the field strength $\vec{E}$ and the fields frequency f. The energy P_V can be evaluated based on the field strength, as indicated by equation 2 [8].

$$P_V = 2 \cdot \pi \cdot f \cdot \epsilon_0 \int_V \epsilon_r' \cdot tan\,\delta \cdot \left|\vec{E}\right|^2 \cdot dV \tag{2}$$

Microwave rubber profile vulcanization emerged in the 1960s to enhance productivity and quality. Early microwave ovens employed either a waveguide or resonant design but faced issues with uniform heating. Due to an inadequate dielectric loss factor and narrow, intricate profiles, satisfactory

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results could not be obtained. Furthermore, certain products had metal cores that acted as antennas for the electromagnetic wave, making microwave heating difficult. Moreover, rapid heating of certain materials caused thermal degradation of the extrudate.

As in 1994 [9], Krieger investigated the microwave heating behavior of rubber extrudates, taking into account the temperature inhomogeneity at the extruder outlet. He found that the areas of the extrudate with higher temperatures are heated more intensively. Thus, temperature differences already present during the shaping of the extrudate are amplified during microwave treatment. In addition, he has already shown that polar rubbers such as acrylonitrile-butadiene rubber (NBR) or polychloroprene rubber (CR) can be heated significantly faster than non-polar rubbers such as natural rubber (NR) or polyisobutylene rubber (IIR). However, he did not describe this behavior in detail but carried out general studies of heating behavior.

In 2010, Makul et al. [10] further investigated the pre-curing behavior of NR using a rectangular waveguide under varying sulfur content. They found that treatment with a microwave frequency of 2.45 GHz in the pre-curing process led to crosslinking of NR already below the vulcanization temperature. It was also shown that the sulfur content had only a minor influence on the absorption behavior of the rubber, while an increase in the carbon black content led to a higher absorption of the microwave energy. Furthermore, an initial basis for a mathematical model of the microwave heating of NR in a stationary process could be generated.

In 2022, Okumura et al. [11] investigated the heating behavior of microwaves in the in-mold tire manufacturing process. They were also able to show that blended carbon black serves as a heat source for microwave vulcanization. As a result, rapid vulcanization was achieved by microwave irradiation compared to conventional processes. However, it should be noted that the heating has an exponential temperature curve over time, which leads to problems in process control. By using a variable frequency microwave between 5.85GHz – 6.65 GHz, this problem could be reduced in the stationary vulcanization process.

Materials

In order to generate a comparatively high absorption behavior of the electromagnetic waves, a material with a high dielectric loss is initially selected for the simulative approach explained in this paper. This material is Nitrile Butadiene Rubber (NBR). The temperature-dependent material parameters permittivity, loss angle, thermal conductivity, specific heat capacity and density have been determined from a real compound. The thermal conductivity was determined using a Laser Flash Analyzer (LFA 467 HyperFlash ©) from NETZSCH-Gerätebau GmbH. The heat capacity was determined by using dynamic differential calorimetry, employing a DSC 3+ apparatus from Mettler-Toledo. The material density was determined using the ME204T/00 analytical balance from Mettler-Toledo. The electrical material parameters, permittivity, and dielectric loss angle were

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measured externally at the Fraunhofer Institute for Chemical Technology (ICT) in the field of microwave and plasma technology. The material parameters thus determined are presented in Table 1.

Table 1. Material parameters for the simulation.

Material Parameter	Unit	Value
Permittivity	-	4.11
Loss angle (at 2.56 GHz)	-	0.04
Thermal conductivity	W/K · m	0.24
Specific heat capacity	J/K · kg	2000
Density	kg/m³	1166

In the simulation environment, a 30 mm x 30 mm x 4 mm cuboid was created based on the material data in Table 1. In addition, a more complex geometry was analyzed based on a sealing profile. The geometry of the sealing profile is shown in the Figure 1.

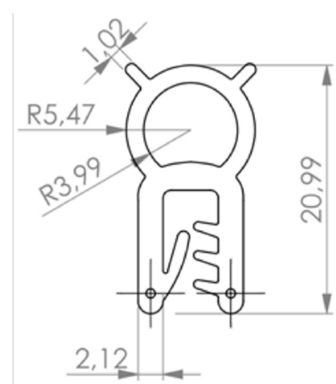

Figure 1. Geometry – Sealing profile (dimensions are given in mm).

Equipment

CST Studio Suite® software is used in this paper for microwave-based heating simulations. This comprehensive software simulates electromagnetic fields and, with additional solvers, can address thermal, mechanical, and other problems. Thermal calculations are facilitated by the CST MPhysics Studio® package, which includes an ACIS-based 3D modeling environment and automatic meshing. A key feature of CST MPhysics Studio® is complete parameterization, allowing easy adjustments of dimensions and automatic maintenance of aspect ratios. Multiphysics simulations in CST Studio Suite® link electromagnetic and thermal models, with options for unidirectional

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or bidirectional transfer of calculated values. If the models depend on each other, e.g., if the field-determining material parameters such as permittivity are temperature-dependent, a bi-directional coupling can be selected. Knowledge of the temperature dependence of the material parameters is critical. For this type of coupling, the number of iterations must be specified, which determines how often both models are to be calculated with the respective changed variables. CST Studio Suite® then proceeds as follows: First, the electromagnetic field is calculated in the model, then the thermal losses are calculated from the simulation results and passed to the thermal solver, which calculates the thermal fields based on the values. The results are used as modified parameters for the new calculation of the EM field. This is repeated for the selected number of iterations. Both solvers base their calculations on the same master model, and global parameters can be defined that are shared between the two subprojects. A schematic representation of the simulation process is shown in Figure 2 [12].

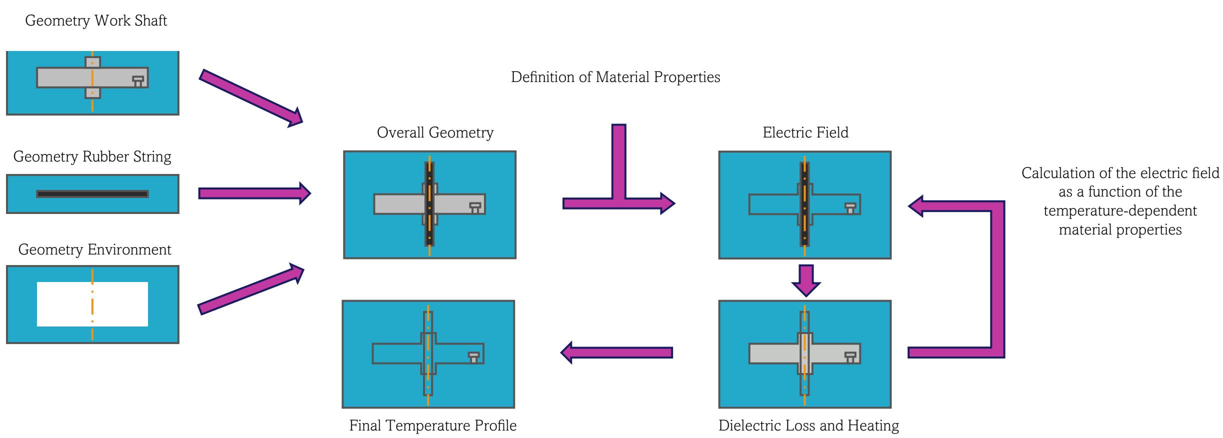

Figure 2. Schematic representation of the iterative heating simulation with consideration of the temperature-dependent material parameters.

Results

The temperature distribution across the cross section of the rubber specimen and the homogeneity of the temperature distribution were used to analyze the simulation results. As described in equation 3, the assessment of the temperature distribution is calculated by the difference between the maximum temperature T_{max} and the minimum temperature T_{min} in relation to the difference between the average temperature T_{mean} and the ambient temperature T_0. This results in an ideal homogeneity of the temperature distribution for a homogeneity index of zero.

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$$Homogeneity\ index = \frac{T_{max} - T_{min}}{T_{mean} - T_0} \quad 3)$$

A rectangular waveguide, a common tool in electrical engineering, was employed in the model to guide the electromagnetic wave. This metallic structure enables the almost loss-free transmission of microwaves while ensuring effective shielding from the surrounding environment. As shown in Figure 3, it was observed that an H_{10} standing wave forms in the rectangular waveguide. The index 10 indicates the number of half waves of the electric field components in the corresponding directions within the rectangular waveguide. Here, “1” means that there is a half-wave in the wider dimension of the rectangle and “0” means that there is no half-wave in the narrower dimension of the rectangle. It should be noted that the field distribution is uneven, particularly in the region near the waveguide opening where the rubber string passes through, compared to the rest of the structure. It was also observed from the electric field that the introduction of a dielectric, in this case rubber, leads to a reduction in the field strength. Both phenomena are shown in Figure 3.

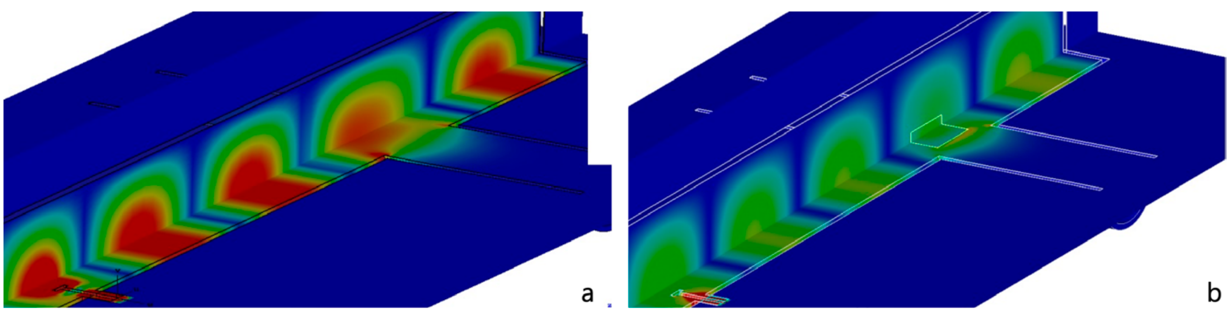

Figure 3. (a) Expansion of the E-field without test specimen (empty waveguide) f = 2450 MHz, (b) Expansion of the E-field with cuboid test specimen f = 2450 MHz.

The process parameters were also optimized. This was done by varying the length of the rectangular waveguide. The output length of the waveguide l_c was extended by an offset as shown in Figure 4. During the simulations, the power consumption was kept constant at 450 W.

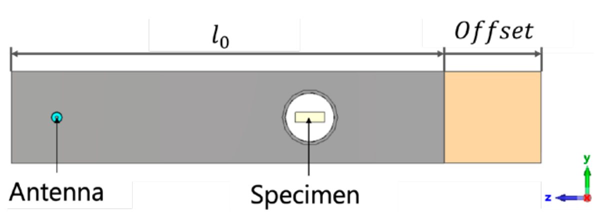

Figure 4. Parametrization of the waveguide length.

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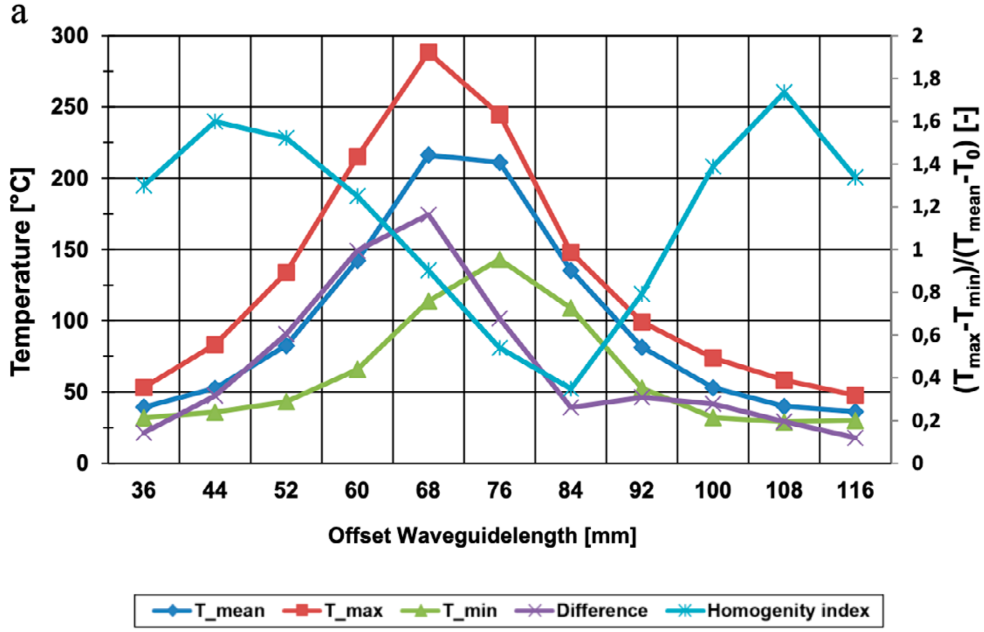
The results of the waveguide length sweep for the cuboid after 80 s of heating at a frequency of 2450 MHz are shown in Figure 5(a). The offset length in mm is shown on the abscissa, the temperature in °C on the left ordinate, and the homogeneity index in dimensionless form on the right ordinate. The simulations show that the mean temperature (dark blue), the maximum temperature (red), and the minimum temperature (green) increase from an offset length of 36 mm to 68 mm. This suggests that the maximum of the e-field at 68 mm is almost entirely in the region of the rubber specimen. This means that maximum temperatures of almost 300°C are reached. The average temperature is about 225°C. As the offset length increases, the temperatures decrease and reach a local minimum at 116 mm. The maximum temperatures there are only about 50°C. The homogeneity index of the heating, shown in light blue, reaches a local maximum of about 1.6 at 44 mm. It decreases with increasing offset length, with the best homogeneity at 84 mm and a homogeneity index of about 0.4. With further increase of the offset length, the homogeneity index increases and reaches a maximum of 1.8 at 108 mm. Thus, for a microwave heating process of a cuboid, an optimized process can be achieved at an offset length of 84 mm. At this point, the highest homogeneity is achieved as well as comparatively high temperatures of about 140°C, on average.

An offset length sweep was also performed for the sealing profile (Figure 5[b]). The cross section of the profile is smaller than that of the cuboid. Since an 80 s heating duration led to significantly higher temperatures, the heating time was subsequently reduced to 28 s. The average, maximum and minimum temperatures also decrease up to an offset length of approximately 32 mm and then increase up to a length of 74 mm. This means that temperatures of about 125°C can be reached on average. The temperature of this profile also decreases as the offset length increases. As with the cuboid, the shift of the field maxima can be observed, with the field maximum in the 74 mm range being very centered in the specimen. The homogeneity is best in the region around 80 mm with a homogeneity index of about 0.3. Therefore, an optimum at 80 mm could also be determined.

a



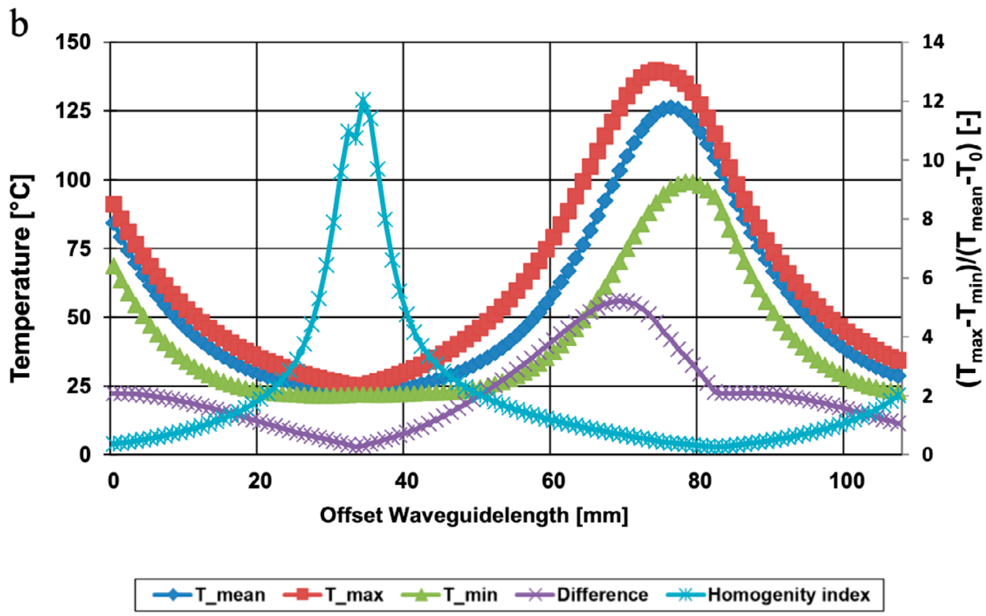


Figure 5. Temperature parameters – parameter sweep waveguide length (a) cuboid – heating time t = 80 s, (b) sealing profile – heating time t = 28 s.

Conclusions and Outlook

The simulation results show a promising approach to facilitate the design of microwave vulcanization systems. The simulation showed that the waveguide length in particular has significant influence on the propagation of the electromagnetic field. As a result, the offset length varied in this model could be optimized to approximately 80 mm for both the cuboid and the sealing profile. Both high energy input and high homogeneity were achieved. The model also showed that smaller geometries experience more homogeneous heating in the single mode process.

The model will now be validated with more complex geometries and then scaled up to industrial scale. The focus will be on optimizing the geometry of the working shaft. Experimental data from an industrial solid-state plant will also be generated to validate the simulated results.

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