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Optimization of the cylindrical CO_2 desorption reactor

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Abstract
Microwave heating offers a promising approach for efficient desorption in carbon capture. The COMSOL Multiphysics simulation study described here optimized microwave cavity design, revealing that optimal dimensions can absorb over 98% of input power. Positioning the waveguide at the cavity's middle height proved most effective, not only absorbing 1.6% more power but, possibly more importantly, providing uniform heating distribution. This configuration is ideal for fluidized bed reactors, potentially enhancing energy efficiency in carbon capture processes.
Keywords: Microwave heating, optimization of desorption reactor.

Introduction
Microwave heating for CO_2 desorption provides fast, low-temperature desorption, lowering energy requirements in carbon capture. According to studies, microwaves generate selective heating, dramatically increasing desorption rates compared to traditional approaches. This new technique shows potential for effective post-combustion carbon capture procedures [1-3].

Governing Equations
The time-harmonic electric field wave equation for the electric field can thus derived from Maxwell's equations and be written as:

$$\nabla \times \frac{1}{\mu_r}(\nabla \times \mathbf{E}) - k_0^2\left(\varepsilon_r - \frac{j\sigma}{\omega\varepsilon_0}\right)\mathbf{E} = 0$$
$$k_0 = \omega\sqrt{\varepsilon_0\mu_0} \qquad ...(1)$$
$$\omega = 2\pi f$$

where E is the electric field strength, where ε_0 is the free space permittivity ($8.854 \times 10^{-12}\ ^{V}/_{m}$), μ_0 is the free space permeability ($4\pi \times 10^{-7}\ ^{H}/_{m}$), ε_r is the material relative permittivity, μ_r is the material relative permeability, σ is the material electrical conductivity, ω is the angular frequency, f is the frequency, and k_0 is the wave number in free space.
The material permittivity can be written as:

$$\varepsilon = \varepsilon_0\varepsilon_r = \varepsilon' - j\varepsilon'' \qquad ...(2)$$

where ε' is the dielectric constant, and ε'' is the dielectric loss factor.

The following equation calculates the total volumetric power generated by the microwave:

$$Q_e = \frac{1}{2}\omega\,\varepsilon_0\varepsilon_r''|\mathbf{E}|^2 \qquad ...(3)$$

To calculate temperature distribution, use the heat transfer equation as follows:

$$(\rho C_p)_{eq}\frac{\delta T}{\delta t} - \nabla\cdot(k_{eq}\nabla T) = Q_e \qquad ...(4)$$

where T is the temperature, $(\rho C_p)_{eq}$ is the equivalent volumetric heat capacity, Q_e is the microwave heat source, and k_{eq} the equivalent thermal conductivity.
The equivalent volumetric heat capacity can be calculated as:

$$k_{eq} = v_s k_s + v_f k_f \qquad ...(5)$$

The equivalent thermal conductivity can be calculated as [1]:

$$(\rho C_p)_{eq} = v_s(\rho C_p)_s + v_f(\rho C_p)_f \qquad ...(6)$$

Boundary conditions
1. Electromagnetic boundary conditions

The rectangular waveguide input port is used to supply the microwave energy to the cavity with 2.45 GHz operating frequency and T_{10} mode of propagation. The impedance boundary conditions, which is used to define the cavity and waveguide walls.
2. Heat Transfer
The thermal insulation boundary condition is used to define the material boundaries

Method
A simulation study was constructed using the COMSOL Multiphysics program to investigate, simulate, and improve the heating process. A parametric sweep was performed for the case where the waveguide was positioned at the center of the microwave cavity to study the effect of the microwave cavity dimensions (inner diameter, outer diameter, and height) on the power absorbed using the RF module. Then, based on the parametric sweep, the dimensions of the microwave cavity were optimized using the RF and optimization modules to maximize the power absorbed by the sorbent material for two cases. In Case One, the waveguide is positioned in the middle of the cavity, and in Case Two, the waveguide is positioned in the top end of the cavity. Then, the heat transfer and RF modules were used to investigate the effect of the

waveguide position on the temperature and electrical field intensity distributions within the sorbent.

Discussion

The microwave cavity's and sorbent bed's dimensions considerably influence its resonance frequency, coupling efficiency, mode distribution, and field uniformity. Figures 2 illustrate the effects of the microwave cavity's inner and outer diameters on the power absorbed by the sorbent material. The microwave cavity's inner and outer diameters are essential in determining how much power the sorbent bed absorbs. Larger diameters often provide lower resonant frequencies and support more electromagnetic modes, resulting in more complicated field patterns. However, they may experience increased radiation losses. Conversely, smaller diameters may offer higher resonant frequencies but can lead to more substantial variations in field strength and higher conductor losses. Optimal diameter selection is crucial in achieving desired performance characteristics for specific microwave cavity applications. Figure 3 shows the effect of the cavity height, which is equal to the sorbent bed height, on the power absorbed by the sorbent bed. A more considerable material height may increase the interaction length between electromagnetic fields and the material, leading to greater power absorption. Similarly, a higher cavity height gives electromagnetic waves a greater area to travel and interact with the material, enhancing power absorption. However, highly tall cavities or materials may result in lower efficiency due to higher losses and reduced field homogeneity. As a result, controlling the material and cavity heights is critical for maximizing power absorption and overall performance in microwave cavity systems.
The results of the optimal microwave cavity dimensions from the parameter optimization to maximize the microwave input power utilization for case one, where the waveguide position at the middle of the cavity, and case two, where the waveguide position at the top-end of the cavity, are shown in Tables 1 and 2, respectively. The optimal microwave cavity and reactor dimensions reduce reflection, maximize the electrical field inside the sorbent material, and assure resonance with the operating frequency, maximizing the power absorbed by the sorbent material and the microwave input power utilization. Using the optimal dimensions can result in absorbing more than 98% of the microwave power input, which results in a more efficient desorption system.
The electrical field distributions within the sorbent material, the electrical field distributions for plane at x=0, and temperature distributions within the sorbent material after 20 seconds heating for cases one and two are shown in Figures 4 ,5, and 6 respectively. Placing the waveguide in the center of the microwave cavity's height results in a more uniform electric field distribution within the sorbent bed. This is because the midway position improves coupling and energy transmission between the waveguide and the processed material, resulting in a more uniform electric field distribution. The power absorbed in case one, which is positioning the waveguide at the middle height of the cavity, absorbed 1.6% more power than case two. A design with a waveguide placed at the middle is suitable for a fluidized bed reactor where the sorbent will be moving along the length of the reactor.

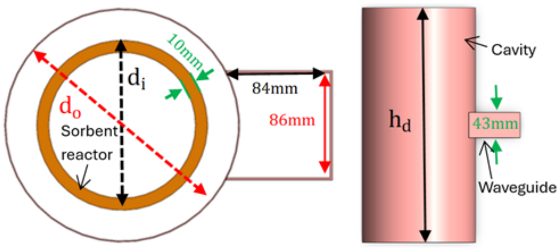

Figure 1. The geometry of the model.

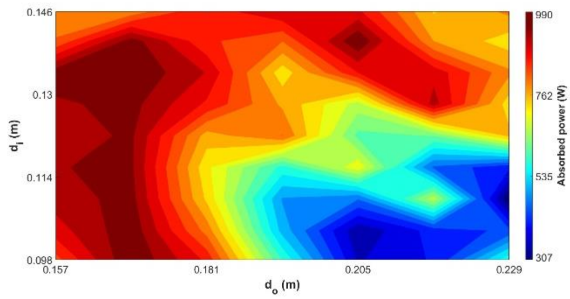

Figure 2. The effects of the cylindrical hole material's inner diameter and the microwave cavity's outside diameter on the power absorbed by the sorbent material.

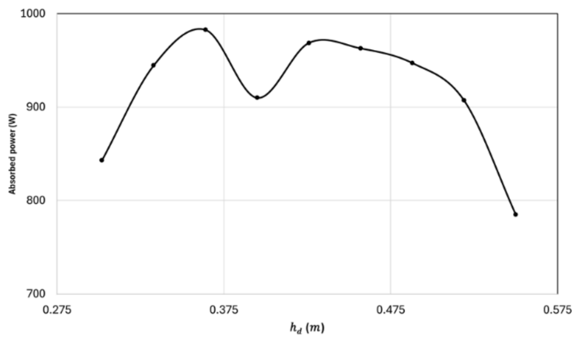

Figure 3. The effect of the cavity height on the power absorbed by the sorbent bed.

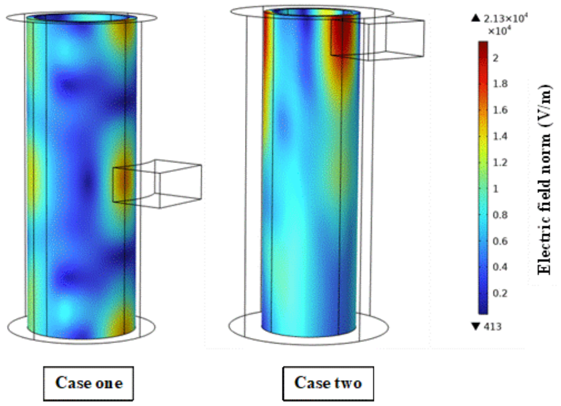

Figure 4. The sorbent material's surface electrical field distributions for case one and case two.

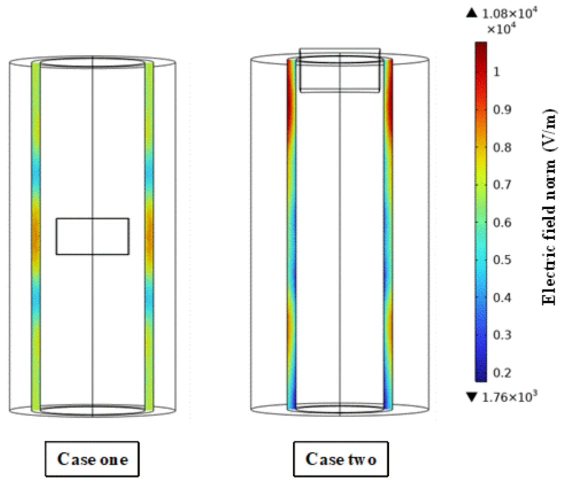

Figure 5. The sorbent material's electric field distribution slice at x=0 for case one and case two.

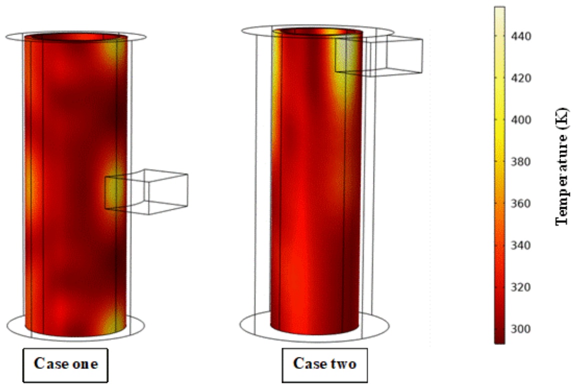

Figure 6. The surface temperature distributions for case one and case two.

Table 1.The optimal dimensions for case one.

The optimal parameter	Value	unit
d_i	139.78	mm
d_o	189.99	mm
h_d	400	mm

Table 2. The optimal dimensions for case two.

The optimal parameter	Value	unit
d_i	120	mm
d_o	202.5	mm
h_d	400	mm

Conclusions

This simulation study using COMSOL Multiphysics has provided valuable insights into optimizing microwave cavity design for carbon capture applications. The research demonstrates the critical role of cavity dimensions and waveguide positioning in maximizing power absorption and achieving uniform heating of the sorbent material.
Key findings include:

- Optimal cavity dimensions can result in over 98% absorption of microwave power input, significantly enhancing system efficiency.
- Waveguide positioning at the middle height of the cavity proved superior, absorbing 1.6% more power than the top-end position and providing more uniform electrical and temperature distribution.
- The middle waveguide position is particularly suitable for fluidized bed reactors, where sorbent material moves along the reactor's length.

These results have important implications for improving microwave desorption energy utilization efficiency in carbon capture processes. By optimizing cavity design and waveguide placement, it is possible to achieve more effective and energy-efficient carbon capture systems.
Future work could focus on experimental validation of these simulation results and exploration of additional parameters to further enhance system performance.

References

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