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Design challenges and solutions

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Coaxial traveling-wave microwave reactors: Design challenges and solutions

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ABSTRACT

Microwave chemistry applications have been investigated for more than three decades. Contrary to common cavity-based microwave applicators, the traveling-wave microwave reactor has the potential to enable the process scale-up, a better coupling of microwave energy with microwave-susceptible catalysts, and consequently highly uniform microwave heating. In this work, the engineering challenges entailed with the design of a traveling-wave microwave waveguide are explained and appropriate solutions developed. A new traveling-wave microwave reactor with a coaxial waveguide structure is presented. Simulation results show that there is no standing wave generated along the structure. Furthermore, in order to keep the impedance matching and minimize the microwave reflections while the reactor is loaded with catalyst samples, new reactor's loading patterns are introduced. Simulation results showed that for the proposed method, microwave-susceptible catalytic fixed-bed could interact more efficiently with microwave energy and produce a uniform heating profile.

Nomenclature

List of symbols

L	Self-inductance (H)
C	Capacitance (f)
μ	Magnetic permeability (H/m)
ε	Electric permittivity (F/m)
ε_r	Relative permittivity
f_c	Cut-off frequency (Hz)
Z_0	Characteristic impedance (Ω)
c	Speed of light in vacuum (m/s)

1. Introduction

Microwave-assisted processes offer several advantagesover the traditional ones in terms of reaction acceleration, volumetric heating, improving product yields and selectivity, and reducing undesired side reactions (Polaert et al., 2017; Oliver Kappe, 2008; Adnadjević et al., 2017; Cherbański, 2011). Besides, operating at a lower bulk gas temperature can lead to a considerable improvement in reaction selectivity that can be maximized by designing microwave-absorbing catalysts (Gabriel et al., 1998; Stefanidis et al., 2014). Despite the obvious intensification effects of the microwave irradiation, one of the main challenges for industrial applications is reliable scale-up of microwave reactors (Stankiewicz, 2006).

Currently, there are three different types of microwave applicators used in material processing laboratories: multi-mode, single-mode (or mono-mode), and traveling-wave microwave reactors (TMR). The applicability of typical multi-mode and mono-mode cavities is limited because both systems suffer from non-uniform heating due to generating standing microwaves and are strongly dependent on the frequency and dielectric properties of the sample (Stankiewicz et al., 2019). Those negative features may not be critical in case of drying or thawing but they are critical for controlling chemical reactions.

In contrast to resonant applicators, i.e., multi-mode and mono-mode cavities, the traveling-wave microwave reactor has the potential to enable highly uniform microwave heating by avoiding resonant conditions (Sturm et al., 2016). The specific purpose is to construct and tune the reactor such that the microwave field inside the reactor travels in

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only one direction to avoid non-uniform electromagnetic interference patterns and non-uniform heating along the reactor. It is envisaged that this particular reactor concept may enable process scale-up beyond the intrinsic restrictions of cavity systems. Indeed, in the traveling microwave reactor, there is no need to have tuning elements to deal with the frequency changes during the process (Mehdizadeh, 2015). The only elements that should be considered in TMR design are the size of the reactor and the microwave reflections throughout the whole system to make sure that there is no standing wave pattern generated along the structure.

Herein, we present a new traveling-wave microwave reactor design, explain the engineering challenges entailed with this design, and provide opportunities to develop solutions required for this type of reactor. In this context, we present the critical factors for the design procedure of a new coaxial traveling-wave microwave reactor and describe its advantages through numerical simulations. Moreover, the effects of the catalyst geometry and loading pattern on its heating profile are studied and optimized to have a more efficient and uniform heating profile along the reactor.

2. Traveling-wave microwave reactor design

2.1. *The characteristic of the waveguide*

The first step in the design of a microwave reactor consists in the selection of the most appropriate type of the waveguide for the given application. TMRs can be implemented in different waveguide types and configurations. The typical types of a waveguide, which can be considered for the required scale, are rectangular, circular and coaxial, where each has some advantages. The concept of TMR with a coaxial cable configuration has been studied in last few years (Sturm et al., 2016; Mehdizadeh, 2015; Gentili et al., 2009; Mehdizadeh, 2009; Longo and Ricci, 2007; Mitani et al., 2016; Durka, 2013). This configuration has several advantages over the other types of the waveguides in terms of having no cut-off frequency for the transverse electromagnetic, TEM, mode of propagation (Kouzaev, 2013; Kapranov and Kouzaev, 2019). In the TEM mode, electric field lines run radially while magnetic field lines run in circles around the inner conductor see Fig. 1b. Consequently, the available operating frequency range of this waveguide is much broader than of other types.

Designing a microwave excitation section in coaxial waveguides is much simpler due to the coaxial nature of the most common microwave generators. Furthermore, the entire inner space of the waveguide can be used for the process functionalities because the electromagnetic field is uniform over the circumferences of conductors in coaxial waveguides, while in the case of rectangular and circular ones, this space is limited to only a portion of their sides. However, it is also important to design the cross-section of the reactor in such a way that the electromagnetic field effectively couples with the catalytic bed inside.

Cross-sectional schematics of a coaxial microwave reactor along the axial and radial direction are depicted in Fig. 1, where, the inner and outer conductors form the coaxial waveguide structure. The microwave energy delivered at the inlet and absorbed by the dielectric material, i.e., microwave absorbing media, and dissipated into heat.

The reactor dimensions are selected based on restrictions imposed by the electromagnetic wave propagation. In that sense, the first requirement is to adjust the impedance matching of different parts to minimize the unwanted microwave field reflections. The second is to make sure that the device works in a single TEM mode by adjusting the cut-off frequency well above the working frequency. The design process considering these two requirements is explained below.

2.1.1. *The dimensions of the waveguide*

Microwave reflection presents an important aspect of reactor performance. A smaller microwave reflection leads to faster heating and less energy loss since more microwave energy penetrates into the dielectric sample (e.g. catalyst). In order to minimize the electromagnetic wave reflections in the coaxial structure reactor, the characteristic impedance of the waveguide should be adjusted to maintain at the characteristic impedance of the feed transmission system. The most common industry standard for the characteristic impedance is 50 Ω since it is a great compromise between power handling and low loss. All the equipment, e.g. microwave generator, used in this study are assumed to be 50 Ω. Characteristic impedance is the ratio of the voltage of the transmission line to the current, which is described for the TEM mode in a coaxial waveguide as follow (Pozar, 2012):

$$Z_0 = \sqrt{\frac{L}{C}} = \frac{\sqrt{\mu/\varepsilon}}{2\pi} \ln\frac{r_o}{r_i} = \frac{60}{\sqrt{\varepsilon_r}} \ln\frac{r_o}{r_i} \tag{1}$$

where, L stands for the total self-inductance of the two conductors, C is the capacitance of two conductors, r_o and r_i are the radii of the outer and inner conductors, respectively, and ε_r is the relative permittivity of the dielectric material placed between the conductors (insulator).

For the case discussed herein, the dielectric material of the waveguide was assumed to be air ($\varepsilon_r \approx 1$). Therefore, considering Eq. (1), in order to keep the characteristic impedance of the customized waveguide equal to 50 Ω, the ratio of the radii of the outer and inner conductors was found to be 2.3.

2.1.2. *Cut-off frequency of the waveguide*

The cut-off frequency of a coaxial transmission line is the frequencies that the excitation of the next unwanted transverse electric, e.g., TE_{11}, mode starts to propagate. This mode has a different propagation velocity and microwave field distribution than the desired TEM mode. These cause perturbations in the electromagnetic behavior of the device and heating pattern of the sample, accordingly. The cut-off frequency in a coaxial transmission line can be calculated using the following formula (Pozar, 2012):

$$f_c = \frac{c}{(r_o + r_i)\,\pi\,\sqrt{\varepsilon_r}} \tag{2}$$

where, c is the speed of light in vacuum. Considering this equation and assuming that air is the filling medium, to adjust the dimensions to have the cut-off frequency above 2.45 GHz, the sum of the radii should be lower than 38.94 mm. Otherwise, microwave reflections are noticeable which lead to a standing wave pattern instead of traveling-wave one.

Combining the results of the constraints, the radii were selected as result in $Z_0 = 50.1\,\Omega$, and $f_c = 2.6$ GHz. It means that only the desirable TEM mode can propagate at frequencies below the cut-off frequency of 2.6 GHz.

2.2. *The microwave transition part and the absorber*

In the previous section, the optimized dimensions of the custom-design coaxial microwave reactor were obtained. The

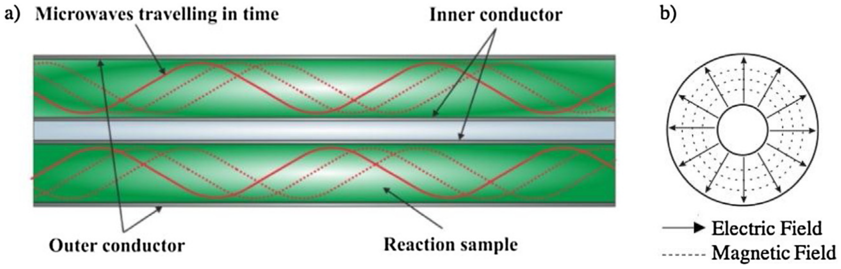

Fig. 1 – (a) Axial and (b) radial electric fields distribution in the coaxial traveling-wave microwave reactor.

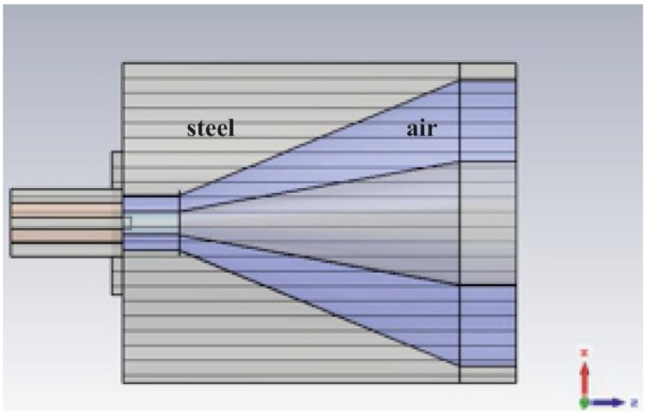

Fig. 2 – Coaxial transition part cross section.

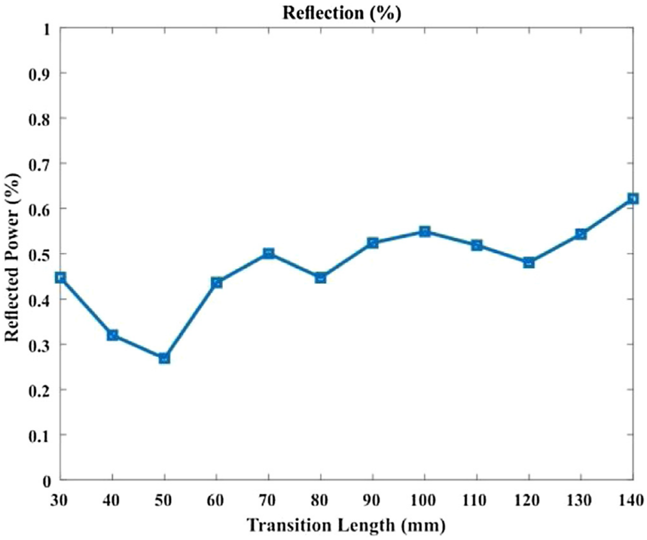

Fig. 3 – The simulated results of a coaxial microwave transition part.

next step is deciding how the microwave field will be introduced into the coaxial microwave reactor. In this sense, designing a microwave transition part is essential to excite the reactor through a standard 50 Ω type-N coaxial connector with minor reflections.

Different methods can be employed in designing the transition section, but the most practical one with the least manufacturing complexity is the tapered coaxial transition. The taper curve can be exponential, logarithmic or even linear, each delivering a compromise between operating bandwidth and transition length (Song and Quan, 2009). In the current study, we are not bound by strict dimensional or bandwidth requirements, thus we can adopt a simple linearly tapered curve in the design of the transition part. This will lead to a conical-shaped coaxial microwave transition, which is placed between the type-N coaxial connector and reactor intersection, see Fig. 2.

Since the dimensions, i.e., the radii of the outer and inner conductors, of the coaxial microwave reactor and type-N connector are already known, the only optimization parameter would be the length of the conical shape microwave transition part. Microwave theory textbooks advise that when two different impedances are expected at each end of a waveguide transition, the length should be extended about one half-wavelength along the impedance change direction. In the present design, the input and output impedances are the same. In fact, the transition is needed to only adapt two physically un-identical 50 Ω coaxial waveguides. In this case, the length of the transition is expected to have less impact on the overall reflection performance. To investigate the effect of transition length on the reflection factor, a full-wave electromagnetic field analysis was performed in the simulation environment using software, CST Studio Suite (CST Studio Suite, 2014). A time-domain method was employed for solving Maxwell equations and obtaining a fast estimation of electromagnetic performance over the desired bandwidth (2.43–2.47 GHz).

The obtained simulation results showed that varying the transition length over a wide range of values has an insignificant effect on the impedance performance of the device, see Fig. 3. Therefore, for the purpose of reducing the length and weight of the overall structure, we have chosen 50 mm as the length of the transition for future analyses. Which has been achieved with acceptable reflection at the input port (less than 0.3% of the input MW power).

As the microwave energy travels along the coaxial microwave reactor, part of this energy is going to be absorbed by microwave-susceptible media, i.e., catalysts or catalyst supports, and dissipated into heat in the reaction zone, and the rest is going to be leaked to the environment. To prevent the unwanted microwave leakage, designing a microwave absorber to be placed at the end of the reactor is crucial to absorb the remaining microwave energy safely.

In this manner, a commercial microwave absorber material, (Eccosorb MF-117, 2019), was selected due to its good permittivity, permeability, and attenuation properties and the easiness of machining. The empty space inside the absorber section was considered air-insulated to have matching waveguide size in the reactor and the absorber intersection. The absorbing part could be designed in a conical shape, see Fig. 4, to have a smooth transition from 50 Ω waveguide to the absorber.

The simulated results for the optimization of the length for each of these two sections are presented in Fig. 5. As it can be inferred from the results, increasing the taper lengths can produce a better input reflection up to a point and after that, there

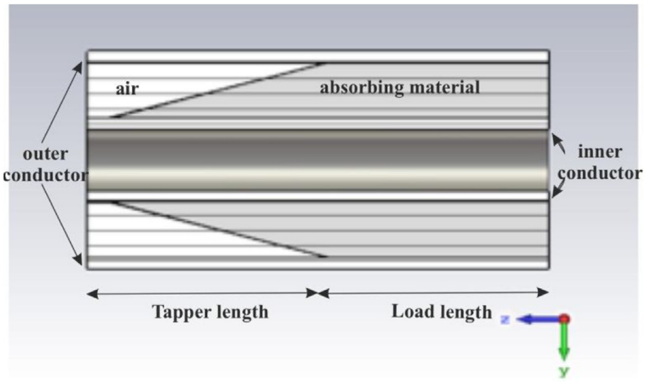

Fig. 4 – Coaxial microwave absorber cross-section.

would be insignificant changes in the performance. However, changing the length of the load part has no meaningful effect on the reflection but can decrease the level of radiation significantly. Considering the optimization results, the taper length and load length parameters are both selected to be 50 mm.

3. Performance characteristics of the integrated system

In the analysis so far, the coaxial microwave waveguide, its connection to the microwave generator system, i.e., the microwave transition part, and the microwave absorber section have been investigated and optimized to produce negligible reflections. In this section, all the above-designed parts have been integrated to constitute a coaxial traveling-wave microwave reactor. The proposed microwave reactor should enable a highly uniform heating profile (Sturm et al., 2014).

The cross-sectional view of the proposed microwave reactor along the axial direction is presented in Fig. 6. Here, the stainless-steel inner and outer conductors form the coaxial waveguide structure. The reaction zone, is the annular space between the two concentric quartz tubes (Øin:27 mm, Øout:46 mm, Length: 300 mm), and the accessible reactor volume is 0.327 L. The quartz tubes form a sealed toroidal reactor inside the waveguide and play the role of the dielectric insulator in the coaxial waveguide. This provides a way to have a relatively high-temperature reactor inside a cooler waveguide structure, while maintaining fluid containment. Different forms of catalysts and/or catalyst supports can be placed in the space between the quartz tubes and the process gases flow in the axial direction along the catalyst section. The conical-shape coaxial transition part, filled with air, is placed between the microwave excitation port and the reactor intersection, in order to adapt the two devices. The tapered coaxial absorber is assigned at the end of the waveguide to prevent any microwave leakage to the environment.

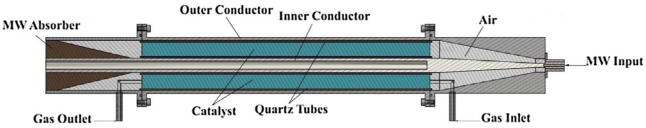

Fig. 6 – A cross-sectional schematic of the proposed traveling-wave microwave reactor.

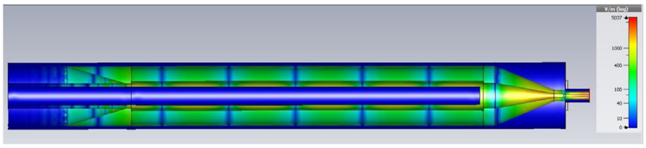

Fig. 7 – Normalized electromagnetic field distribution of the optimized reactor.

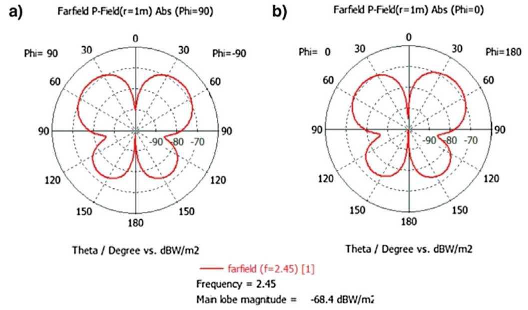

Fig. 8 – Radiation pattern in the environment for a) phi = 90 and phi = 0.

The electromagnetic field simulation software of CST Studio Suite was used for the analysis of the reactor characteristics. The simulated results of the normalized microwave field distribution inside the reactor without a catalyst bed inside are presented in Fig. 7. The simulation results reveal that in the optimized design, the microwave field is perfectly traveling along the reactor, and the remaining energy is dissipated in the absorber section.

Fig. 8 depicts the radiation pattern of the proposed design in the three-dimensional cylindrical coordinates. Assuming the reactor to be extended along the z-axis, it is customary to evaluate the radiation pattern in two orthogonal planes, i.e., phi = 0 and phi = 90°, while sweeping theta value. This can offer an acceptable approximation for the three-dimensional radiation pattern of any device. The presented results show

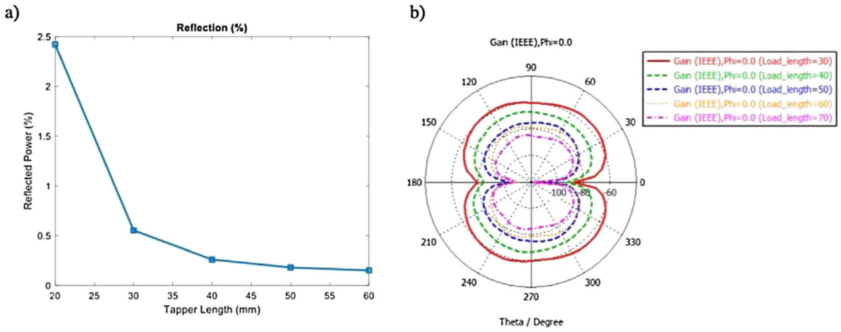

Fig. 5 – The simulated results of a coaxial microwave absorber (a) Effect of changing Taper Length in the Absorbing Section on the input reflection (Load Length = 50 mm) and (b) Effect of varying Load Length of Absorbing Section on the external radiation (Taper Length = 50 mm).

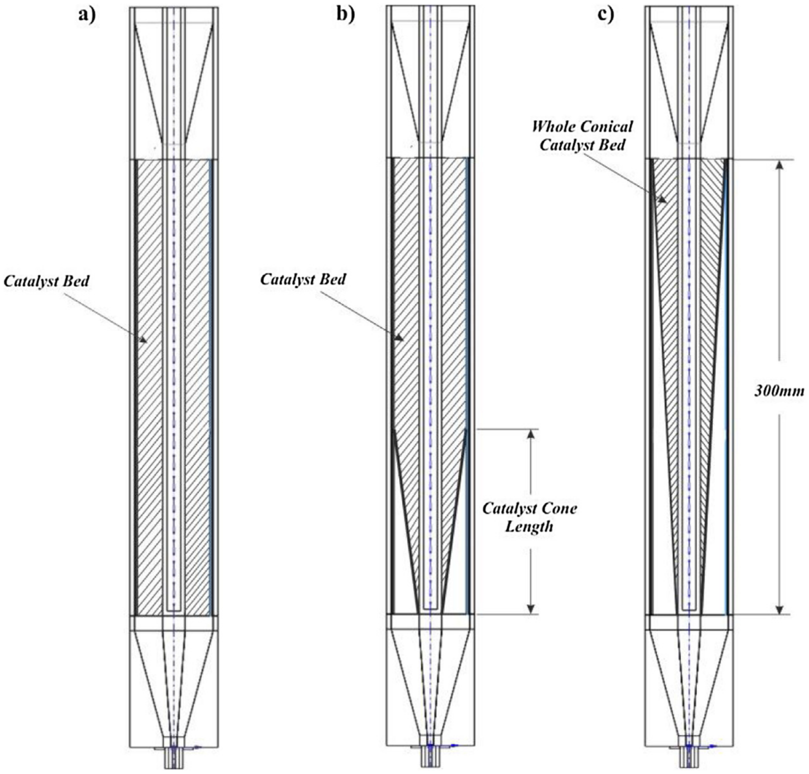

Fig. 9 – Schematic diagram of different catalyst loading pattern (a) Fully loaded, (b, c) Gradual increasing the catalyst concentration cone length from 50 to 300 mm.

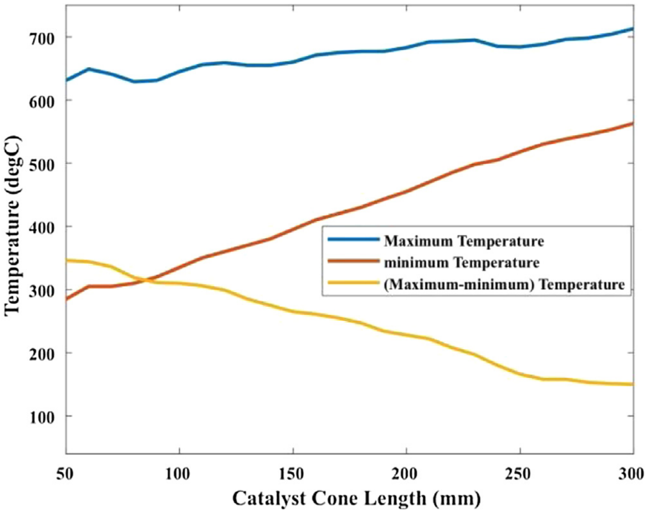

Fig. 10 – Effect of catalyst cone length on the heating profile of the catalyst bed and its homogeneity.

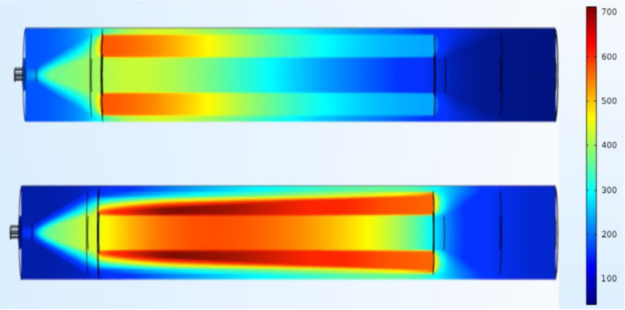

Fig. 11 – Catalyst heating profile of different loading patterns: (a) Fully (b) Gradually loaded by the catalyst.

that the leaked waves from different parts of the reactor are at least −65 dB (3×10^6 times) weaker than the source-generated power. This is well below the FDA and European directive approved range of safe radiation for microwave heating devices (U.S. Food & Drug Administration, 2019; European Union Law).

Obtaining proper traveling-wave waves inside the reactor requires a good impedance matching between the parts of the structure. Simulation results show that the reflection coefficient of the overall structure is approximately −20 dB (≈ % 1) at the working frequency of 2.45 GHz. This is a proof that there is no standing wave generated along the structure.

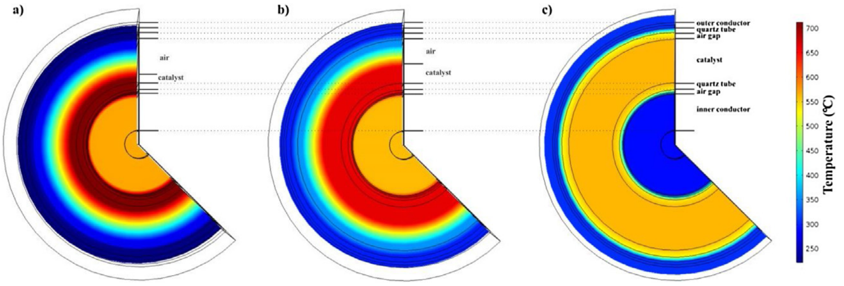

Fig. 12 – Catalyst heating profile of gradually loading pattern in different axial locations: (a) z = 73 mm (where we have the maximum temperature of the catalyst bed), (b) z = 150 mm (at the middle of the bed), and (c) z = 300 mm (at the end of the bed).

4. Controlling the catalyst heating profile

The simulation results discussed so far concerned with an empty traveling-wave wave reactor system, optimized for impedance matching. This way, the microwave reflections could be minimized. In a reactor loaded with a catalyst as a microwave absorbing media, the impedance matching should obviously be retained. To this end, the catalyst volume/mass should increase gradually over the reactor length, avoiding any sudden impedance changes. Otherwise, it would behave as a mirror at the intersection on the way of the microwave and reflect a considerable amount of the incident microwave. This would result in creating a standing-wave pattern inside the waveguide, which leads to a non-uniform heating profile and hot spots formation. Moreover, for the case where catalyst evenly and longitudinally filled along the reactor, the microwave field intensity and consequently the heating rate would attenuate exponentially.

To illustrate the effect of the impedance matching in the reactor loaded with catalyst, different loading schemes were studied with the length of the catalyst cone ranging from 50 mm to 300 mm with 5 mm intervals, see Fig. 9.

The heating profiles were simulated for all the case studies, and the minimum and maximum temperature of the catalyst bed is extracted and compared, see Fig. 10. In all cases, the reactor was loaded with platinum on carbon, Pt/C catalyst, with temperature-dependent dielectric properties provided by Gangurde et al. (2017). Heat transfer and electromagnetic field equations were coupled using COMSOL Multiphysics 5.3 simulation environment (Comsol Multiphysics, 2012) and MW power input is 400 W.

As can be seen in Fig. 10, both maximum and minimum temperatures for the whole conical-shaped catalyst bed are higher than the other cases. This is mainly due to the good impedance matching of the catalytic bed with the MW system. Fig. 11, compares the heating profile of the normal and conical (gradually increased catalyst concentration) loading pattern. As illustrated in Fig. 11(a), due to significant microwave reflections, the catalyst cannot interact with the electromagnetic waves efficiently and even with the same energy input the catalyst cannot be heated properly (570 °C at most). On the other hand, in the case presented in Fig. 11(b), where, with the intention of keeping the impedance matching, the catalyst load is gradually increased. In this case, the maximum temperature achieved is much higher (above 700 °C) and the temperature profile is distributed much more smoothly without forming hot spots. Also, the uniform heating zone is much larger.

To examine the heating uniformity in the radial direction, the temperature at three different axial positions (i.e., z = 73 mm, 150 mm, and 300 mm) is plotted in Fig. 12. It can be seen from the figure that even in the radial direction, the catalyst zone is heated up quite evenly.

In fact, two latest figures show that in the current design, the temperature distribution in both axial and spatial directions is almost uniform and no hot spots occur along the catalyst bed. However, from the simulation results and the heating profile depicted in Fig. 11, the temperature in the absorber section is considerably lower than the reactor section. On the other hand, the amount of power which reaches the absorber is practically negligible and this proves the efficiency of the design.

5. Conclusion

This paper addresses the critical aspects of designing a traveling-wave microwave reactor. A coaxial structure traveling-wave microwave reactor is proposed as a potential solution to the process scale-up and catalyst heating profile issues. Simulated results demonstrate that the reflection coefficient of the overall structure is −20 dB (≈% 1) at the standard working frequency of 2.45 GHz. This proves that there is no standing wave generated along the structure. Additionally, a catalyst loading pattern is proposed in order to keep the impedance matching and minimize the microwave reflections. Simulation results show that the proposed loading pattern enables more efficient coupling between the microwave energy and the catalyst which leads to having a more uniform temperature profile distribution inside the bed.

Declaration of interests

None.

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