Core-shell biochar-bearing iron ore powder model for calculation of effective electrodynamic parameters

Anton P Anzulevich¹, Svetlana N Anzulevich¹, Igor V Bychkov¹, Vasilii D Buchelnikov¹, Leonid N Butko¹, Dmitry A Kalganov¹, Dmitry A Pavlov¹, Sergey G Moiseev²,³ and Zhiwei Peng⁴

¹ Chelyabinsk State University, 129 Br. Kashirinykh Str., Chelyabinsk 454021, Russia
² Ulyanovsk State University, 42 L. Tolstoy Str., Ulyanovsk 432017, Russia
³ Kotelnikov Institute of Radio Engineering and Electronics of Russian Academy of Sciences, Ulyanovsk Branch, 48/2 Goncharov Str., Ulyanovsk 432011, Russia
⁴ Central South University, Changsha, Hunan, China
E-mail: anzul@list.ru

Abstract. The simplified model of biochar-bearing iron ore with binder was studied. It was considered to be a mixture of two types of core-shell particles, iron ore - binder particles and biochar - binder particles. The expressions to calculate complex effective permittivity and permeability was derived by effective medium approximation (EMA). The corresponding dependencies on volume fraction of iron ore in the mixture are provided.

1. Introduction
In this work, we consider biochar as a carbon-containing filler of iron ore. By using biochar, which is obtained via low-temperature pyrolysis of waste, abundant and sustainable biomass, to replace coal and coke, faster reduction and low reduction temperature can be expected with much lower emission of CO2 and hazardous gas (such as SO2). If the biochar-bearing pellets are heated by microwave energy which is characterized by volumetric heating, selective heating and non-thermal effect, reduction temperature and time can be further reduced with better quality of reduced pellets. The metallized pellet can then be used as a good raw material for steelmaking in electric arc furnace.

Given that biochar is a relatively new material, a huge amount of publications [1,2] studying the possibilities of its application in various fields of science and technology can be observed. In work [2], the absorbing capacity of biochar with respect to heavy metal oxyanions (Cr(VI)) was improved by impregnating the negatively charged surface of the biochar with Fe₃⁺ particles to neutralize the surface. In addition, a composite consisting of carboxymethylcellulose, iron sulfide and biochar (CMC-FeS@biochar) as an absorber of heavy metal particles such as Cr(VI) was proposed in [3]. Using a composite of polyvinyl alcohol and biochar as a part of pressure sensors is proposed in [4]. In [5], the influence of the pyrolysis temperature of biochar and the distribution of metal oxyhydrochlorides on the surface of biochar particles pretreated with Al and Fe trichlorides on the ability to exchange ions in a neutral medium is investigated. Finally, a review [6] considers all possible aspects of the use of biochar as a catalyst.
Figure 1. Simplified model of biochar-bearing iron ore powder compacted by binder.

In connection with the foregoing, the theoretical calculations of electrodynamic parameters of biochar-bearing materials are of particular interest and modeling the propagation of electromagnetic radiation of a wide frequency range in such composite structures is topical.

2. Theoretical model
Let us consider the following simplified theoretical model of biochar-bearing iron ore compacted with addition of binder - see figure 1.

Here $\varepsilon_b$ is permittivity of binder, $\varepsilon_c$ - permittivity of biochar, $\varepsilon_m$ - permittivity of iron ore; $R_{1m}$ - core radius of iron ore particle, $R_{2m}$ - radius of entire core-shell iron ore - binder particle, $R_{1c}$ - core radius of biochar particle, $R_{2c}$ - radius of entire core-shell biochar - binder particle. Both types of particles are identical except of values of permittivity, permeability, and radius. Hence, the solutions of Maxwell equations with standard boundary conditions for core-shell particles look like following [7]:

$$
\vec{E}_{m,c} = \frac{9\varepsilon_b\varepsilon_{eff}\zeta_{m,c}}{2\alpha_{m,c}\varepsilon_{eff} + \beta_{m,c}\varepsilon_b}\vec{E}_0, \ r < R_{1m,1c},
$$

$$
\vec{E}_{bm,bc} = \frac{3\zeta_{m,c}\varepsilon_{eff}}{2\alpha_{m,c}\varepsilon_{eff} + \beta_{m,c}\varepsilon_b} \times 
\left[ (\varepsilon_{m,c} + 2\varepsilon_b - (\varepsilon_{m,c} - \varepsilon_b) \frac{R_{1m,1c}^3}{\rho^3}) \vec{E}_0 + 
+ 3(\varepsilon_{m,c} - \varepsilon_b) \frac{R_{1m,1c}^3}{\rho^3} r (\vec{E}_0 \cdot \vec{r}) \right], R_{1m,1c} < r < R_{2m,2c},
$$

Here $bm$ and $bc$ indexes correspond to the field inside the shell of iron ore particle and biochar particle correspondingly;

$$
\zeta_{m,c} = (R_{2m,2c}/R_{1m,1c})^3 = (1 + l_{m,c})^3,
\alpha_{m,c} = (\zeta_{m,c} - 1)\varepsilon_{m,c} + 2(\zeta_{m,c} + 1)\varepsilon_b,
\beta_{m,c} = (2 + \zeta_{m,c})\varepsilon_{m,c} + 2(\zeta_{m,c} - 1)\varepsilon_b,
$$
In EMA we have deal with a mixture of two types of spherical particles, which are randomly distributed in the effective medium. In this paper, we deal with three types of particles. Two of them are identical and considered above. As third type of particles we will consider spherical inclusions of gas (vacuum). It is considered that the permittivity of such a composite is equal to the permittivity of the effective medium. These gas particles can be any radius so that to fill all the remaining space. They are spherical and electric field inside of them is determined as:

\[ \vec{E}_g = \frac{3\varepsilon_{eff}}{\varepsilon_g + 2\varepsilon_{eff}} \vec{E}_0, \]  

(4)

Here \( \varepsilon_g \) is the permittivity of gas or vacuum. According to the EMA an average value of electric displacement of effective medium connects with an average value of electric field strength as:

\[ \langle \vec{D} \rangle = \varepsilon_{eff} \langle \vec{E} \rangle = \varepsilon_{eff} \vec{E}_0, \]  

(5)

After substitution of electrical fields (1), (2) and (4) into Eq. (5) and their integration we can find the final equation for calculation of the effective permittivity:

\[
(1 - p_m \zeta_m - p_c \zeta_c) \varepsilon_g - \varepsilon_{eff} + \\
+ p_m \zeta_m \frac{\varepsilon_b [3 \varepsilon_m + (\zeta_m - 1) (\varepsilon_m + 2 \varepsilon_b)] - \varepsilon_{eff} [3 \varepsilon_b + (\zeta_m - 1) (\varepsilon_m + 2 \varepsilon_b)]}{2 \varepsilon_m \varepsilon_{eff} + \beta_m \varepsilon_b} + \\
+ p_c \zeta_c \frac{\varepsilon_b [3 \varepsilon_c + (\zeta_c - 1) (\varepsilon_c + 2 \varepsilon_b)] - \varepsilon_{eff} [3 \varepsilon_b + (\zeta_c - 1) (\varepsilon_c + 2 \varepsilon_b)]}{2 \varepsilon_c \varepsilon_{eff} + \beta_c \varepsilon_b} - \\
- p_m \zeta_m \frac{\varepsilon_b (\varepsilon_m - \varepsilon_b) \ln (1 + l_m)}{2 \varepsilon_m \varepsilon_{eff} + \beta_m \varepsilon_b} - \\
- p_c \zeta_c \frac{\varepsilon_b (\varepsilon_c - \varepsilon_b) \ln (1 + l_c)}{2 \varepsilon_c \varepsilon_{eff} + \beta_c \varepsilon_b} = 0, \]  

(6)

where \( p_m \) and \( p_c \) are volume fractions of iron ore and biochar in effective medium mixture.

3. Results and discussion

This equation (6) can be used to determine the complex effective permittivity of biochar-bearing iron ore if permittivities and concentrations of initial components are known. Effective permeability of this mixture can be determined by the same equation (6) replacing \( \varepsilon \) with \( \mu \).

On the basis of the following papers [8–10], let’s consider that monolithic biochar (containing 85% of C) and iron ore (containing 65% of Fe in oxide form) have following complex values of permittivity and permeability:

\[ \varepsilon_m = 14.2 + i 0.2, \mu_m = 1.8 + i 0.9, \varepsilon_c = 3 + i 0.12245, \mu_c = 1, \]
\[ \varepsilon_b = 1.2, \mu_b = 1, \varepsilon_g = 1, \mu_g = 1, \]
\[ R_{1m} = 25 \mu m, R_{1c} = 30 \mu m \]  

(7)

We considered that \( \varepsilon = \varepsilon' + i \frac{4 \pi \sigma}{\omega} \) and \( \omega = 2 \pi \nu \) where \( \nu \) is frequency of microwave radiation that equals to 2.45 GHz. Taking into account that volume fraction of binder is about 1-2% it is easy to calculate that \( l_m \approx l_c \approx 0.0060227 \). Volume fraction of biochar component is assumed to be \( p_c = 0.9 - p_m \).

Eventually, on figure 2 we can see that wave impedance \( Z = \sqrt{\frac{\mu_{eff}}{\varepsilon_{eff}}} \) decreases from 0.6 to 0.38 when volume fraction of iron ore in the mixture increases from 0 to 1.
Figure 2. Real (black) and imaginary (red) parts of effective permittivity (left) and permeability (right) of biochar-bearing iron ore powder on volume fraction of iron ore $p_m$.

4. Conclusion
Using the obtained on figure 2 dependencies it is possible to optimize matching of impedances on the surface of studied biochar-bearing iron ore powder by changing volume fraction of iron ore depending on depth. That will allow to improve penetration of microwave radiation into the volume of powdered sample and enhance heating and, hence, reduction of iron ore.

Acknowledgments
This work was supported by the Russian Foundation for Basic Research (Project No. 18-58-53055, 16-29-14045, 17-02-01382) and by the Ministry of Education and Science of the Russian Federation (State Contract No. 3.5698.2017/9.10).

References
[1] Zhiwei Peng, Jiann-Yang Hwang, and Matthew Andriese, Absorber Impedance Matching in Microwave Heating, Applied Physics Express 5 (2012) 077301, pp. 1-3
[2] Wang H., Tian Z., Jiang L., Luo W., Wei Z., Li S., Cui J., Wei W., Highly efficient adsorption of Cr(VI) from aqueous solution by Fe3+ impregnated biochar, Journal of Dispersion Science and Technology, Volume 38, Issue 6, 3 June 2017, pp. 815-825
[3] Lyu H., Tang J., Huang Y., Gai L., Zeng E.Y., Liber, K., Gong Y., Removal of hexavalent chromium from aqueous solutions by a novel biochar supported nanoscale iron sulfide composite, Chemical Engineering Journal, Volume 322, 15 August 2017, pp. 516-524
[4] Nan N., DeVallance D.B., Development of poly(vinyl alcohol)/wood-derived biochar composites for use in pressure sensor applications, Journal of Materials Science, Volume 52, Issue 13, 1 July 2017, pp. 8247-8257
[5] Lawrinenko M., Jing D., Banik C., Laird D.A., Aluminum and iron biomass pretreatment impacts on biochar anion exchange capacity, Carbon, Volume 118, 1 July 2017, pp. 422-430
[6] Lee J., Kim K.-H., Kwon E.E., Biochar as a Catalyst, Renewable and Sustainable Energy Reviews, Volume 77, 1 September 2017, pp. 70-79
[7] V.D. Buchelnikov, D.V. Louguine-Luzgin, A.P. Anzulevich, G. Xie, N. Yoshikawa, M. Sato, I.V. Bychkov, A. Inoue. Heating of metallic powders b microwaves: Experiment and theory, Journal of Applied Physics, College Park, MD: AIP, 2008, 1, 104, pp 1-10. ISSN 1089-7550 / ISSN 0021-8979
[8] V.A. Sotskov, A.N. Zabavin, Experimental study of concentration dependence of the permittivity in three-component disordered systems, Journal of Technical Physics, 2012, Volume 82, Issue 7, pp. 137-139
[9] M.P., Dielectric constant and magnetic permeability of various ferrites at ultrahigh frequencies, Physics-Uspekhi (UFN), 50, pp. 152-155, doi: 10.3367/UFNr.0050.195305j.0152
[10] Randeep S. Gabhi, Donald W. Kirk, Charles Q. Jia, Preliminary Investigation of Electrical Conductivity of Monolithic Biochar, Carbon, 11678, 21 January 2017, doi: 10.1016/j.carbon.2017.01.069