## FORMATION/ACCUMULATION RATE ESTIMATION OF TARGET CHEMICALS FROM MUSROOMS THROUGH A NOVEL NUMERICAL PROCEDURE

Emoke Dalma Kovacs<sup>1</sup>, Radu Trîmbițaș<sup>2</sup>, Lukacs Arpad Imre<sup>1</sup>

<sup>1</sup>Chemistry and Chemical Engineering Faculty, Babes-Bolyai University, Romania. <sup>2</sup>Faculty of Mathematics and Computer Science, Babes-Bolyai University, Romania.

\* Kovacs Emoke Dalma: Fax: +40 264 590818 Email: dalma\_kovacs2005@yahoo.com

Keywords: ODEs, formation/accumulation rate estimation, mushroom.

## ABSTRACT

Numerous species of wild growing mushroom are widely used both in culinary purposes as healthy foods that are low in calories, fats and high in vegetable proteins, vitamin and minerals as well in pharmaceutical purposes due to their rich antioxidant chemical constituents that made them able to prevent human body from oxidative damage.

The aim of this study was to propose a numerical procedure which estimate the highest formation/accumulation rate (R) of interest nutritional and pharmaceutical compounds on the entire anatomic compartments of a mushroom body. Such data could lead to improve the technological flows performance both in food industry (manufacture of food supplements) as well in pharmaceutical industry (manufacture of drugs), allowing the extraction of the interest chemical compounds directly from the anatomical part of the mushroom which is the most abundant in it, thus being possible the avoidance of increased financial and time consumption procedures.

Estimation process was built on the following differential equation:

$$\frac{d(p\Phi(z)\chi C(z))}{dz} - \frac{d}{dz} \left[ p\Phi(z)(W_c - \overline{ET}) \frac{dC(z)}{dz} \right] + p\Phi(z) Up_f(C(z) - BA_f) = R$$

which includes elements that may affect the rate of formation/accumulation of as: height (z),

diameter ( $\Phi$ ), porosity (p), hydration coefficient ( $\chi$ ), saturated hydration factor ( $W_c$ ), evaporation-transpiration coefficient ( $\overline{ET}$ ), uptake factor ( $Up_f$ ) and bioaccumulation factor ( $Ba_f$ ).

R, the solution of the equation is the rate of formation/accumulation for the interest chemical compound.

The model was supported by concentration data (C) of the target compounds, which were measured in laboratory from cross sections taken at every 2 mm over the whole body of the studied mushroom species.

The numerical method for target compounds formation/accumulation rate estimation was implemented into MATLAB solver where the proposed equation was solved numerically using bvp4c function.

Approximation of differential operators from the left side of the proposed equation has been solved using smoothing spline functions.

Model validation was performed by solving the differential equation on the interval given by extreme values of z and comparing with the measured values of C. There is a good concordance.