Plugin ***pharmaceuticals_v0.1***

Technical documentation

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Contents

General overview

This plugin allows to simulate pharmaceuticals' concentration in surface water.
Based on the pharmaceutical's concentration measured at the inlet of a surface stream and on the average velocity of water in the stream, the concentration of the pharmaceutical at a certain distance from the inlet along the stream profile (outlet) is simulated (Figure 1).
Transport processes which are assumed to occur along the stream profile are advection and degradation. No dispersion nor diffusion processes are assumed to affect the fate of the pharmaceutical. Also, no source/sink terms are taken into account. As such, the solute transport equation solved along the stream profile (e.g., in the 1D domain) is:

$$\frac{\partial C(x;t)}{\partial t} = -v\frac{\partial C(x;t)}{\partial x} - \kappa C(x;t), \tag{1}$$

where, in a reference system where the Cartesian x axis is oriented along the stream profile:

- $C(x;t)$ [M/V] is the pharmaceutical's concentration along the stream profile, time-dependent;
- v [L/T] is the average velocity of water in the stream (it is assumed to stay constant in space and time);
- κ [1/T] is the degradation rate coefficient for the pharmaceutical. It can be calculated as $\ln 2/T$, where T is the half-life time of the pharmaceutical.

With reference to Figure 1, the following boundary condition can be set:

$$C(x=0;t) = C_{inlet}, \tag{2}$$

where C_{inlet} [M/V] is the pharmaceutical's concentration measured at the inlet.
Also, the following initial condition occurs:

$$C(x;t=0) = C_{inlet}. \tag{3}$$

Using the method of characteristics (Appendix 1), the solution to equation (1), given (2) and (3), is:

$$C(x;t) \quad = \quad C_{inlet} \cdot e^{-\kappa t}.$$

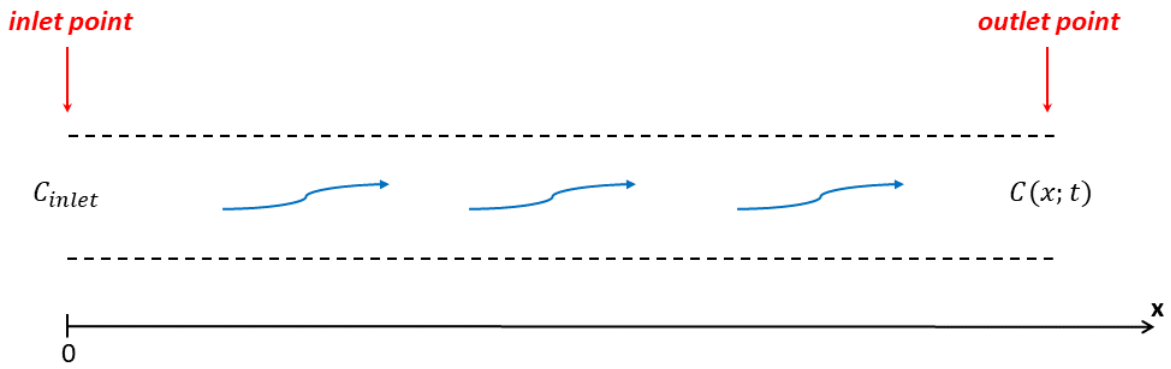


Figure 1: Sketch of the problem.

Installation requirements

This plugin has been programmed for Python 3. Python 3 can be installed through QGIS3.
To run this plugin, installing the *pandas* and *matplotlib* Python libraries is required. To install these libraries, the OSGEO4W Shell (which comes with QGIS3 installation) can be used. The following steps must be performed (Figure 2):

- run the OSGEO4W Shell **AS ADMINISTRATOR** (i.e., righ-click on the OSGEO4W Shell executable and *Run as administrator*);
- type *python -m pip install pandas* (lower-case letters and respect the spaces) and press Enter. The depencies will be installed in few seconds (Note: this step requires connection to the Internet);
- type *python -m pip install matplotlib* (lower-case letters and respect the spaces) and press Enter. The depencies will be installed in few seconds (Note: this step requires connection to the Internet).

Figure 2: Installation procedure of the *pandas* and *matplotlib* Python libraries.

Example of application

Input needed

To run this plugin, an input csv file is needed. This csv file must contain **AT LEAST** the following fields (the order is not important):

- sample ID (arbitrary format);
- measured pharmaceutical's concentration at the inlet (arbitrary units of measurements). It is suggested to indicate the name of the pharmaceutical and unit of measurements in the heading of this field;
- date and time of measurement (required format: YYYY-mm-dd hh:mm:ss);
- average velocity of water in the stream (values expressed in m/s).

An example on the structure of the input csv file is shown in Figure 3.

Running the plugin

The provided plugin folder (**pharmaceuticals_v0.1**) can be pasted in any folder.
To run the plugin, the ***run_pharmaceuticals_v0.1.bat*** file must be run by simply double-clicking on it. The *Pharmaceuticals* dialog opens (Figure 4).

input_csv_file.csv

```
1  Sample ID;Date and Time;Avg velocity (m/s);Diclofenac (ng/l)
2  1;2018-05-28 07:05:00;0.026;348
3  2;2018-05-28 09:32:00;0.025;391
4  3;2018-05-28 12:10:00;0.026;420
5  4;2018-05-28 13:20:00;0.021;433
6  5;2018-05-28 16:42:00;0.029;363
7  6;2018-05-28 18:32:00;0.028;305
8  7;2018-05-28 21:05:00;0.029;352
```

Figure 3: Structure of the input csv file.

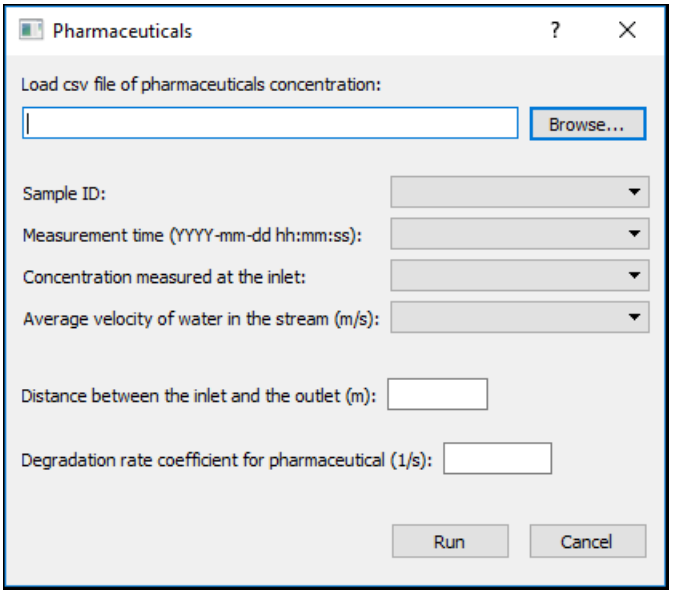


Figure 4: The *Pharmaceuticals* dialog.

First of all, you must load the input csv file by using the *Browse...* button. As an example, you can use the ***input_csv_file.csv*** file provided in the folder **documentation/example_application** (Figure 5).

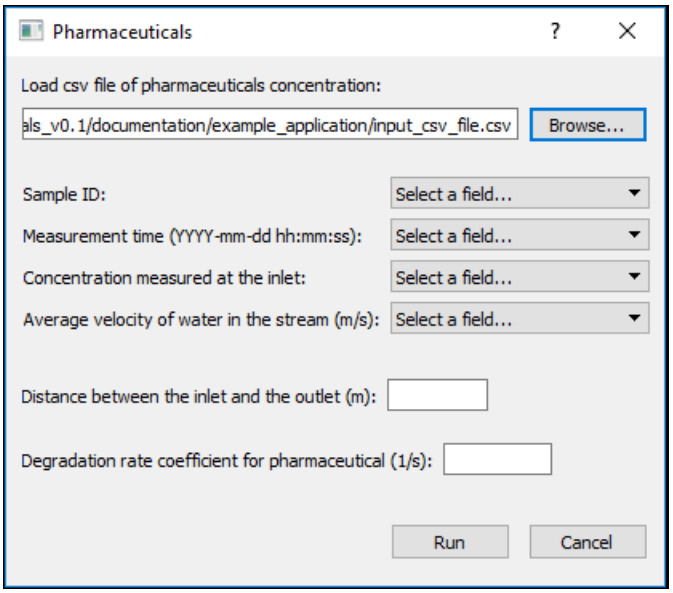


Figure 5: Loading the input csv file.

The drop-down menus *Sample ID*, *Measurement time (YYYY-mm-dd hh:mm:ss)*, *Concentration measured at the inlet* and *Average velocity of water in the stream (m/s)* fill with the headings of the input csv file. You must thus select which fields contain information about *Sample ID*, *Measurement time (YYYY-mm-dd hh:mm:ss)*, *Concentration measured at the inlet* and *Average velocity of water in the stream (m/s)* (Figure 6).

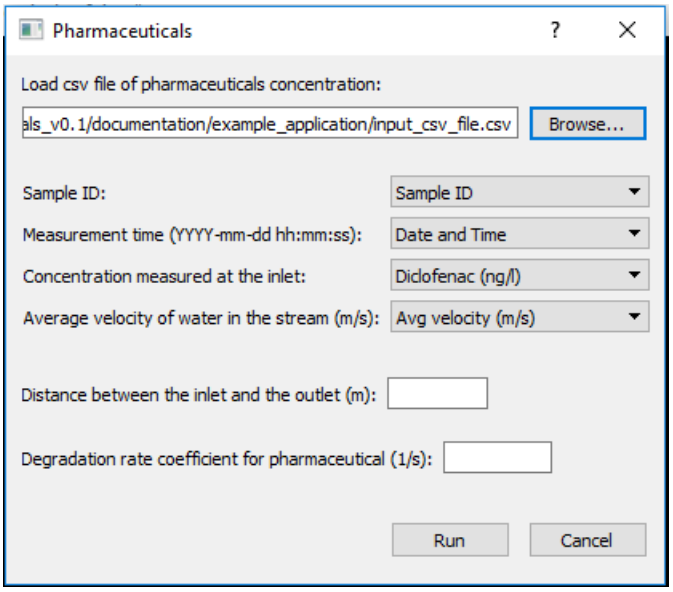


Figure 6: Selecting fields from the input csv file.

The *Distance between the inlet and the outlet (m)* and the *Degradation rate coefficient for pharmaceutical (1/s)* must then be input (Figure 7).

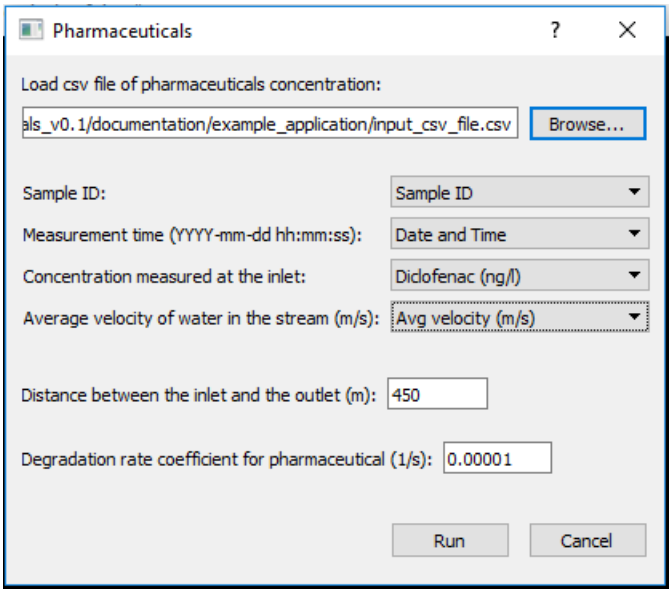


Figure 7: Inputing the *Distance between the inlet and the outlet (m)* and the *Degradation rate coefficient for pharmaceutical (1/s)*.

Output plot

After clicking on *Run*, a plot showing concentration measured at the inlet and concentration simulated at the outlet vs. time is produced (Figure 8).
The sample ID is displayed as a label for the blue points (concentration measured at the inlet), while the string id_out (where id is the sample ID) is displayed as a label for the orange points (concentration simulated at the outlet).
The title of the plot and the label of the y axis are retrieved from the heading of the field corresponding to *Concentration measured at the inlet* in the input csv file.

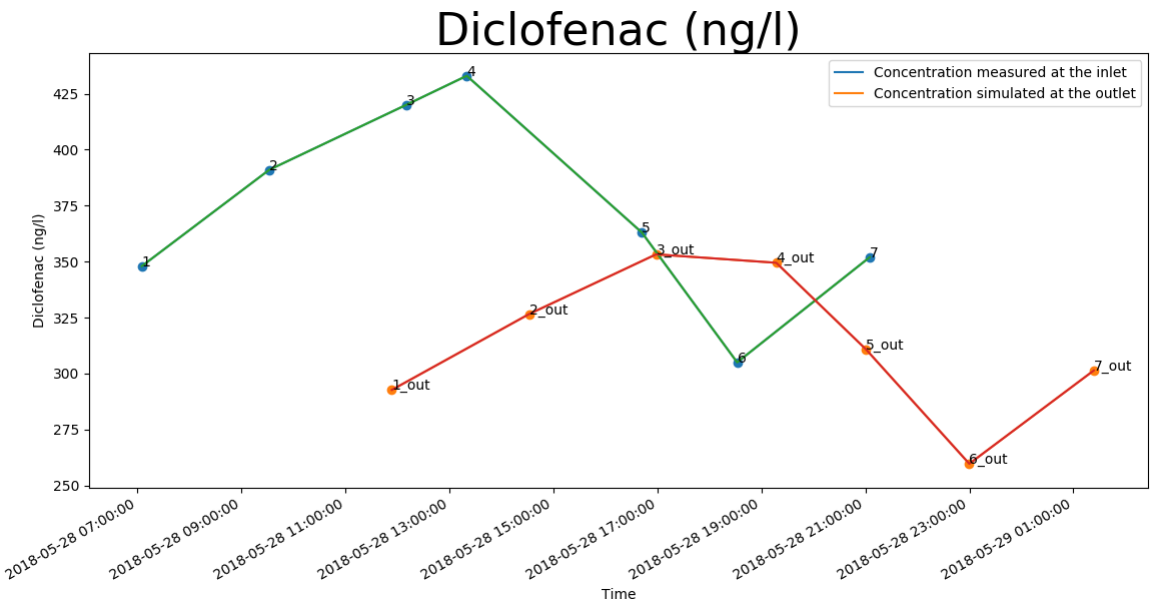


Figure 8: Output plot.

Acknowledgements

This plugin has been developed within the framework of the PHARM-SWAP MED (removal of PHARMaceuticals from treated wastewaters in the Soil-Water-Plant continuum in the MEDiterranean basin) project.
This project has received funding from the Italian Ministry of Foreign Affairs and International Cooperation and the Israelian Ministry of Science Technology and Space, in the framework of the cooperation agreement between Italy and Israel in the field of research and industrial, scientific and technological development (Scientific Track).

Appendix 1 - Resolution of the transport equation by the method of characteristics

Equation (1) can be rewritten as:

$$\frac{\partial C(x;t)}{\partial t} + v\frac{\partial C(x;t)}{\partial x} + \kappa C(x;t) = 0. \tag{4}$$

Equation (4) can be solved with the method of characteristics, provided the following initial condition (equation (3)):

$$C(x;t=0) = C_{inlet}. \tag{5}$$

By using a simplified coordinate system $[(x;t) \rightarrow (s;\tau) \Rightarrow x = x(s;\tau)$ and $t = t(s;\tau)]$, the following characteristics equations can be written:

$$\begin{cases} \frac{dx}{ds} = v \\ \frac{dt}{ds} = 1. \end{cases} \tag{6}$$

Integrating equations (6) gives:

$$\begin{cases} x(s) = v \cdot s + c_1 \\ t(s) = s + c_2, \end{cases} \tag{7}$$

where, given definitions for s and τ, constants c_1 and c_2 can be obtained by the following:

$$\begin{cases} x(s=0) = c_1 = \tau \\ t(s=0) = c_2 = 0. \end{cases}$$

Equations (7) thus become:

$$\begin{cases} x = v \cdot s + \tau \\ t = s, \end{cases}$$

or:

$$\begin{cases} t = \frac{x-\tau}{v} \\ s = t. \end{cases} \tag{8}$$

The initial PDE (Partial Differential Equation; equation (4)) can be written as an ODE (Ordinary Differential Equation) as follows:

$$\frac{dC(s;\tau)}{ds} + \kappa C(s;\tau) = 0. \tag{9}$$

The initial condition for the ODE (9) can be written by solving equations (8) for $t = 0$, which gives:

$$\begin{cases} x = \tau \\ s = 0. \end{cases} \tag{10}$$

Given equations (10), the initial condition (3) can be written for the ODE (9) as:

$$C(x; t = 0) \rightarrow C(\tau; s = 0) = C_{inlet}. \tag{11}$$

Integrating equation (9) gives:

$$\lg C(s;\tau) \quad = \quad -\kappa s + c_1,$$

or

$$C(s;\tau) = c_1 \cdot e^{-\kappa s}. \tag{12}$$

Given the initial condition (11), the following holds: $c_1 = C_{inlet}$. Equation (12) can be thus written as:

$$C(s;\tau) = C_{inlet} \cdot e^{-\kappa s},$$

or, in the $(x;t)$ coordinate system (i.e., by taking into account equations (8)):

$$C(x;t) = C_{inlet} \cdot e^{-\kappa t}. \tag{13}$$

Appendix 2 - Details on the *pharmaceuticals_v0.1* code

Hereinafter, the workflow of the *pharmaceuticals_v0.1* code is reported (Figure 9).

Workflow - step 1. The *Browse...* button (**QPushButton** object) triggers the opening of a window renamed "Select input csv file", which allows to browse the folder where the input csv file is and to load such input csv file.
If the User closes the "Select input csv file" window prior to select the input csv file, an error is produced and the *Pharmaceuticals* dialog closes.

Workflow - step 2. Once loaded the input csv file, its whole path is dispayed in the corresponding bar (**QLineEdit** object). This triggers the reading of the selected input csv file in the form of a Python dictionary whose keys are given by the headers of the fields within the input csv file itself. This also triggers the filling of four drop-down menus corresponding to *Sample ID*, *Measurement time (YYYY-mm-dd hh:mm:ss)*, *Concentration measured at the inlet* and *Average velocity of water in the stream (m/s)* (**QComboBox** objects). Each drop-down menu contains a list of the keys of the above-mentioned dictionary (i.e., the headers of the fields within the input csv file). The first elements of these lists consist of the string "Select a field...", which is first displayed indeed in the drop-down menus.

Workflow - step 3. Once the User select in the drop-down menus the headers corresponding to the *Sample ID*, *Measurement time (YYYY-mm-dd hh:mm:ss)*, *Concentration measured at the inlet* and *Average velocity of water in the stream (m/s)* fields in the input csv file, this triggers the reading of corresponding values in the above-mentioned dictionary. Such values are stored in four different lists, made of string elements.

Workflow - step 4. Once the User types values for the *Distance between the inlet and the outlet (m)* and the *Degradation rate coefficient for pharmaceutical (1/s)* (**QLineEdit** objects), pushing the *Run* button (**QPushButton** object) triggers:

a. a check on the content of the above-mentioned **QComboBox** objects. If the cintent of at least one of them corresponds to "Select a field...", then an error message appears informing which combo box needs to be properly filled;

b. the reading of the content of the **QLineEdit** object corresponding to the *Distance between the inlet and the outlet (m)*;

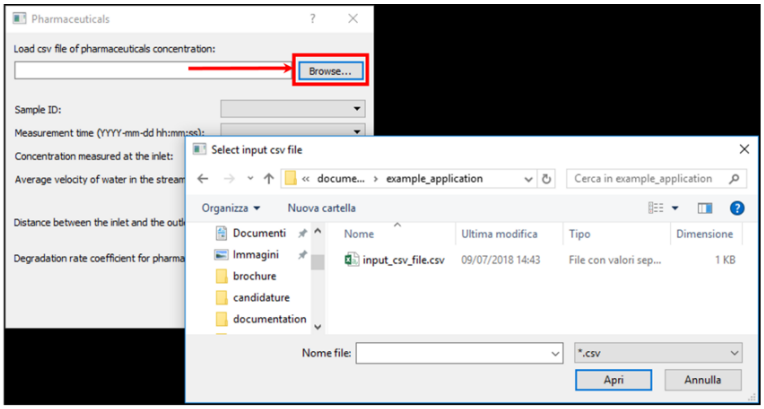
c. the calculus of the time instant when the sample collected at the inlet of the stream reaches the outlet, assuming that $t = 0s$ is the time instant when the sample is collected at the inlet (i.e., the *Measurement time (YYYY-mm-dd hh:mm:ss)* combo box). This calculus is based on the average velocity of the stream (i.e., the *Average velocity of water in the stream (m/s)* combo box) and on the *Distance between the inlet and the outlet (m)*. This calculus is performed for each sample collected at the inlet of the stream: a list of time instants is thus obtained. This list is made of string elements;

d. the reading of the content of the **QLineEdit** object corresponding to the *Degradation rate coefficient for pharmaceutical (1/s)*;

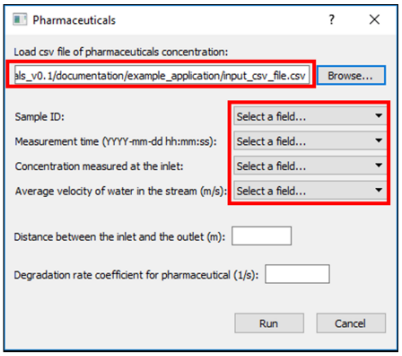
e. the calculus of the simulated concentration for the specific pharmaceutical using equation (13), using the *Concentration measured at the inlet* values read from the input csv file as C_{inlet}, the *Degradation rate coefficient for pharmaceutical (1/s)* input by the User as κ, and the time instant mentioned in item c. as t. This calculus is performed for each sample collected at the inlet of the stream: a list of simulated concentrations is thus obtained. This list is made of string elements;

f. the plotting of the measured and simulated concentrations for the specific pharmaceutical vs. time. The plot will contain two curves: (1) measured concentrations for each sample (values read from the *Concentration measured at the inlet* field of the input csv file) vs. time (values read from the *Measurement time (YYYY-mm-dd hh:mm:ss)* field of the input csv file); (2) simulated concentrations for each sample (values retrieved from calculus made in item e.) vs. time (values retrieved from calculus made in item c.). The points plotted on curve (1) are labeled with values read from the *Sample ID* field of the input csv file as labels. The points plotted on curve (2) are labeled with values read from the *Sample ID* field of the input csv file, plus the "_out" string. The title of the y axis and the title of the plot correspond to the content of the **QLineEdit** object corresponding to the *Average velocity of water in the stream (m/s)*.

All calculus and plotting described in items a. to f. require translating string elements of the lists involved in float numbers or date/time objects.



Workflow – step 1.



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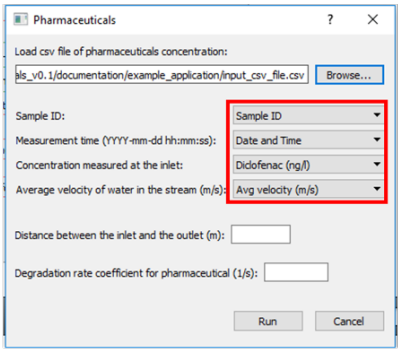
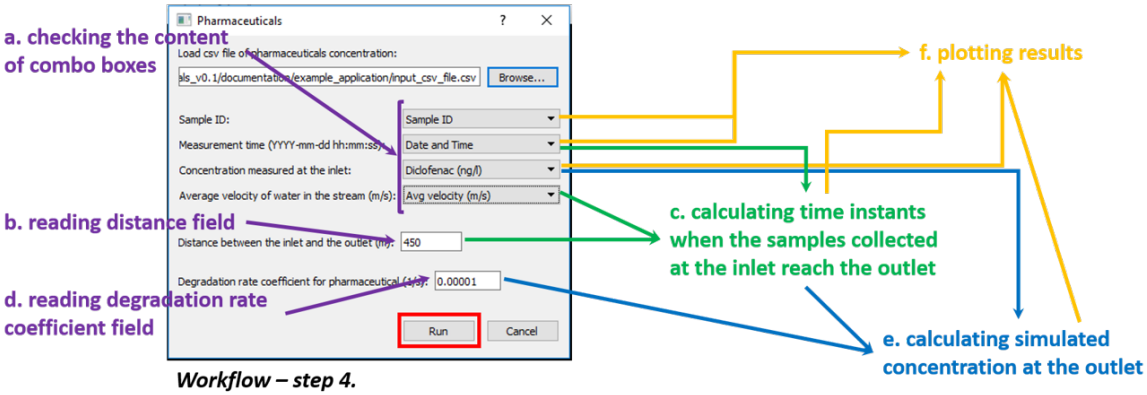


Workflow – step 3.



Workflow – step 4.

Figure 9: Workflow of the *pharmaceuticals_v0.1* code.

Documentation history

2018/07/31 release of v0.1