MATHEMATICAL MODELING AND SIMULATION OF WATERCOURSES CONSIDERING FLOWRATE AND TEMPERATURE DYNAMICS

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ABSTRACT – Due to the importance of the natural watercourses preservation, a mathematical model of heat and mass transfer dynamics of a fixed-geometry watercourse is fully developed. The mathematical model is derived from first principles and consists of both partial differential and algebraic equations. Semi empirical equations are applied to calculate the physicochemical properties, heat loads and mass transfer coefficients. The model is implemented and solved using gPROMS (*General Process Modeling System*).

In this context, the proposed dynamic mathematical model predicts the temperature profile of the watercourse under study, as well as the waterbed one, while considering every major heat flux which impacts on the system (including radiation and non-radiation terms). The obtained results are compared against a well-known river and stream water quality modeling implementation, which allows concluding that a good calibration of the watercourse dynamics mathematical model is here achieved.

1. INTRODUCTION

Nowadays, preservation and purgation of rivers is considered by national and international organizations which are responsible of quality control and preservation of water resources. Water pollution from human activities, either industrial or domestic, and accidental spillages, is a major problem in many countries (Tchobanoglous and Burton, 1991). So it is clear that estimation and simulation of flow and contaminant in river and water systems have more significance in water resources management in order to control and predict water quality.

In addition, water resource temperature is a very important variable in ecological studies. Changes in its temperature can significantly impact its inherent resources dynamics (Caissie, 2006). It is therefore important to understand the thermal regime of rivers for an effective management of aquatic resources.

Deterministic models are efficient tools to understand the dynamics and contribution of the heat and flow rate components (Maheu et al., 2013). This modeling approach consists of both partial differential and algebraic equations of heat and mass transfer processes into a fixed-geometry. Such models can be extremely complicated to solve, involving a large number of parameters and variables, but their main advantage is their closely approximation of reality.

In this context, the primary objective of the present work is to introduce a complete mathematical model to describe temperature profiles of water resources taking into account mass and heat transfer equations, while considering a comprehensive description of the radiation and non-radiation heat transfer terms. Radiation terms including solar shortwave radiation, atmospheric longwave radiation and water longwave radiation are considered. On the non-radiation terms side, the model considers convection, evaporation and condensation. Real measurements of the heat fluxes of a watercourse are used to calibrate the model performance.

2. MATHEMATICAL MODEL

2.1. Watercourse Flowrate Dynamics

The mass balance for the watercourse is expressed in Equation (1), which represents a one-dimensional model for the flowrate dynamics of the system, as represented in Figure 1, with no chemical reaction neither substances addition.

$$\rho \left(\frac{\partial \omega_a}{\partial t} + v_x \frac{\partial \omega_a}{\partial x}\right) = \rho\, D_{AB} \left(\frac{\partial^2 \omega_a}{\partial x^2}\right) \tag{1}$$

This expression of the unsteady-state mass balance is a first-hand approach to the actual behavior of the watercourse; even though, its early inclusion in the overall model should prove quite useful when studying the effects of spillages in future works.

2.2. Watercourse Temperature Dynamics

The time-dependent heat balance is given in Equation (2). Therefore, the temperature of the watercourse depends on the net heat exchanged with the atmosphere and the sediment, as expressed in Equation (3).

$$\rho\, C_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x}\right) = k \left(\frac{\partial^2 T}{\partial x^2}\right) + Q_{Net} \tag{2}$$

$$Q_{Net} = J_{snt} + J_{longat} - J_{back} - J_{conv} - J_{evap} + J_{sed} \tag{3}$$

The heat fluxes considered in the model are summarized next:

- Solar Shortwave Radiation (J_{snt}): the model computes the amount of solar radiation entering the water at a particular latitude and longitude on the earth's surface, which is a function of the radiation at the top of the earth's atmosphere, attenuated by atmospheric transmission, cloud cover, reflection, and shade.

- Atmospheric Longwave Radiation (J_{longat}): the downward flux of longwave radiation from the atmosphere is one of the largest terms in the surface heat balance, and can be computed using the Stefan-Boltzmann law. Thus, it depends upon the effective emissivity of the atmosphere and its temperature, the longwave reflection coefficient and the sky opening fraction.

- Water Longwave Radiation (J_{back}): the back radiation from the water surface to the atmosphere can also be represented by the Stefan-Boltzmann law; as a function of the emissivity of water and its temperature, and the sky opening fraction.

- Convection (J_{conv}): this is the heat transfer that occurs due to the mass movement of fluids. For the watercourse, it occurs at the air-water interface, in the direction given by the positive temperature gradient between both of them. Dependence on wind speed is also considered.

- Evaporation and Condensation (J_{evap}): the heat loss due to evaporation (or heat gain due to condensation) can be represented by Dalton's law, being proportional difference between the saturation vapor pressure at the water surface and the air vapor pressure.

- Sediment Conduction (J_{sed}): the conduction heat flux from the sediments to the water is computed as a function of the temperatures difference between both of them, as well as the effective thickness of the sediment layer and its properties (conductivity, diffusivity, density).

2.3. Watercourse-Sediment Interaction

For the interaction between the watercourse and the sediment at its bottom, Equation (4) describes the associated heat transfer phenomena, and therefore, the dynamic influence over the sediment temperature.

$$\frac{\partial T_s}{\partial t} = -\frac{J_{sed}}{H_{sed}\, {}^{k_s}/_{\alpha_s}} \tag{4}$$

2.4. Implementation and Solution Method

The whole set of equations describing the dynamic behavior of the watercourse is solved using gPROMS (gPROMS, 2001), which is a software package for process modeling and simulation, and acts as a high-level PDE package which allows symbolic specification of PDAEs, boundary conditions, initial conditions and appropriate coefficients. The system of PDAE is numerically solved using the method of lines family of numerical methods (which involves discretisation of the distributed equations with respect to all spatial domains, which reduces the problem to the solution of a set of time depending DAEs).

gPROMS modeling language allows the user to specify the type of the spatial approximation method (e.g. finite difference or finite elements) and the order (e.g. first, second, etc.) of the approximation, where numerical discretization is applied automatically. The resulting system of DAE is integrated over time by employing SRADAU solver (which implements a variable time step, fully-implicit Runge-Kutta method; and it has been proved to be efficient for the solution of problems arising from the discretization of PDAEs with strongly advective terms, in general, highly oscillatory ODEs, and models with frequent discontinuities). SRADAU is included in gPROMS, and automatically adjusts the time step size as well as the integration order to maintain the error of integration within user-specified tolerance.

In this work, first order backward finite difference method, 400 discretization intervals and an absolute and relative tolerance of 10^{-5} are used. All simulations are performed on a 3.7 GHz Core i3 processor with 2 GB RAM.

3. RESULTS AND DISCUSSION

Simulation results obtained from the watercourse dynamics mathematical model are presented in this section. In addition, the obtained results are compared with the ones obtained through the module rTemp included in QUAL2Kw (Pelletier and Chapra, 2001), which is a well-known Excel Workbook for river and stream water quality modeling.

Figure 1 represents every heat flux considered in Equation (3), across 6 days for the selected location, where each day spans across 1440 minutes in local time.

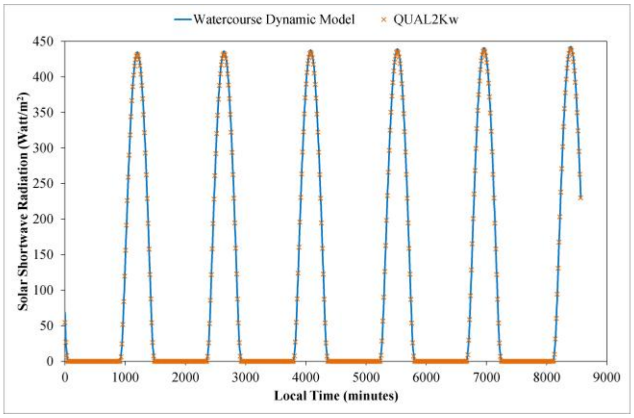
Figure 1.a introduces the solar shortwave radiation. As expected, the contribution from the sun is only noticeable after sunrise and until sunset. Across each day, the solar radiation varies as a function of the solar azimuth and elevation, as well as the shadow and reflection components given by the local atmospheric conditions.

Atmospheric longwave radiation is introduced in Figure 1.b, where it exhibits a direct relationship of air temperature. In addition, it becomes larger as the reflection coefficient decreases, while it also increases as the sky opening fraction does.

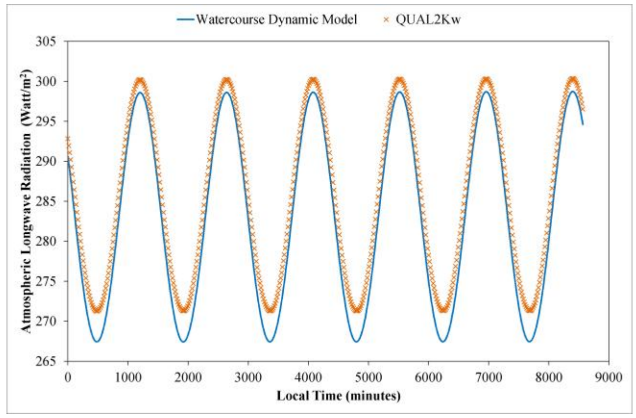
Figure 1.c plots the time-dependent variation of the water longwave radiation, which follows the same trend as the watercourse temperature (as it will be shown further ahead), while it also presents a positive correlation upon the sky opening fraction.

Convection heat transfer between water and atmosphere is represented in Figure 1.d. Since the air temperature is always higher than the watercourse’s, the heat transfer occurs towards the latter. Moreover, convection is favored by increasing wind speeds, whereas the Brady, Graves and Geyer correlation is used to represent such functionality.

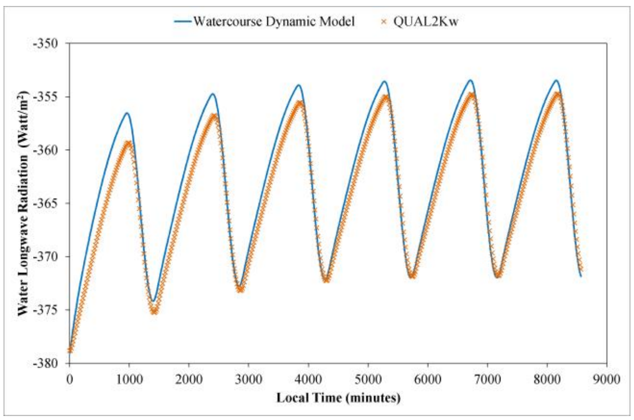
Figure 1.e introduces the heat transfer flux due to evaporation or condensation effects. In this case study, the air temperature remains always higher than de watercourse’s, thus only an evaporative heat flux takes place.



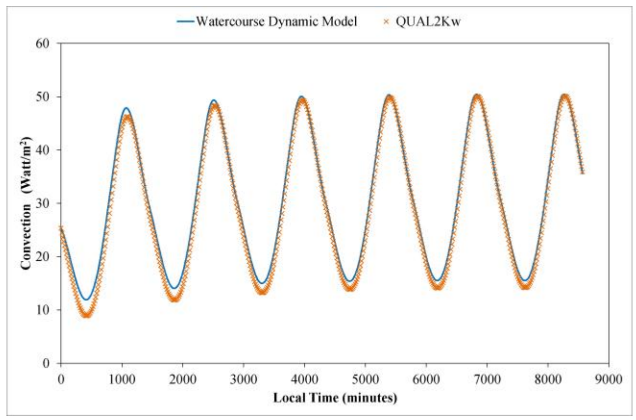
a. Solar Shortwave Radiation.



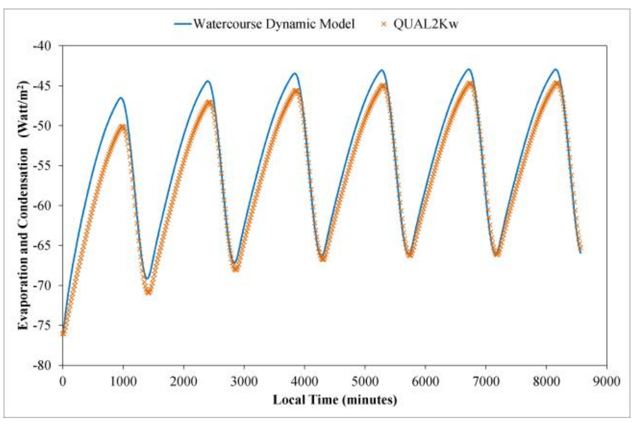
b. Atmospheric Longwave Radiation.



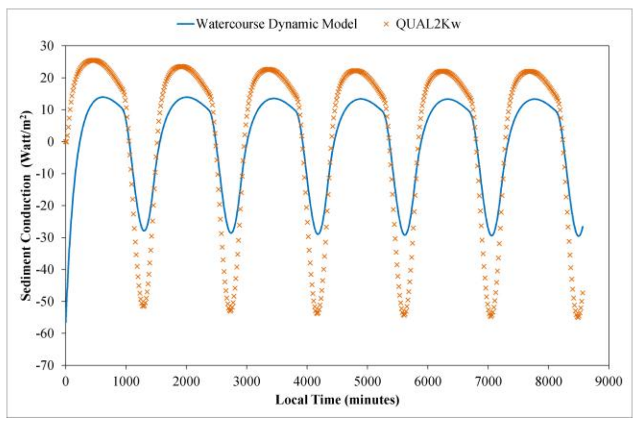
c. Water Longwave Radiation.



d. Convection.

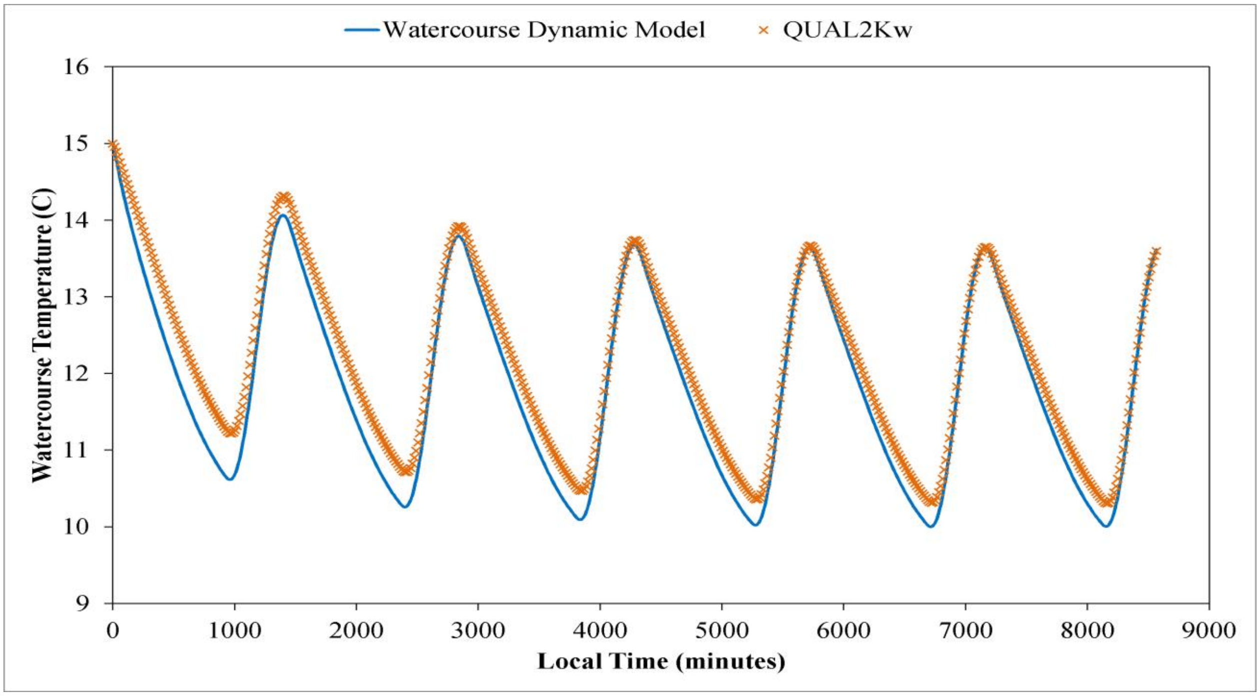


e. Evaporation and Condensation.

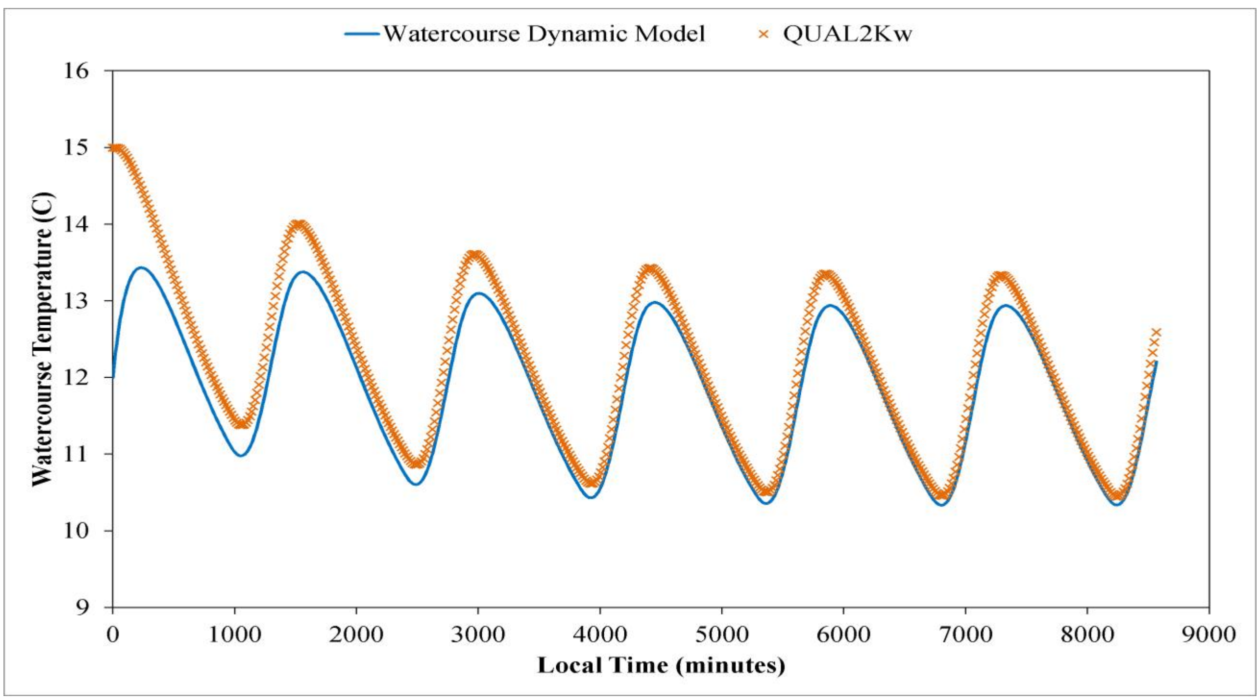


f. Sediment Conduction.

Figure 1 - Calculated heat fluxes and comparison.



a. Watercourse Temperature.



b. Sediment Temperature.

Figure 2 - Obtained temperature profiles and comparison.

The direction of the sediment conduction heat flux varies across the time horizon, as presented in Figure 1.f. Due to the different time-dependent thermal behavior of the watercourse and the sediment layer, associated to their respective physicochemical properties, the temperatures difference shifts its sign, as does the direction of the heat transfer.

Figure 2.a shows the obtained temperature profile for the watercourse, which is governed by Equation (2). It is observed that the radiation terms exert the larger influence in its dynamic behavior; and consequently, the water temperature raises during the daytime, while decreases across dark hours. On the other hand, the non-radiation heat fluxes are one order of magnitude smaller, thus significantly less impacting upon the observed trend for the watercourse thermal response.

The temperature profile for the sediment layer closely follows the watercourse one, as presented in Figure 2.b. As consequence of Equation (4), the larger thermal inertia of the sediment implies a delay on its response to the unsteady state variation of the water temperature.

In addition, the calibration errors between the watercourse dynamics mathematical model here presented, and the values provided by the module rTemp included in QUAL2Kw, are reported for each variable in Table 1. These differences are computed by means of the correlation coefficient between both of them, which reveal the good calibration level here achieved for the proposed formulation.

Table 1 - Calibration errors

Variable	R^2
Solar Shortwave Radiation	0.9999
Atmospheric Longwave Radiation	1.0000
Water Longwave Radiation	0.9711
Convection	0.9962

Variable	R^2
Evaporation and Condensation	0.9707
Sediment Conduction	0.8442
Watercourse Temperature	0.9843
Sediment Temperature	0.9333

4. CONCLUSIONS

The here proposed unsteady state mathematical model for the prediction of watercourses' mass and temperature dynamic profiles exhibits good values of the calibration errors when compared with a well-known free-available software. Therefore, the presented formulation allows determining the main heat fluxes which impact on the system thermal behavior, while delivers accurate estimations of the temperature evolution for the watercourse and its associated stream bed.

This model is the first and priority step to study spillages of toxic substances into watercourses. In future works, the authors intend to build a useful tool to analyze the affectation distances as well as temperature influence regarding climatic events and other possible external factors for different type of spillages, such as chronic or sporadic, and continual or pulse.

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LIST OF TERMS FOR THE DIFFERENTIAL EQUATIONS

$\rho \frac{\partial \omega_a}{\partial t}$	Rate of increase of mass of substance A per unit of volume
$\rho\, v_x \frac{\partial \omega_a}{\partial x}$	Rate of addition of mass of substance A due to convection per unit of volume
$\rho\, D_{AB} \left(\frac{\partial^2 \omega_a}{\partial x^2}\right)$	Rate of addition of mass of substance A due to diffusion per unit of volume
$\rho\, C_p \frac{\partial T}{\partial t}$	Rate of increase of watercourse's temperature per unit of volume
$\rho\, C_p\, v_x \frac{\partial T}{\partial x}$	Rate of increase of watercourse's temperature due to convection per unit of volume
$k \left(\frac{\partial^2 T}{\partial x^2}\right)$	Rate of increase of internal energy due to heat conduction per unit of volume
Q_{Net}	Rate of addition of energy due to external sources per unit of volume
$\frac{\partial T_s}{\partial t}$	Rate of increase of sediments' temperature
$\frac{J_{sed}}{H_{sed}\, {}^{k_s}/_{\alpha_s}}$	Rate of addition of energy due to sediment-water heat flux

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