



An INCA model for pathogens in rivers and catchments: Model structure, sensitivity analysis and application to the River Thames catchment, UK



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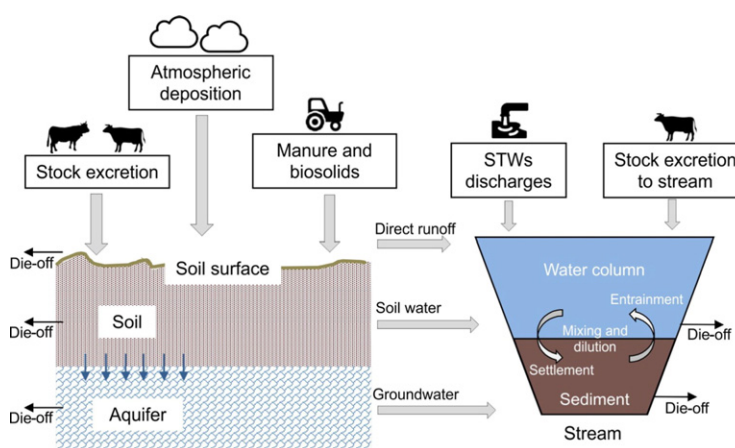
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HIGHLIGHTS

- INCA Pathogens is a process dynamic model for the simulation of pathogens in catchments.
- The model can be used to simulate fluxes of pathogen from both diffuse and point sources.
- The model incorporates all the key processes occurring in soils and water.
- The model has been evaluated using a Monte Carlo sensitivity scheme.
- The model has been applied to 22 reaches of the River Thames in the UK.

GRAPHICAL ABSTRACT



Schematic representing the sources, transport mechanisms and stores of pathogens in the environment.

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ABSTRACT

Pathogens are an ongoing issue for catchment water management and quantifying their transport, loss and potential impacts at key locations, such as water abstractions for public supply and bathing sites, is an important aspect of catchment and coastal management. The Integrated Catchment Model (INCA) has been adapted to model the sources and sinks of pathogens and to capture the dominant dynamics and processes controlling pathogens in catchments. The model simulates the stores of pathogens in soils, sediments, rivers and groundwaters and can account for diffuse inputs of pathogens from agriculture, urban areas or atmospheric deposition. The model also allows for point source discharges from intensive livestock units or from sewage treatment works or any industrial input to river systems. Model equations are presented and the new pathogens model has been applied to the River Thames in order to assess total coliform (TC) responses under current and projected future land use. A Monte Carlo sensitivity analysis indicates that the input coliform estimates from agricultural sources and decay rates are the crucial parameters controlling pathogen behaviour. Whilst there are a number of uncertainties associated with the model that should be accounted for, INCA-Pathogens potentially provides a useful tool to inform policy decisions and manage pathogen loading in river systems.

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1. Introduction

Pathogens are a generic name for the primary microbial agents that cause many illnesses and contagious diseases. These micro-organisms can be microscopic bacteria, sub-microscopic viruses or larger protozoa. In general, pathogens derive from warm blooded animals and humans and can originate from both diffuse sources in catchments, such as runoff from livestock, as well as point sources, such as sewage treatment works (STWs). Pollution of water resources by pathogens is a serious health risk, and pathogens are recognised as one of the primary pollutants of concern in the world (Domingo et al., 2007). Water bodies contaminated with pathogens are responsible for the spread of many contagious, water-borne diseases (Chapra, 2013). This is particularly of concern where water is used for municipal water supply, crop irrigation, and recreational purposes (Environment Agency, 2003, Amirat et al., 2012). Furthermore, the contaminants of wastewater can exacerbate biodiversity loss, such as invertebrates, fish and shellfish (European Commission, 2013).

The European Commission has highlighted the need for continual improvement of wastewater treatment in their seventh implementation report (2013) of the 1991 Urban Waste Water Treatment Directive. According to the most recent Water Framework Directive 2000/60/EC implementation report (2015), point source pollution from sewer overflows remain one of the main pollution sources in urban areas, requiring significant investment in the coming years across the EU. Diffuse pollution significantly affects 90% of river basin districts, 50% of surface water bodies, and 33% of groundwater bodies across the EU. The agricultural sector is the primary source of diffuse pollution. In England and Wales there have been many incidents associated with consumption of contaminated public and private drinking water (Nichols et al., 2009), with the implicated pathogens being *Giardia* spp., *Cryptosporidium* spp., *Escherichia coli* 0157, *Salmonella typhi*, *Salmonella paratyphi*, *Campylobacter* spp. and *Streptococcus moniliformis*. Also the evidence suggested that both low and high river flow conditions can give rise to pathogen-associated drinking water problems, due to reduced dilution of point sources under low flows, and the flushing of pathogens from diffuse sources during high flows and rainfall events (Wilkinson et al., 1995a, 2011). There is also growing evidence of microbial contamination of groundwater, which is often used as an untreated private supply among many communities in the developed world (Kay et al., 2007b; Feighery et al., 2013). For example, testing of private water supplies in England and Wales during 2014 shows that water supplies, in many cases, continues to be of unsafe microbiological quality, with 22.2% of samples (N = 12,885) containing coliform bacteria, 13.4% (N = 7829) containing enterococci, and 12.8% of samples (N = 13,828) containing *E. coli* (DWI, 2015). These results demonstrate that groundwater contamination with faecal matter from birds, animals or humans is widespread, and there is a high risk of private water supplies causing illness (DWI, 2015). There are well established methods of measurement of pathogens and the unit of measurement for bacteria using culturing methods is colony forming units (cfu) per 100 ml of sample. These numbers can be large from STWs with up to 100 million cfu/100 ml for effluents and even higher levels from manures and animal sources (Kay et al., 2008). Thus, filtration and chlorination of public water supplies are generally essential to ensure potable drinking water.

Future predictions of climate change, land-use change and population growth are likely to exacerbate existing pressures on the world's river systems (Alcamo et al., 2007; Whitehead et al., 2009). Climate change is predicted to increase the risks water-borne diseases with a very high confidence (IPCC, 2014). For example, temperature increases and precipitation pattern changes associated with climate change will affect the growth, survival and transport of enteric bacteria (Liu et al., 2013). In order to understand land-use, climate change, and population growth impacts on river pathogen concentrations, scientific and modelling studies on both point and diffuse pathogen sources, and their transport dynamics and survival at the catchment scale, are required. Models

can be used to develop informed health risk assessments, evaluate policy reforms and land-use change options, as well as study management practices (Wilkinson et al., 1995a, 1995b, Kay et al., 2008).

In this paper we consider the transport mechanisms and dynamic processes affecting pathogens in river catchments and develop a new generic version of the INtegrated CAatchment Model INCA (Whitehead et al., 1998, 2011; Wade et al., 2002a, 2002b). The model is subjected to an uncertainty analysis to evaluate the parameter sensitivity and is applied in a case study of the River Thames to investigate the transport, survival, and management of the indicator species total coliforms (TC). Lastly, the potential impacts of land-use change are investigated to assess future potential changes in total coliforms in the River Thames catchment.

2. Pathogen sources, modelling and die-off dynamics

An understanding of pathogen dynamics in the natural environment is necessary in order to model their fate, protect water sources and manage contamination (Meays et al., 2004). Sources of pathogens can be divided into two categories, point and diffuse sources, each of which varies spatially in relation to land use and human population. Point sources are STWs discharges of domestic and industrial wastewater, urban runoff and storm water drainage, and agricultural effluent drainage systems (Wilkinson et al., 1995b). Diffuse sources include surface runoff and drain flow, subsurface flow, and leaching of wildlife and domestic livestock excreta, inputs from nesting or roosting bird colonies, and land application of livestock slurry or manure from indoor sheds, and human biosolids (Wilkinson et al., 1995b).

With the exception of effluent ponds and storage tanks, stores of pathogens principally exist within three medium: 1) the soil system; 2) the river system, within the water column and within the riverbed sediment; and to a lesser extent 3) the groundwater system. The transport of pathogens from the soil system to river systems is related to hillslope hydrological processes, and movement within the river is due to fluvial processes, river morphology and groundwater interactions. Riverbed sediment can act as a repository of pathogens, and entrainment of sediment associated high velocity storm events can introduce pathogens from previous contamination events back into the water column (Domingo et al., 2007). A schematic of the sources and transport mechanisms of pathogens in the environment is illustrated in Fig. 1.

There are many approaches to modelling environmental systems and the review by de Brauwere et al. (2014) highlights the real difficulties with modelling pathogens or indicators of pathogens. This is mainly because of the limited knowledge of process dynamics in soils, sediments, rivers and groundwaters, linked to the paucity of terrestrial and aquatic field data. The situation is further complicated by the wide range of pathogens (protozoa, bacteria, viruses), which display different behavioural and response patterns, making dynamic modelling difficult (Chapra, 2013). Early work by Thomann and Mueller (1987) gave a good summary of the extent and scope of the modelling needs, but mainly focus on indicators of pathogens. More recent approaches include export coefficient and regression analysis (McGrane et al., 2014; Kay et al., 2008) and these approaches are often used especially where data is limited or where broad policy advice is required. Chapra (2013) describes a process based approach in rivers considering the growth and die off dynamics linked to a pathogens budget. This approach forms the basis of most stream models (Ludicello and Chin, 2015; Coffey et al., 2013 and Ferguson et al., 2007) and has been extended to include terrestrial components as part of the Soil and Water Assessment Tool (SWAT) applied to whole catchments (Coffey et al., 2013). The dominant factors affecting the survival of pathogens in the water column are settling, solar radiation (and turbidity), and temperature and these have been modelled in rivers and catchments by Wilkinson and colleagues (Wilkinson et al., 1995a, Wilkinson et al., 1995b; Collins and Rutherford, 2004). Risk based approaches have also been utilised taking

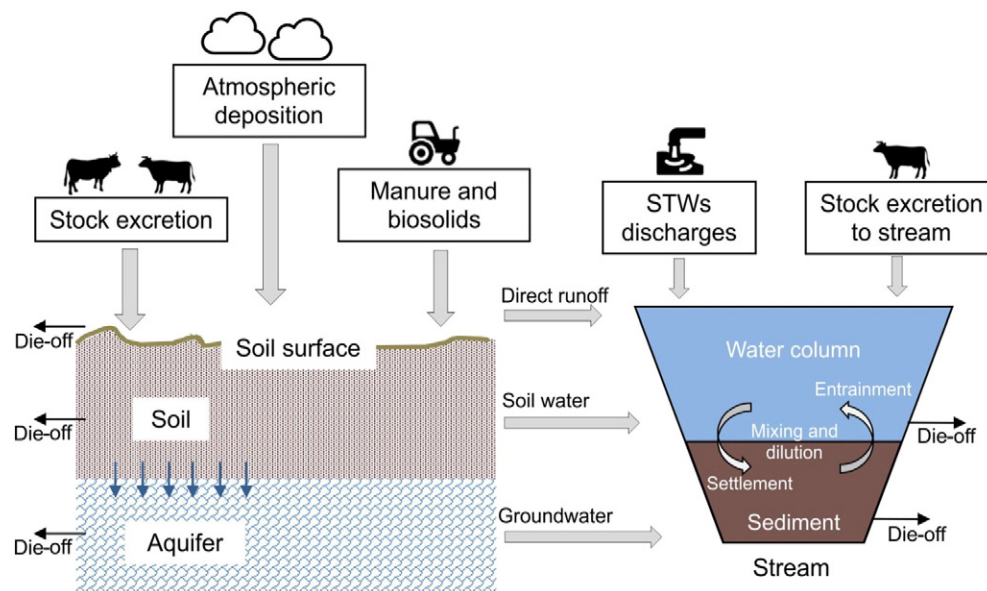


Fig. 1. Schematic representing the sources, transport mechanisms and stores of pathogens in the environment.

advantage of Monte Carlo Techniques to address parametric uncertainty (Muirhead et al., 2011).

The reported fate of pathogens in the environment ranges from extended persistence to rapid decline. The die-off or decay of pathogens varies depending on the medium in which they are located (soil, water column, river bed sediment or groundwater), and a number of other environmental factors. The factors affecting the survival of pathogens in the aquatic and terrestrial environment include temperature, suspended sediment in the water column and sediments in the river bed, exposure to solar radiation and oxygen levels. In addition, hydrological conditions, shear velocity in streams, and the dynamic interaction with hosts such as humans, domestic animals or wild animal populations (Maszle et al., 1998) play a major role in pathogen dynamics and mechanisms. Gonzalez (1995) explains that die-off curves are typically non-linear, but can be approximated as a first order exponential decay with a characteristic decay rate. There is contradictory evidence on the length of time that pathogens can survive in soils with estimates of decay rates of Faecal Indicator Bacteria (FIB) ranging from 0.025 day^{-1} at 5°C in a saturated sandy loam with a pH of 6.8–8.3 (Sjogren, 1994), to 0.7 day^{-1} during warm, dry summer conditions in a coarse loam, rich in organic materials (Donsel et al., 1967). Reported survival of FIB in UK soils range from 4 days (Nicholson et al., 2005) to 5–6 months (Avery et al., 2004). The survival of pathogens in soil is primarily limited by soil moisture and texture, and exposure to sunlight. In the water column, published decay rates of FIB in the water column range from 0.60 to 6.64 day^{-1} . In the River Exe, Devon, UK, measured decay rates (day^{-1}) of FIB range from 0.3 – 0.9 day^{-1} depending on the season (Wilkinson et al., 1995b). In the River Ribble, northern England, the average FIB decay rates during daylight hours was measured as 6.64 day^{-1} (Kay, 2014, pers. comm.). In contrast, measured FIB decay rates under dark conditions were much reduced at 0.60 day^{-1} (Kay, 2014, pers. comm.). Turbidity reduces the ability of light to penetrate through the water column, as does water depth, and thus indirectly increases the survival of pathogens (Wilkinson et al., 1995a).

Pathogen survival within riverbed sediment stores remains poorly understood (Wilkinson et al., 1995a, Collins and Rutherford, 2004, Domingo et al., 2007, Garzio-Hadzick et al., 2010), although they can persist longer, and in greater concentrations, in riverbed sediments than in the overlying water column (Garzio-Hadzick et al., 2010). Published decay rates of pathogens in riverbed sediment range from 0.021 day^{-1} at 4°C to 0.3 day^{-1} at 26 – 34°C . Little is known about

the survival of pathogens in groundwater. Groundwater is vulnerable to contamination (Personné et al., 1998, Entry et al., 2000), although pathogens are generally found in concentrations several times lower than surface concentrations, due soil filtration (Entry et al., 2000). It is also known that pathogens in groundwater are capable of surviving for extended periods due to the absence of solar radiation in comparison to surface waters (Keswick et al., 1982).

3. INCA modelling of pathogens in catchments

In this paper we utilise the INCA Model as the main platform for a new pathogens model. INCA is a catchment scale process based model to calculate pollutant transfer from diffuse sources and point sources to the catchment outlet, as shown in Fig. 1. To date, the INCA model family includes simulation of nitrogen, phosphorus, sediments, chloride, carbon and mercury (Whitehead et al., 1998, White, 2011, 2013; Wade et al., 2002a, 2002b, Lazar et al., 2010; Futter et al., 2007, 2012; Jin et al., 2012 and Crossman et al., 2013). Many of the parameters and processes that have previously been successfully validated in other versions of INCA, also apply to modelling for pathogens, such as the hydrology, pathways, sediment settlement and entrainment, and flushing out components. Due to the dynamic nature of the model, variations in rainfall and temperature, and changes of inputs, such as STW discharges and manure from livestock, can be investigated. This means the effects of climate change, population growth, land use change, and mitigation measures on the concentration of pathogens in the environment can be evaluated. A full description of the equations and processes of INCA is given by Wade et al. (2002a, 2002b).

The INCA-Pathogens Model has been designed to simulate the transport pathways and fluxes of generic pathogens in the land, water column, riverbed sediment, and groundwater phases. By generic we mean that the model equations have been written so that, in theory, any pathogen can be simulated provided the appropriate input sources and die-off and regrowth rates are utilised in any model application. The processes of both suspended sediment deposition, and riverbed sediment entrainment are simulated based on the INCA-Sediment model (Lazar et al., 2010) and this is used as the core of the model together with the underlying hydrological model (Whitehead et al., 1998; Wade et al., 2002a, 2002b). The model framework is the same as other versions of INCA with different scales from which data flows in INCA: from a 1 km^2 cell containing process mass balance equations of water

and pathogens for each land use; to the sub-catchment scale summing the fluxes from the different land uses, and diffuse and point sources; and lastly to the catchment scale where multiple sub-catchments are summed to give a cumulative representation of in-stream pathogen concentrations, as shown in Fig. 2.

3.1. The simulation of water flow and pathogens in the landscape

The landscape mass balances of water and pathogens are based on a 1 km² cell and the inputs to the model and the model constants can vary on a sub-catchment basis and according to soil or land-use type. These two factors allow the mass stored, process rates and hydrological pathways to vary spatially based on preconceived notions of variations in soil moisture, temperature, adsorption potential and land management practices. The water volumes and the mass of pathogens are summed based on the relative amounts of each land use or soil type within a sub-catchment and the output passed to the instream routing model (Fig. 2).

It is assumed there can be rapid drainage or storm flow from the land surface and that there are two main sub surface stores: the soil and groundwater zones (Whitehead et al., 1998). The flow of water through the two zones is given by the following two equations:

Soil zone:

$$\frac{dq_{sz}}{dt} = \frac{P_{eff} - q_{sz}}{T_{sz}} \tag{1}$$

Groundwater zone:

$$\frac{dq_{gz}}{dt} = \frac{\beta q_{sz} - q_{gz}}{T_{gz}} \tag{2}$$

where q_{sz} and q_{gz} are the outflows from the soil and groundwater zones (m³ s⁻¹ km⁻²); P_{eff} is the hydrologically effective rainfall (m³ s⁻¹ km⁻²); β is the base flow index (\emptyset); t is time and T_{sz} and T_{gz} are the response times associated soil and groundwater zones (days).

Within the soil zone it is assumed the water can be partitioned into two volumes: drainage and retention. The drainage volume represents the water stored in the soil that responds rapidly to water inflow and drains under gravity; it may be thought of as macropore or drain flow (i.e. the flow that most strongly influences the rising hydrograph limb). The soil zone retention volume represents the water stored or retained in the soil after gravity drainage; it responds more slowly than the drainage water and represents the majority of water in the soil.

3.2. Equations for the transport, storage and transformations of pathogens in the landscape

The change in numbers of pathogens in the soil, m_{sz} (No. km⁻²) and groundwater, m_{gz} (No. km⁻²) stores are given by Eqs. (3) and (4) and the diffuse pathogens sources from the land phase, m_{in} (No. km⁻²) are:

$$m_{in} = \text{manures (either aerial spreading or injection application)} \\ + \text{atmospheric deposition} + \text{livestock animal inputs} \\ + \text{wild animal inputs}$$

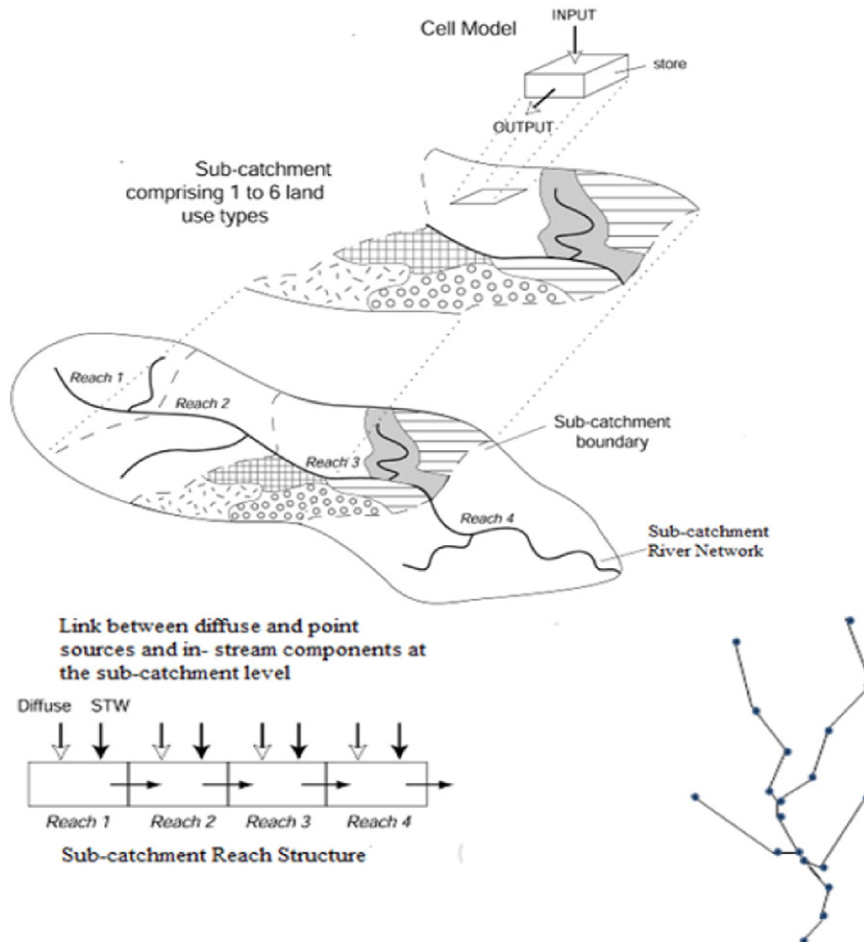


Fig. 2. Schematic representing the structure and different scales of the INCA and showing a typical multi-reach branched structure (bottom-right part of the figure) that can be set up within INCA.

with soil zone dynamics:

$$\frac{dm_{sz}}{dt} = \frac{m_{in}q_{sz}86400}{V_D + V_R} - \frac{m_{sz}q_{sz}86400}{V_D + V_R} - \frac{\beta m_{sz}q_{sz}86400}{V_D + V_R} - C_3 m_{sz} + C_4 m_{sz} \quad (3)$$

with groundwater zone dynamics:

$$\frac{dm_{gz}}{dt} = \frac{\beta m_{sz}q_{sz}86400}{V_{gw}} - \frac{m_{gz}q_{gz}86400}{V_{gw}} - C_5 m_{gz} + C_6 m_{gz} \quad (4)$$

where, C_3 and C_5 (day^{-1}) are the rates of pathogen die-off in the soil and aquifer. V_D and V_R represent the volume of the direct soil zone and the volume of the direct runoff respectively. V_{gw} is the volume of the groundwater zone. The rate parameter describing pathogen die-off or decay in the soil is both temperature dependent and solar radiation dependent, such that

$$C_3 = C_d (1.07^{\theta_w - 20}) + C_{sr} \quad (5)$$

where θ_w is the water temperature ($^{\circ}\text{C}$) which is driven by input air temperature, C_d (day^{-1}) is the decay rate at 20°C and where C_{sr} is a light enhanced decay rate (day^{-1}), where

$$C_{sr} = \alpha \cdot SR \quad (6)$$

and where α is a proportionality constant and SR is the solar radiation (Thomann and Mueller, 1987).

It is assumed that the decay rate in the groundwater is temperature dependent only so that

$$C_5 = C_d (1.07^{\theta_w - 20}). \quad (7)$$

It is assumed that C_4 and C_6 are growth parameters which would enable the growth of pathogens under certain favourable temperature conditions (such as for legionella), as follows:

$$C_4 = C_e (1.07^{\theta_w - 20})$$

and

$$C_6 = C_f (1.07^{\theta_w - 20}).$$

Whereby, C_e and C_f are the growth rates in the soils and groundwaters and subject to temperature controls.

3.3. Water flow and storage in the river

The reach residence time constant, T_{reach} (days) is calculated as:

$$T_{reach} = \frac{L}{aq_{reach,out}^{b, 86,400}} \quad (8)$$

where L is the reach length, $q_{reach,out}$ is the discharge from the reach and a and b are parameters relating the reach velocity to the discharge. The parameters a and b are determined through calibration, though typically b has a value of 0.67. The parameters can also be determined from tracer measurements. The change in the reach flow is calculated from the input–output mass balance of the form

$$\frac{dq_{reach,out}}{dt} = \frac{q_{reach,in} - q_{reach,out}}{T_{reach}} \quad (9)$$

where $q_{reach,in}$ is the sum of the input flows from the upstream reach, point source effluent, diffuse inputs from the rapid overland flow or

drainflow, flow from the soil and groundwater zones and any losses via abstraction.

3.4. Pathogen process equations for the river system

In the river, the key pathogen processes are sedimentation to the river bed, subsequent resuspension under high flows and decay in both the water column and in the river bed sediment. The reach mass balance includes the upstream water quality together with diffuse inputs from the soil and groundwater zones, as well as direct effluent discharges and abstractions. A key concept in the water column is that pathogens are not all bound to sediments but can float freely in the stream. However, they can flocculate and combine to form clusters which can be deposited on the stream bed (Chapra, 2013). They are also subject to decay in the water column and this decay can be temperature and solar radiation dependent.

The pathogen numbers, m_{reach} present in the water column in a river reach is given by:

$$\frac{dm_{reach}}{dt} = \frac{m_{reach-in}q_{reach,out}86400}{V_{reach}} - \frac{m_{reach}q_{reach,out}86400}{V_{reach}} - C_7 m_{reach} - C_8 m_{reach} + C_9 m_{sed} + C_{10} m_{reach} \quad (10)$$

And for the sediment bed:

$$\frac{dm_{sed}}{dt} = C_8 m_{reach} - C_9 m_{sed} - C_{11} m_{sed} + C_{12} m_{sed} \quad (11)$$

where, Eq. 10 is the mass balance over a reach. The pathogen mass into the reach, $m_{reach-in}$ (No. day^{-1}) is the sum of the upstream input, point source effluent and the diffuse inputs from the soil and groundwater. The second term on the right hand side of Eq. (10) represents the mass transfer downstream with the flow of water; the third term represents any the mass loss due to decay; the fourth term represents the sedimentation of the pathogen onto the river bed; the fifth term represents the resuspension of pathogens from the sediment bed and the sixth term represents a growth rate of the pathogens in the reach.

The rate parameter describing pathogen decay C_7 in the water column is both temperature dependent and solar radiation dependent, such that

$$C_7 = C_g (1.07^{\theta_w - 20}) + C_{sr} \quad (12)$$

where θ_w is the water temperature ($^{\circ}\text{C}$) which is assumed driven by input air temperature, C_g (day^{-1}) is the decay rate at 20°C and C_{sr} is a light decay rate (day^{-1}), where

$$C_{sr} = \alpha \cdot SR. \quad (13)$$

And, where α is a proportionality constant, and SR is the solar radiation (Thomann and Mueller, 1987).

C_8 is the in loss rate of pathogens moving from the reach to the sediments.

It is assumed that the resuspension rate of pathogens from the sediments bed to the water column, C_9 , is triggered at a threshold water velocity such that:

$$\text{If } (Vs > Vks) \quad C_9 = C_{9k} \quad (14)$$

where Vs is the shear velocity calculated by the model and Vks is the user supplied threshold shear velocity above which resuspension is triggered at a rate C_{9k} .

Also, the pathogen growth terms are temperature dependant as follows

$$C_{10} = C_i (1.07^{\theta_w - 20}) \quad (15)$$

$$C_{12} = C_j(1.07^{0w-20}) \quad (16)$$

and C_{11} represents the die-off of pathogens in the riverbed sediments and is temperature dependant as follows

$$C_{11} = C_k(1.07^{0w-20}). \quad (17)$$

Whereby, C_i and C_j are the pathogen growth rates (subject to temperature controls) in the water column and in the riverbed sediments and C_k is the die-off rate in the sediments.

The equations are a set of ordinary differential equations that are solved numerically using a 4th order Runge and Kutta Algorithm using a Merson variable step length routine. This ensures a stable solution to the equations. Model outputs will be the same as current versions of INCA, namely times series at each reach boundary, profiles along the river system, frequency distributions (and hence probability of occurrence), 3D plots, loads and also times series data for subsequent application to downstream groundwater models.

4. Application of INCA-Pathogens to the River Thames

The River Thames has been subject to several INCA studies for nutrients such as N and P, and details of the catchment characteristics are given by Jin et al. (2012); Crossman et al. (2013) and Whitehead et al. (2013). The geology of the River Thames catchment is mainly of highly permeable, dual-porosity chalk, although the upper part of the catchment is characterised by low permeability clays, and the lower part characterised as sands and sandstone (BGS, 2014). The catchment has

an average base flow index of about 0.65 and land use is mainly intensive agriculture or pasture for grazing of sheep and cattle. Significant progress has been made to improve the water quality and ecosystem health of the River Thames over the years but FC and TC problems remain with incidents of pollution from STWs and agriculture, particularly during high rainfall events when combined sewer overflows operate more frequently and runoff from agriculture is induced (Lang et al., 2007, Amirat et al., 2012).

As in previous INCA studies of the River Thames, a 22 reach catchment description has been used, as shown in Fig. 3. For the purposes of this study, TC was chosen as the pathogen indicator because of its acceptability as an effective indicator of pathogens from soils and mammals and due to the availability of TC data from the UK Environment Agency. An overview of input data required for INCA and their sources are presented as Table 1. The INCA-Pathogens model was applied for the time period 2002–2008.

4.1. Input time series data

The daily time series of actual precipitation, hydrological effective rainfall (HER), soil moisture deficit (SMD), air temperature, and solar radiation were sourced and derived from the Meteorological Office and the PERSiST conceptual rainfall–runoff model (Futter et al., 2014). PERSiST, the Precipitation, Evapotranspiration and Runoff Simulator for Solute Transport, is a semi-distributed, watershed-scale hydrological model suitable for simulating terrestrial runoff and streamflow across a range of spatial scales from headwaters to large river basins (Futter et al., 2014).

For INCA-Pathogens, land use in the River Thames catchment was classified as one of five types: Urban, Intensive agriculture, Non-

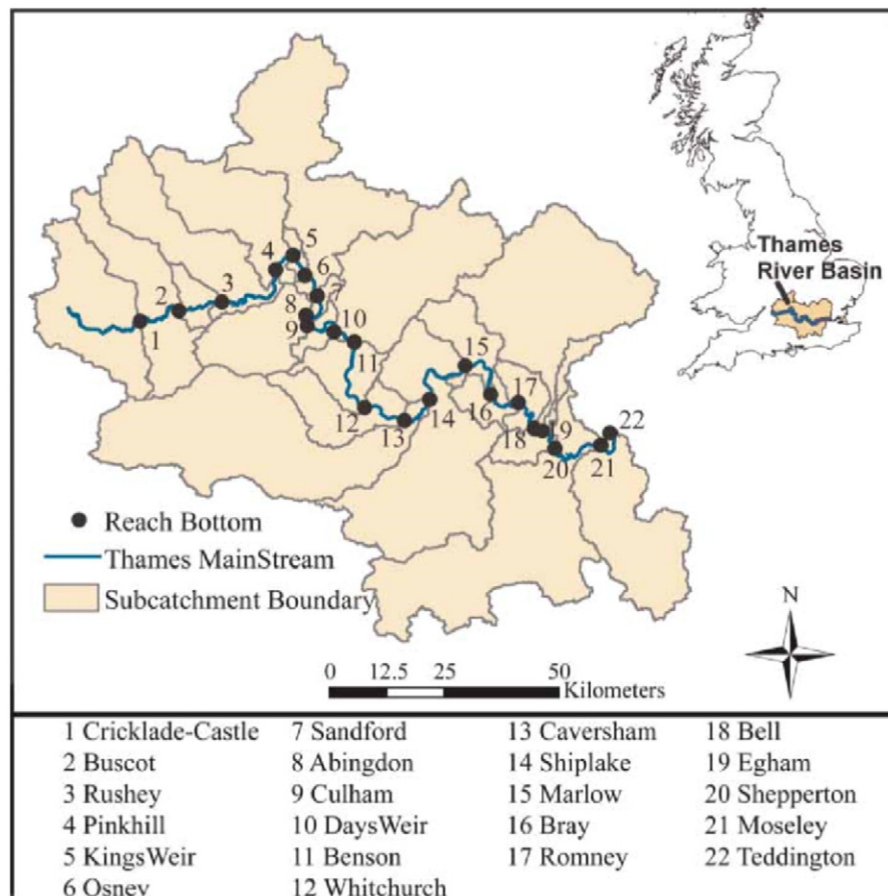


Fig. 3. Study location map of the River Thames catchment and the 22 reaches of the main river used for INCA-Pathogens set-up.

Table 1
Data sources for INCA-Pathogens.

Data	Data description	Data source
Observed hydrological data		
Precipitation, temperature, and solar radiation	Daily time series	Met office
Discharge	Daily time series	Environment Agency
Flow rates	Daily measurements in Reaches 4, 9, 10, 13, 17, 20, 22	Environment Agency
Base flow index	Derived from flow gauges and extrapolated to other tributaries	Wade et al. (2002a, 2002b)
Soil moisture deficit (SMD) and hydrologically effective rainfall (HER)	Daily time series	Estimated for the Thames catchment based on the PERSiST rainfall runoff model (Futter et al., 2014)
Groundwater residence time	For each sub-catchment	Jin et al. (2012), Crossman et al. (2013)
Observed water quality data		
TC concentrations	Routine sampling and event sampling in Reaches 3, 10, 11, 12, 14, 15, 20, 22.	Environment Agency
Land use and livestock data as TC diffuse inputs		
Land use data	Ecological land classification and land use classifications GIS layer	LCM2000 land coverage map, Centre for Hydrology (Crossman et al., 2013)
Animal numbers	Numbers of cattle, sheep, poultry, and pigs for each sub-catchment, based on year 2008	Crossman et al. (2013), DEFRA (2014)
Coliforms from animals	Derived from average manure production and TC	Kay et al. (2010)
STW data as TC point source inputs		
Discharge rates	STW discharge rates for each reach	Environment Agency
FC and TC	numbers for UK sewage and treated effluent	Kay et al. (2008)
Future scenario data		
Land use change	Ecological land classification and land use classifications GIS layer	LCM2000 land coverage map, Centre for Hydrology (Crossman et al., 2013)

intensive agriculture, Wetlands, and Forest. In this study, land-use type 'intensive agriculture' was defined as arable (i.e. used for the purposes of growing crops). Therefore, all diffuse livestock sources of TC were attributed to land-use type 'non-intensive' agriculture. The reach lengths, sub-catchment areas, and land use percentages used as inputs for INCA-Pathogens application to the River Thames are presented by Jin et al. (2012). Diffuse sources of TC from agriculture were calculated per reach by multiplying the number and type of livestock, by the number of TC produced per animal per day. These values were apportioned by sub-catchment depending on the percentage of non-intensive agriculture land use. It was assumed that poultry were chicken. For the purposes of this study, it was assumed that whether livestock graze outdoors, or were housed indoors, the manure from livestock was returned to the land and incorporated into the soil. The total TC from diffuse livestock sources to the River Thames catchment surface was assumed to be 1.4×10^{16} CFU/100 ml/day, which when divided by the catchment area (1 M ha), the TC from livestock becomes 1.4×10^{10} CFU/100 ml/ha/day. However, it is recognised that only a small percentage of coliforms from livestock makes it to the river, due to die-off and soil filtration (Chapra, 2013). The livestock input parameter was adjusted with this in mind during the calibration procedure to get best model fit. Major STW discharges are located in 13 of the 22 reaches of the River Thames (Table 2). The majority of STW discharges to the River Thames and its tributaries are treated to the secondary level in accordance with the European Wastewater Treatment Directive 91/271/EEC (EU, 2013). In accordance with this level of treatment, TC numbers from STWs were assumed to be 1.4×10^4 CFU/100 ml (Kay et al., 2008), and were multiplied by the daily discharge rates of the STWs (Table 2).

5. Model calibration and dynamics

Simulated daily flow over the calibration period (2002–2008) provided an acceptable reproduction of the observed flow ($R^2 = 0.67$) at Reach 22, as shown in Fig. 4 and similar results are given elsewhere for the INCA application to the Thames (Jin et al., 2012, Futter et al., 2014). The livestock input, light proportionality constant for water column TC die-off, and sediment settlement and entrainment coefficients, were calibrated to get the best model fit and Table 3 shows the decay

rates and input parameters. The percentage of TC from deposition of livestock manure on the soil surface that reached the river channel was calibrated at 0.01%, corresponding to an input number of 1.4×10^6 cfu/100 ml/ha/day. The best fit light proportionality constant, and the settlement and entrainment coefficients, were in agreement with values calculated by Thomann and Mueller (1987) and Chapra (2013) respectively.

Using the fixed literature input parameters outlined in the previous section, and the adjusted best fit parameters presented in Table 3, the simulated TC concentrations in the water column over the calibration period broadly matched that of the observed data, as shown in Fig. 4, with an R^2 of 0.83 at Reach 20 and R^2 of 0.57 at Reach 22. This degree of correlation is comparable to that of other microbial water quality models developed, such as the Collins and Rutherford (2004) model with an R^2 of 0.71, and Wilkinson et al. (2011) with an R^2 of 0.54. Peak concentrations of TC were broadly linked with diffuse pollution and storm events in winter and spring, and STW discharge with low flow in summer. However, there was limited storm event data for TC in the River Thames with which to calibrate the model. There were some discrepancies between the simulated and observed concentrations, particularly during winter storm events, as might be expected given the wide range of uncertainty

Table 2
Daily STWs flows in the main reaches of the River Thames catchment.

Reach	Flow (m ³ /s)
1	0.00864
3	0.00098
5	0.04507
7	0.076
9	0.12406
10	0.107
11	0.0056
12	0.0348
13	0.015
15	0.02834
16	0.22525
18	0.07393
22	0.715

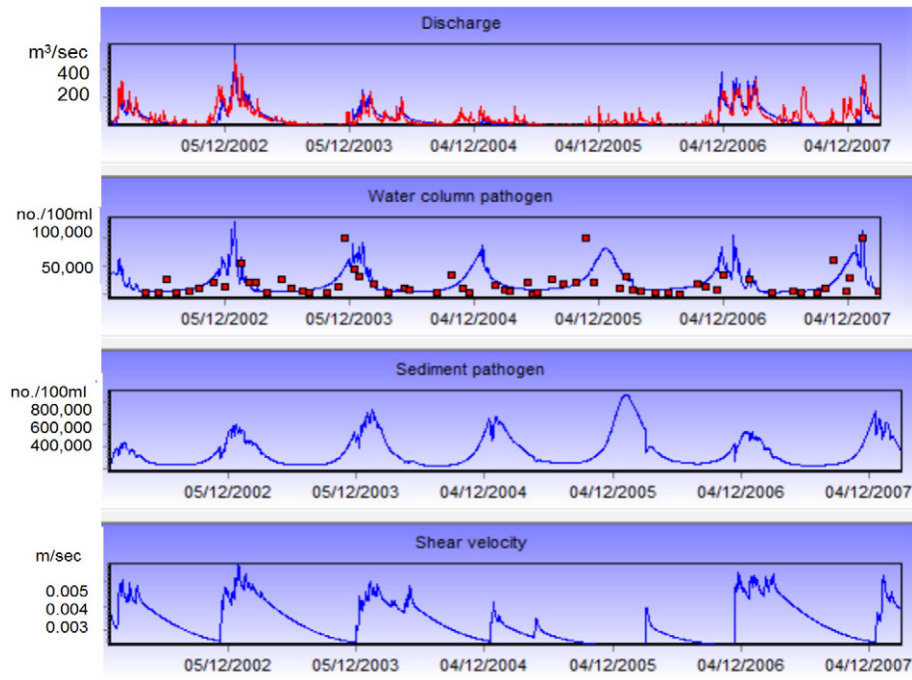


Fig. 4. Comparison of simulated (red) and observed (blue) flow rates, simulated (blue line) and observed (red dots) TC concentrations in the water column and riverbed sediment, and shear velocity, at Teddington (reach 22).

on the inputs, especially from diffuse sources, and the lack of TC data during such events. The mean simulated TC concentration of all reaches over the period 2002–2008 was 5.0×10^4 CFU/100 mL, within the same order of magnitude of mean TC concentrations recorded in the UK study by Kay et al. (2007a). It appears that sediment entrainment may play a significant role in the water column TC concentration of the River Thames, as there is a marked depletion of the riverbed sediment TC store following high river flows in winter.

5.1. Sensitivity analysis

A sensitivity analysis was performed to assess the sensitivity of INCA-Pathogens to changes in the input parameters that affect water column TC concentrations. Whilst it is recognised that there are uncertainties with other processes that affect the model outputs, the hydrological dimension of INCA has been subject to extensive sensitivity, uncertainty and Monte Carlo analysis in earlier studies (e.g. McIntyre et al., 2005, Rankinen et al., 2006, Crossman et al., 2013), giving high correlation between observed and simulated flow for the Thames (Crossman et al., 2013). A further Monte Carlo analysis has been undertaken following the methods outlined in Futter et al. (2014) to identify the most sensitive parameters controlling INCA- pathogen's performance. Parameter sensitivity was assessed using Pearson correlation, Nash-Sutcliffe efficiency (NS) and log (NS) statistics for modelled and observed pathogen concentrations at reaches TR03, TR20 and TR22. Performance statistics were weighted by the number of observations

Table 3
Adjusted best-fit parameters for input into INCA-Pathogens.

Parameter	Calibrated input value
Livestock coliform input (cfu/100 ml/ha/day)	1.4×10^6
Light proportionality constant for water column coliform die-off	0.5
Settlement rate (per day)	0.5
Entrainment rate (per day)	0.1

available for each reach. One hundred iterations of the Monte Carlo analysis were performed. Each iteration consisted of 500 model runs, for a total of 50,000 simulations. Posterior parameter distributions were identified based on the best performing parameter set from each iteration. Parameter sensitivity was assessed using Kolmogorov–Smirnov d statistic comparing the posterior distribution to a rectangular prior. Parameters related to pathogen growth and die-off rates as well as effluent and animal inputs were evaluated. As Table 4 illustrates, pathogen model performance was sensitive to the light decay proportionality constants, effluent inputs, and livestock inputs in the ‘non-intensive agriculture’ land cover type. This analysis suggests a role for both urban effluent and rural animal faecal waste control strategies in order to reduce river pathogen levels, and suggests that UV disinfection of STWs effluent may prove an effective mitigation measure.

6. Land use change scenario analysis

As part of the River Thames case study, an assessment was undertaken of the likely effects of land use change on TC in the catchment. The future land use scenario was developed by Castellazzi et al. (2010) and represents sub-versions of an IPCC storyline, considering food security as a main driving force for land use change. In this scenario, it is

Table 4
List of most sensitive parameters and associated Kolmogorov–Smirnov d statistic.

	Location (reach or land use type)	Parameter name	d
1	TR19	Light decay proportionality constant	0.62
2	TR21	Effluent concentration	0.54
3	Non-intensive Ag	Light decay proportionality constant	0.44
4	TR02	Light decay proportionality constant	0.43
5	TR02	Effluent concentration	0.38
6	TR21	Light decay proportionality constant	0.37
7	TR18	Light decay proportionality constant	0.37
8	Urban	Animal addition rate	0.36
9	TR01	Light decay proportionality constant	0.31
10	Non-intensive Ag	Animal addition rate	0.29

assumed that world food demand increases, raising grain prices and the UK farmers respond by switching to more intensive arable farming. The land use modelling by Castellazzi et al. (2010) suggests an increase in 'intensive agriculture' (arable) land use from 35.5% to 50%, and a decrease in the amount of 'non-intensive agriculture' (livestock farming) by 14.5%. This change is particularly accentuated in the upper catchment, where intensive agriculture increases by greater than 60%, in contrast to the lower catchment where the change is less than 35%. Such land use change significantly reduces the area for grazing of livestock, and would reduce the sources of diffuse pollution. The dominantly rural sub-catchments of reaches 1, 11, and 12, change prime non-intensive grassland by 20% to intensive agricultural (arable) use. The predominantly urban sub-catchments of the lower reaches 20–22, undergoing a 10% change from grassland to arable use. Within INCA these land use changes can be investigated by altering the land use percentages in the model, re-running the model, and comparing the outputs to the baseline conditions. The land use changes significantly altered the water column coliform concentrations with a mean reduction of 46%, with the greatest reductions in reaches 1 and 11, associated with the higher losses of livestock to arable land use, and reach 19, which had a relatively low sub-catchment area and high livestock density. Reach 12, despite having a 25% reduction in non-intensive agricultural land use, had little impact on TC concentrations because of the low livestock numbers in this sub-catchment. One aspect not considered here is the likelihood that the change to land use could mean that cattle are raised in intensive indoor units thereby effectively becoming a point source of pollution. This could be considered in a future modelling study.

7. Discussion and conclusions

A new model to simulate pathogen transport, dynamics and distribution has been developed and applied to the Thames. As might be expected, there are uncertainties associated with the pathogen modelling structures, equations and parameters. There are also uncertainties associated with pathogen field observations, which have high natural variability and are difficult to measure. There is also limited understanding of the factors that influence pathogen survival and regrowth, particularly in sediment and groundwater and assumptions have to be when considering TC numbers in livestock manure and human effluent. Where possible, input parameters were based on the best available data from published literature, and adjusted when necessary to achieve a calibration with observed data. The sediment settlement rate, entrainment rate, light proportionality constant, and the TC from livestock manure that actually made it to the river system, were all estimated and the latter two parameters were also the most sensitive parameters to change in the model. The application of INCA-Pathogens to the River Thames catchment is a complex task, requiring the consideration of many variables, and is constrained, in many cases, by the lack of quantitative microbiological data for input parameters, and for model calibration and validation. In addition to suffering from "poor" microbial water quality, the River Thames catchment is already classified as under "severe water stress" (Rodda, 2006), which will be further exacerbated by the effects of climate change and population growth. This will inevitably impact on the ability of the river system to provide sufficient high quality water to Thames Catchment and London residents, and irrigation for improving agriculture production. The dominant sources of TC to the River Thames throughout the majority of the year were of agricultural origin, and coincided with rainfall events and runoff from livestock pasture. Future scenarios of land use change have high uncertainties of their own and with a growing population and high demand for space in the UK, land will be devoted to the most economically viable use, and one which will give the highest energy production per unit area. Future land use change, under a global food security scenario, will encourage the conversion of prime land used for tertiary food production (meat), to more economically viable intensive primary production (high yield

crops). Modelling indicates that this land use conversion to arable use will subsequently result in the loss of livestock, and therefore reductions in diffuse pollution from livestock available for runoff to the river system. Further research is required to build confidence and reduce uncertainties in this type of modelling, and such uncertainties should be considered when making policy decisions. Nevertheless, the INCA pathogenic water quality model is an emerging tool that will prove particularly valuable in predicting and managing pathogen loading in an uncertain world of future climate change, and global food and water security.

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