EVALUATION OF THE SOIL AND WATER ASSESSMENT TOOL (SWAT) TO SIMULATE PESTICIDE DYNAMICS IN THE GUAYAS RIVER BASIN (ECUADOR)

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I, NAOMI CAMBIEN, declare that this is the result of my own work and that no previous submission for a degree has been made here or elsewhere. Works by others, which served as sources of information, have been duly acknowledged by references to the authors.

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Abstract
The current agricultural intensification in the Guayas River basin is an important stimulant for Ecuador’s economy but, at the same time, it affects the ecological value of the river system. As the increased use of pesticides poses a particular threat to the freshwater ecosystem, it is urgent to gain more insight into the impact of pesticide practices within the basin. Hydrological watershed models extended for pesticide simulations are potentially appropriate tools to obtain this insight and to provide useful information for river management. In this thesis, the use of the Soil and Water Assessment Tool (SWAT) to simulate pesticide dynamics within the Guayas River basin is evaluated. For this purpose, required data were gathered and SWAT was applied to develop a hydrological model, which was subsequently calibrated and validated for streamflow. This model was then used to run simulations for two pesticides (pendimethalin and fenpropimorph) and to do a system analysis. The hydrological model was evaluated as performing well on a monthly basis. In addition, the pesticide simulations provided useful insights, e.g. the seasonal variation and the influence of slope and pesticide properties. These insights should, however, be confirmed by field measurements. In addition, the identification of the Vinces catchment as a potential risk area can help to prioritise river management. SWAT was evaluated to be a suitable tool to investigate the impact of pesticide use in the Guayas River basin, based on its strengths and limitations as experienced during this study and considering the boundary condition of limited data availability. Recommended for future studies is to focus on the optimisation of the model development and the collection of pesticide application data. Provided that key suggestions for further improvement are considered, the developed model has valuable future applications in view of protecting and restoring the freshwater ecosystems of the basin. This case study demonstrates the potential of SWAT to estimate the impact of agriculture on surface water quality in areas with limited data availability.
Samenvatting

De huidige intensivering van de landbouw in de Guayas River basin is een belangrijke stimulans voor Ecuador ’s economie. Echter, tegelijkertijd tast het de ecologische waarde van het rivierbekken aan. Aangezien het toenemende gebruik van pesticiden in het bijzonder een bedreiging vormt voor het zoetwaterecosysteem, is het verhogen van het inzicht over de impact van het pesticide gebruik in het bekken een dringende noodzaak. Hydrologische stroomgebied modellen uitgebreid voor het simulieren van pesticiden zijn mogelijk geschikt om dit inzicht te verwerven en nuttige informatie voor rivierbeheer te verlenen. Het gebruik van de Soil and Water Assessment Tool (SWAT) om pesticide dynamieken binnen de Guayas River basin te simuleren wordt geëvalueerd in deze thesis. Hiervoor werden de benodigde data verzameld en werd SWAT toegepast om een hydrologisch model te ontwikkelen, dat vervolgens gekalibreerd en gevalideerd werd voor debietsimulaties. Hierna werd dit model gebruikt om simulaties voor twee pesticiden (pendimethalin en fenpropimorfo) te runnen en een systeem analyse uit te voeren. De prestatie van het hydrologische model op maandelijkse basis werd geëvalueerd als goed. Daarenboven verschaften de pesticide simulaties nuttige inzichten, bijvoorbeeld de seizoensgebonden variatie en de invloed van helling en pesticide eigenschappen. Deze inzichten dienen echter bevestigd te worden aan de hand van veldmetingen. Bovendien kan de identificatie van het stroomgebied van de Vinces Rivier als mogelijke risico zone helpen bij het scherpstellen van rivierbeheer. SWAT werd beoordeeld als een geschikte tool om de impact van het pesticide gebruik in de Guayas River basin te onderzoeken, gebaseerd op de krachtpunten en beperkingen ervan als ervaren tijdens deze studie en rekening houdende met de gelimiteerde data beschikbaarheid. Het is toekomstige studies aangeraden te focussen op het optimaliseren van de model ontwikkeling en het verzamelen van pesticide applicatie data. Indien de belangrijkste suggesties voor verdere verbetering worden opgevolgd, biedt het ontwikkelde model waardevolle toekomstige toepassingen gericht op het beschermen en herstellen van het zoetwater ecosysteem van het bekken. Deze casus toont aan dat SWAT potentieel heeft om de invloed van landbouw op de kwaliteit van oppervlaktewater in te schatten, zelfs wanneer de beschikbaarheid van data beperkt is.
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1 Introduction

Water is widely considered as one of the world’s most vital resources. Freshwater of high quality, more specifically, is indispensable in many aspects, by virtue of the numerous ecosystem services\(^1\) it provides. The use of freshwater is fundamental to agriculture, industry, energy generation and drinking water production. In addition, freshwater ecosystem services include biodiversity, water quality, disturbance regulation, commodities, recreational services and aesthetic services.

Unfortunately, the quality of freshwater is threatened by agricultural intensification. This intensification – i.e. making a fixed unit area more productive in response to a growing world population, changing consumption patterns and bioenergy development – often implies the use of irrigation, fertilisers, pesticides and mechanisation. Pesticides, applied because of their toxic effect on target species, are particularly suspects in aquatic ecosystem damage. In developing countries, where legislation is weak and data are scarce, the increasing use of pesticides poses an acute problem. The reasons for, and environmental consequences of, pesticide use are the topics of chapter 2.

To gain insight into the impact of pesticide use on freshwater quality, a suitable tool is required. Hydrological watershed models extended to simulate pesticide dynamics aim to assess the impact of agriculture on water quality. Numerous hydrological model tools exist, with varying input requirements and output detail. The implementation of the hydrological processes and a comparison of four tools will be given in chapter 3. This thesis analyses the use of the Soil and Water Assessment Tool (SWAT) to estimate the impact of agricultural intensification on pesticide dynamics in a context of data scarcity. Advantages, disadvantages and applications of SWAT will be discussed in chapter 4.

As a case study, this research focusses on the Guayas River basin, the most important riverine system in Ecuador. The economic benefits of agricultural intensification in this watershed are in conflict with the environmental consequences. Thus, insight and proper actions are needed to solve or mitigate this conflict. However, in the basin available data are low in quantity and quality and knowledge on the effects of pesticide use is limited. As a first attempt to improve this situation:

1. Data, required for model development and simulation, are gathered. In addition, methods to deal with data limitations are explored.
2. A hydrological model of the basin is developed and calibrated for streamflow. To our best knowledge, this is the first model developed using SWAT at the extent of the Guayas River basin.
3. With this model, simulations for two pesticides and a system analysis are done.
4. Case-specific opportunities and limitations of SWAT are discussed and advise for future model refinement is formulated.

Steps 1 to 3 will be described in chapter 5, whereas steps 1 to 4 are the topics of the discussion (chapter 6). In the final chapter, a conclusion will be formulated.

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\(^1\) i.e. the benefits humans obtain from ecosystems.
2 Pesticides
The use of pesticides, characteristic of agricultural intensification, has both productivity benefits as well as harmful consequences. In this chapter, the benefits of pesticide use will be discussed first. Thereafter, processes leading to the transport of pesticides to receiving waterways will be described. This transport results in the occurrence of pesticides in surface water (section 2.3) and determines the intensity of the harmful effects (section 2.4). The next section will focus on the use of pesticides in developing countries. The last part, finally, will outline mitigation strategies to counteract the consequences of pesticide use for surface water quality.

2.1 Benefits
The widespread use of synthetic pesticides has its origins in the discovery of dichlorodiphenyltrichloroethane (DDT) in 1939, by Nobel prize winner Paul Müller (Pimentel and Peshin, 2014). Since then, the global use of pesticides has increased dramatically, driven by its direct benefits. These are mainly the improvement of crop quality and productivity, associated with increased food supply security and economic income. The world food productivity doubled in the past 40 years, largely due to the control of weeds, insects and other pests (Oerke, 2006; Popp et al., 2013). It is estimated that globally each dollar invested in pesticide control returns about five dollars of economic benefits, that is, if one turns a blind eye to the environmental costs (Pimentel, 2009).

2.2 Transport
A part of the employed amount of pesticides will end up in the environment, depending on land use and management, pesticide characteristics and environmental conditions (soil, meteorology, topography) (Love et al., 2011). Rivers, often located in the proximity of farmlands, are especially vulnerable to unintended pesticide inputs (Schulz, 2004; Schwarzenbach et al., 2006). This occurs either at one specific location, as a point source, or along the water stream, as a diffuse source. Common point sources are accidental spills and improper practices, e.g. during the filling of spraying equipment. They can contribute largely to the occurrence of pesticides in surface water. However, their impact is relatively easy to manage because of their local characteristics (Holvoet, 2006; Tang et al., 2011).

Main input pathways for diffuse sources are depicted in Figure 1 and described in Holvoet (2006). Surface runoff or overland flow is generally considered to be the most important transport route (Bach et al., 2001; Boithias et al., 2011; Huber et al., 1998; Neumann et al., 2002). Below, surface runoff will be referred to as runoff. During runoff events, pesticides are transported both in solution as attached to sediment particles. The detachment and entrainment of particles, also called soil erosion, is caused by the combined effect of rainfall impact and runoff flow. Where the fraction of pesticides transported in the dissolved phase mostly dominates, the transfer via erosion is non-negligible for pesticides with a high adsorption capacity (Holvoet, 2006; Tang et al., 2011). Additionally, rapid pesticide transfer via drains can cause temporary peak concentrations in small streams (Brown et al., 2004; Leu et al., 2004). Once in the river, the pesticides are subject to several processes influencing their bioavailable concentration. A detailed description of these reactions can be found in Holvoet (2006).
2.3 Occurrence in the aquatic compartment

Data on surface water pesticide concentrations are scarce for financial and technical reasons (Guzzella and Pozzoni, 2006; Wang et al., 2016). The extensive literature research of Stehle and Schulz (2015) pinpoint this: for approximately 90% of the highly intensive agricultural areas no insecticide concentration data were found. Data that are available, however, demonstrate the worldwide occurrence of pesticides in surface water. In the study of Stehle and Schulz (2015), for example, 70% of investigated areas located around the world had insecticide concentrations exceeding the regulatory threshold level of the United States (US) and the European Union (EU). During the US Geological Survey’s National Water Quality Assessment Program from 1992 until 2001, moreover, pesticide compounds were detected in streams in urban and agricultural watersheds for over 90% of the time (Gilliom, 2007). It is important to note that pesticide concentrations are typically highly dynamic. Peak concentrations, occurring during major rainfall events and shortly after application, are seldom captured. Therefore, results do often not indicate the maximum exposure of ecosystems to pesticides (Schulz, 2004; Stehle and Schulz, 2015). Next to the water concentration, the fraction adsorbed to the sediment is important as well. Sediments can be an important sink of the contamination, thereby slowing down degradation rates and forming a secondary source (Radović et al., 2016; Summerfelt and Laird, 2001). Finally, groundwater pollution is less common but can persist longer (Love et al., 2011; Vonberg et al., 2014).

2.4 Effects on freshwater ecosystems

The worldwide use of pesticides, which are applied because of their toxic effect on target species, imposes a major stress on freshwater ecosystems (Schäfer et al., 2012). The functioning of these ecosystems relies on a complex and vulnerable network of interdependencies where the direct effect on one population can have major and unpredictable consequences for the whole system (Warren et al., 2003). Reported effects are (sub-)lethal, more specifically the reduction of reproduction, biomass and activity of aquatic organisms, caused by sensory, hormonal, neurological and metabolic system malfunctioning (Bessa da Silva et al., 2016; Scott and Sloman, 2004; Shuman-Goodier and Propper, 2016; Sturve et al., 2016; Sura et al., 2012). The mode of action determines the specificity of pesticides. As many insecticides (e.g. pyrethroids, organophosphates, neonicotinoids) are neurotoxic and the nervous system shows similarities among all animals having one, they are of major concern to aquatic arthropods and vertebrates (Sánchez-Bayo et al., 2011). Herbicides, on the other hand,
target physiological functions specific to plants, e.g. photosynthesis. Nevertheless, direct and indirect effects of herbicides on animals are observed too, e.g. reduced reproduction and implications of reduced food sources and dissolved oxygen concentrations (Hostovsky et al., 2014; Pimentel, 2005). Apart from the toxicity, the degree of effect also depends on the bioavailability, bioaccumulation tendency and persistence of the pesticides (Warren et al., 2003). In addition, the cocktail effect of mixtures, the toxicity of degradation products, the long-term effect of field conditions and the interaction at higher levels of biological organisation are recently receiving more attention in ecotoxicological studies (e.g. in mesocosm studies) (Hasenbein et al., 2016; Ieromina et al., 2016; Kohler and Triebskorn, 2013; Naidu et al., 2016).

2.5 Pesticide use in developing countries

The use of pesticides in developing countries, which has been strongly encouraged in the past because of economic reasons, is especially of concern (Grung et al., 2015). Applied doses are often higher than recommended to guarantee high production levels and because of weak or non-existing legislation (Orozco et al., 2013; Stehle and Schulz, 2015). In addition, extremely and highly hazardous pesticides (World Health Organization classification), e.g. pyrethroids, are frequently used and this use is positively linked with poverty and lower education (Orozco et al., 2013; Wee et al., 2016). Pesticides that are banned since the Stockholm Convention on Persistent Organic Pollutions are still being used illegally (Dores et al., 2016). Data to estimate the effect of this overuse on pesticide pollution are scarce (De Gerónimo et al., 2014; Stehle and Schulz, 2015).

2.6 Mitigation of surface water pesticide pollution

2.6.1 Legislative context

Legislation concerning pesticide use, forming a central part in the protection of water resources, appeared at the beginning of the 20th century (Stehle and Schulz, 2015). Worldwide, a wide variation in restrictive legislation is observed, with in general a stricter regulation in developed countries/nations (Handford et al., 2015). In the EU, to give an example, Directive 91/414/EEC and REACH (Registration, Evaluation, Authorization and Restriction of Chemicals) are important for the registration of pesticides (European Commission (EC), 1991, 2006). The sustainable use of pesticides, in addition, is encouraged by Directive 2009/128/EC (European Commission (EC), 2009). The pesticide concentrations in surface water, finally, are controlled by the European Water Framework Directive (EWFD) (European Commission (EC), 2000). A more detailed overview can be found in Pinto et al. (2016).

In Brazil, a developing country and currently the largest consumer of pesticides, the pesticide legislation framework is law 7802, enacted in 1989 (Albuquerque et al., 2016; Fang, 2016). However, the implementation and enforcement of this law is plagued by several issues, including the prioritisation of economic interests, the lack of financial resources and the possibility to appeal against a non-registration (Pelaez et al., 2013). An overview of implementing decrees and supporting regulations is given by Fang (2016).

2.6.2 Mitigation strategies

Mitigating pesticide pollution and achieving legislative goals can be accomplished at two levels: either via a more sustainable use of pesticides (application related measures) or by minimising the transfer to the aquatic compartment (landscape related measures) (Figure 2). A more sustainable use of pesticides, on the one hand, can be accomplished by reducing the application rate, e.g. via green
cane trash blanketing or precision application (Davis and Pradolin, 2016; Fillols and Callow, 2011). Product substitution, via the elimination or restriction of certain pesticides (e.g. Stockholm convention) and a registration procedure (e.g. REACH), in addition, should guarantee the use of less harmful pesticides. However, new generation pesticides seem not always to reduce environmental risks (Stehle and Schulz, 2015). On the other hand, it is possible to minimise the transfer of pesticides to the aquatic compartment by the implementation of landscape related measures such as vegetated retention ponds which reduce runoff (Bereswill et al., 2014).

Figure 2: Classification of pesticide pollution mitigation strategies (Bereswill et al., 2014).

2.6.3 Tools to assess the effect of pesticide use on surface water quality

Considering the wide variety of pesticides, transport routes and mitigation strategies, the investigation of the link between pesticide use and surface water concentrations is challenging. Necessary insight can be obtained via monitoring and modelling, either to get a rough understanding and/or to support decision making. Because running model simulations is faster and cheaper than water quality monitoring, modelling enables:

1. to extensively analyse the given system, which allows to stipulate e.g. major polluting sources, risk areas, main transfer routes, data gaps
2. to provide water quality parameters (distributed in time and space) in data scarce conditions
3. to compare different scenarios, e.g. a priori best management practices (BMP) comparison.

The development of a mathematical model\(^2\), on the contrary, is not possible without experimental data. Water quality monitoring thus remains obligatory (Holvoet, 2006). In addition, it is important to keep in mind that even the most complex models are simplified representations of the reality, and are, therefore, unable to capture each phenomenon (Nopens, 2014).

\(^2\) Model consisting of a set of mathematical equations (Nopens, 2014).
Modelling the effect of agriculture on pesticide dynamics

This chapter will outline the use of mechanistic watershed models to investigate the effect of agricultural intensification on pesticide dynamics. First, a brief overview of model classification and mechanistic model characteristics will be given. Next, model requirements related to the objectives of this study will be specified. A last part will focus on hydrological models capable of pesticide simulations at the watershed scale by discussing relevant processes and comparing four candidate tools.

3.1 Model classification

There are many different ways to classify the variety of mathematical models (Huber et al., 2004). One way is to differentiate between statistical and mechanistic models. Statistical or data-driven models, on the one hand, use empirically derived relationships between variables to make predictions (Nopens, 2014). A synonym, “black-box models”, refers to the generation of an output based on given inputs, without understanding the physical processes responsible for the generation of this output (Huber et al., 2004). The advantage of using these models is their relative simplicity (Booker and Woods, 2014). However, they are not capable of detailed predictions and they depend on the quality and range of the available observation data (Borah and Bera, 2003; Gamble and Babbar-Sebens, 2012). Moreover, extrapolation to other systems is limited (Devi et al., 2015).

Mechanistic or white-box models, on the other hand, aim to describe which driving processes are present in the system. They are able to make detailed predictions in both time and space and can potentially be extrapolated to other areas and scenarios, provided that the same processes are dominant (Table 1). However, the development of these models is time, data and cost intensive. Moreover, the numerical solutions of the physically based equations are often computationally intensive. Because not every detail of the complex driving processes is understood, many mechanistic models include empirical components. Therefore, most of them are sensu stricto not mechanistic but hybrid or grey-box models. All mechanistic models require some parameterisation and their calibration can be challenging (Booker and Woods, 2014; Borah and Bera, 2003; Devi et al., 2015; Gamble and Babbar-Sebens, 2012; Nopens, 2014; Pandey et al., 2016).

Table 1: Advantages and disadvantages of mechanistic models.

<table>
<thead>
<tr>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Understanding of the system</td>
<td>Data, time and cost intensive development</td>
</tr>
<tr>
<td>Detailed predictions</td>
<td>Computationally intensive</td>
</tr>
<tr>
<td>Extrapolation</td>
<td>Challenging calibration</td>
</tr>
</tbody>
</table>

Other classifications are based on the spatial scale (field scale versus watershed scale models), the temporal scale (single event versus continuous or long-term models) and the spatially explicit character (distributed versus lumped models) (Pandey et al., 2016). In distributed models, the area consists of spatially explicit units with spatially defined model variables and processes. This enables the generation of detailed outputs, distributed in space, but requires a high number of inputs and parameters. In lumped models, on the contrary, the area is represented as one homogeneous unit, modelling an average state. A compromise between both are the semi-distributed models which subdivide the area into several, homogeneous (lumped) regions (Jajarmizadeh et al., 2012).
3.2 Model requirements

The choice between the numerous models is not a straightforward one. Every model has coupled advantages and disadvantages and its suitability depends strongly on the application objectives (required output accuracy, time and spatial scale, state variables of interest and dependencies to be included) (Nopens, 2010). Taking into account the desired degree of detail a trade-off has to be sought between model complexity, on the one hand, and its computational efficiency, on the other hand. Furthermore, the required data are often an important selection criterion. Finally, a decision has to be made between either the development of a new model or the application and eventual adaptation of one or multiple existing models (Huber et al., 2004; Tuo et al., 2015).

With respect to the objectives of this study, a model is required to estimate the effect of agricultural practices on surface water pesticide dynamics at the watershed scale,

- simulating: - the transfer to and routing within river channels
  - on a long-term basis
  - with spatially variable, dynamic outputs

- considering the influence of: - the spatial variability of soil, land use, climate and topography
  - pesticide properties

- given: - the extent of the river basin
  - data scarce conditions
  - the presence of water regulating structure, i.e. hydropower dams.

Based on these requirements, the use of a mechanistic model seems appropriate though the modelling exercise might be hindered by the data availability (quality and quantity). As the hydrology of a watershed has a major impact on the transport and fate of solutes and sediments, the inclusion of the main hydrological processes is essential (Koch et al., 2013; Migliaccio and Srivastava, 2007; Novotny and Olem, 1994). However, this hydrological watershed model should be extended to enable pesticide modelling, which is more complex than hydrological modelling (Holvoet, 2006).

3.3 Hydrological models extended to simulate pesticide dynamics

Various hydrological models exist, differing strongly with respect to their spatial and temporal complexity, data requirements and application range (El-Nasr et al., 2005; Huber et al., 2004). Common to all, however, is the mathematical description of (some of) the main hydrological processes and their interaction with climate, soil and land use (Jajarmizadeh et al., 2012). Climate determines the amount of precipitation a land surface receives and it influences the amount that will evaporotranspirate again. The degree of infiltration into the soil is, among others, dependent on soil characteristics and land use. The amount that does not evaporotranspirate nor infiltrate is available for runoff. The actual hydrological processes that are accounted for differ among the models but the major hydrological components, represented in Figure 3, are implemented in most of the models (Migliaccio and Srivastava, 2007; Tuo et al., 2015). The return flow or baseflow, depicted on this figure, is the fraction of the streamflow that originates from groundwater. The lateral flow is the flow originating from the unsaturated soil zone (Neitsch et al., 2011).

Below, common implementation techniques of processes relevant to pesticide modelling will be discussed. Thereafter, a comparison between four tools used to develop hydrological watershed models extended for pesticide modelling will be given.
3.3.1 Processes relevant to pesticide modelling

3.3.1.1 Evapotranspiration

Evapotranspiration [mm day$^{-1}$] is the combined result of all processes contributing to the formation of atmospheric water vapor at the earth’s surface (evaporation, transpiration and sublimation) (Neitsch et al., 2011). It is a major component of the hydrological cycle, globally 60% of the terrestrial precipitation is evapotranspired again (Oki and Kanae, 2006). Hence, it is essential to simulate this process accurately (Bouraoui and Dillaha, 1996). Because the actual evapotranspiration rate is difficult to determine, the reference evapotranspiration ($ET_0$) was introduced by the Food and Agriculture Organization of the United Nations (FAO) as “the rate of evapotranspiration from an extensive surface of 8 to 15 cm tall green grass cover of uniform height, actively growing, completely shading the ground and not short of water” (Doorenbos, 1977; Jiang et al., 2016). This rate is only dependent on climatic conditions. To account for specific characteristics of the actual crops, the $ET_0$ is multiplied by a crop coefficient (Allen et al., 1998). Subsequently, the actual evapotranspiration rate can be estimated as a function of e.g. soil moisture (Bingner et al., 2015). $ET_0$ is often called the “potential evapotranspiration rate”. However, this name is discouraged by the FAO and is therefore not used here (Allen et al., 1998).

Four common methods that implement the evapotranspiration processes exist. The equations can be found in the appendix (A.1-A.4). The Penman method, first, combines an energy (radiation) term and a ventilation (transport) term, each multiplied by a weighting factor (Penman, 1948; Stigter, 1978). The Penman-Monteith equation, secondly, was developed based on this equation and is probably the one most used (Monteith, 1965; Verhoest et al., 2014). It modifies the Penman equation by adding two resistances in series (r$_c$ and r$_a$, Figure 4). This is done by using the big-leaf concept where the vegetation is represented as one single surface transpiring at one specific height (Fleischer et al., 2015; Shaw et al., 2010). In the FAO version of the Penman-Monteith equation, these resistances are calculated for a hypothetical reference crop with fixed values for crop height, surface resistance and albedo (Allen et al., 1998). This reference crop closely resembles the grass from the FAO $ET_0$ definition (Verhoest et al., 2014).
3.3.1.2 Infiltration and runoff

The amount of rainfall that can infiltrate into the ground is limited by the infiltration capacity of the soil and its moisture status. When precipitation exceeds infiltration on a sloping surface, the remaining part flows overland as (surface) runoff. Runoff contributes largely to pesticide transport (section 2.2). By calculating either infiltration or runoff, the other one is determined too and can be obtained using a simple mass balance (Neitsch et al., 2011).

Implementation methods can be empirical or physically based and estimate either infiltration or runoff (Migliaccio and Srivastava, 2007). A commonly used empirical method to calculate runoff is the soil conservation service curve number (SCS CN) method (Neitsch et al., 2011). As this method will be used in this study, it will be discussed below. Alternatives include the empirical Chezy-Manning equation for runoff and physically based methods for infiltration, e.g. the Green and Ampt method (Green and Ampt, 1911; Johanson et al., 1984).

The SCS CN procedure makes use of equation 3.1 to simulate runoff (USDA, 1972):

\[
Q_{\text{surf}} = \frac{(P-I_a)^2}{(P-I_a+S)} \quad \text{if} \ P > I_a, \text{otherwise} \ Q_{\text{surf}} = 0
\]  

(3.1)

Where \(Q_{\text{surf}}\) the accumulated runoff [mm day\(^{-1}\)], \(P\) the precipitation [mm day\(^{-1}\)], \(I_a\) the initial abstractions (surface storage, interception, infiltration) prior to runoff [mm day\(^{-1}\)] and \(S\) the retention parameter [mm day\(^{-1}\)].

In order to account for the runoff response characteristics of a given system, the CN [-] is introduced. First, three main CNs are determined, corresponding to three antecedent soil moisture classes. These numbers are a function of land use, management, soil and slope. In a second step, the retention parameter is calculated as a function of the soil water content and CN\(_1\) and CN\(_3\), such that \(S\) varies smoothly from the maximum value at the wilting point via the average value associated with CN\(_2\), to a minimum value at field capacity (Bingner et al., 2015; Cronshay, 1986; Neitsch et al., 2011; Verhoest et al., 2014).
Advantages of this method are its computational efficiency, the use of readily available input data and the inclusion of the effect of soil type, land use and management. However, it does not account for rainfall intensity (Williams et al., 2008b).

### 3.3.1.3 Streamflow routing

When (surface) runoff reaches a channel, it continues its movement through the channel network towards the outlet of the basin. The time this takes is estimated by a mathematical procedure called streamflow routing. This makes it possible to correct for the time lag between the generation of the runoff and its exit out of the watershed (Loosvelt, 2013). In order to do so, the discharge \([\text{m}^3 \text{s}^{-1}]\) is estimated. Routing methods can be divided into two main categories, being hydrologic (lumped) and hydraulic (distributed) routing. While the discharge in hydraulic routing techniques is calculated as a function of both time and space, hydrologic techniques calculate the discharge as a function of time only, for one specific location (Verhoest et al., 2014).

Hydraulic routing methods, on the one hand, are mostly based on the solution of the de Saint-Venant equations (St. Venant) (Barre de Saint-Venant, 1871). These two equations for unsteady, one-dimensional open channel flow express the conservation of mass and momentum. Since the dynamic wave approach, which includes all terms of partial differential equations, is complex and computationally intensive, the diffusive and kinematic wave model were proposed by Chow et al. (1988) to simplify the momentum equation. The equations may be solved numerically by using finite-difference approximations (DHI, 2009).

Hydrologic routing models, on the other hand, are only based on the continuity equation (conservation of mass) (Fread, 1976). In its simplest form, this equation can be written as:

\[
\frac{dWS(t)}{dt} = I(t) - Q(t)
\] (3.2)

Where \(WS(t)\) the water storage in the channel \([\text{m}^3]\), \(t\) the time \([\text{s}]\), \(I(t)\) the flow rate at the inlet of the channel \([\text{m}^3 \text{s}^{-1}]\) and \(Q(t)\) the flow rate at the outlet of the channel \([\text{m}^3 \text{s}^{-1}]\).

As both \(Q(t)\) and \(S(t)\) are unknown, an additional relationship between the variables is needed. This can be a linear relationship between \(S(t)\) and \(Q(t)\), which is the case with the linear reservoir model (Nash and Farrel, 1955). In this conceptual model, the channel network is represented as a succession of reservoirs through which the water is routed (Figure 5-a). In the Muskingum model, alternatively, \(S(t)\) is a linear function of \(I(t)\) and \(Q(t)\). In this model, the storage volume is represented as the combination of a prism, with constant cross section, and a wedge, which is positive or negative depending on the difference between inflow and outflow rate (Figure 5-b) (Neitsch et al., 2011).
3.3.1.4 Sediment yield and routing

Because pesticides are transported both in the dissolved phase and adsorbed to the sediment (section 2.2), pesticide simulations require the implementation of sediment yield and routing. Physically based models that simulate soil erosion and sediment yield are mostly based on concepts of the Universal Soil Loss Equation (USLE). Nonetheless, these models are empirical (Pandey et al., 2016). USLE expresses the daily sediment yield as a function of rainfall energy taking into account the influence of soil properties, topography, land use and management (Wischmeier and Smith, 1965; Wischmeier et al., 1978). MUSLE, the Modified Universal Soil Loss Equation, on the contrary, is based on the runoff amount to calculate the sediment yield (Williams, 1975). Description of both equations can be found in Neitsch et al. (2011).

Once the amount of sediment yield is calculated, the sediment is routed through the channel network. Major processes of influence are sedimentation and channel erosion, with relative importance depending on stream power, sediment particle size, bed geometry etc. (Neitsch et al., 2011). Channel erosion, however, is not considered in every model (Pandey et al., 2016). Again, different implementation techniques exist as is outlined by Pandey et al. (2016).

3.3.1.5 Pesticide-specific processes

The implementation of water and sediment processes forms an essential backbone to water quality modelling. However, in order to simulate transport and fate of pesticides, models should be extended with pesticide-specific processes (Holvoet, 2006). First of all, the amount available for pesticide loss needs to be determined, considering the influence of e.g. application technique, rate and timing and pesticide properties. In addition, pesticide transfer processes have to be implemented, with runoff as the main transport route (section 2.2). Next, pesticide-specific routing methods are required. These are mostly implemented conceptually, using simple mass balances and considering the water and sediment layer as cascades of well mixed, separate but linked reactors (continuous stirred tank reactors) (Bingner et al., 2015; Borah and Bera, 2003; Neitsch et al., 2011).

For each of these processes, it is crucial to consider the partitioning of pesticides between dissolved and adsorbed phase. This will influence the degradation rate, transfer pathways, routing characteristics etc. However, many models are not able to simulate this accurately and sometimes the adsorbed fraction is even ignored (Luo and Zhang, 2011; Tang et al., 2011). Implementation of partitioning can be done by using a (non-)linear, pesticide-specific adsorption isotherm and assuming an instantaneous equilibrium (Laroche et al., 1996; Neitsch et al., 2011). Accordingly, the fraction in each phase is calculated based on the suspend solid concentration.
3.3.2 Comparison of four candidate tools

There is a wide variety of models simulating surface water pesticide concentrations, ranging from simple screening tools to complex watershed models (Holvoet, 2006). The extensive reviews of Quilbé et al. (2006) and Mottes et al. (2014) illustrate this. However, the number of models that agrees with the requirements of this study (section 3.2) is limited. Four candidate tools were found, all being used to develop long-term, hydrological watershed models extended for pesticide modelling. They are compared in Table 2 and discussed in this section. It is important to keep in mind that these tools are not static. Due to continued developments, shortcomings can be solved and tools can be improved.

Table 2: Comparison between four tools to develop hydrological watershed models extended for pesticide modelling.

<table>
<thead>
<tr>
<th>Model</th>
<th>AnnAGNPS</th>
<th>HSPF</th>
<th>MIKE SHE</th>
<th>SWAT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spatial representation</td>
<td>Distributed</td>
<td>Lumped</td>
<td>Distributed</td>
<td>Semi-distributed</td>
</tr>
<tr>
<td>Evapotranspiration method</td>
<td>Penman</td>
<td>Input</td>
<td>Input</td>
<td>Penman-Monteith/</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Priestly-Taylor/</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Hargreaves</td>
</tr>
<tr>
<td>Runoff method</td>
<td>Curve number</td>
<td>Chezy-Manning</td>
<td>Manning equation/</td>
<td>Curve number/</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>St. Venant equations</td>
<td>Green and Ampt</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(diffusive wave)</td>
<td></td>
</tr>
<tr>
<td>Routing method</td>
<td>Manning equation</td>
<td>St. Venant equations</td>
<td>MIKE 11 submodel (a):</td>
<td>Manning equation +</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>St. Venant equations</td>
<td>variable</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(dynamic/ diffusive/</td>
<td>storage routing</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>kinematic wave)</td>
<td>method/</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>MIKE 11 submodel (b):</td>
</tr>
<tr>
<td>Erosion method</td>
<td>Revised USLE (b)</td>
<td>Power relation with</td>
<td>EUROSEM module (c)</td>
<td>Muskingum method</td>
</tr>
<tr>
<td></td>
<td></td>
<td>water storage and flow</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pesticide component</td>
<td>Modified version of GLEAMS (e)</td>
<td>PRZM (f) or GLEAMS</td>
<td>DAISY (g)</td>
<td>GLEAMS and EPIC (h)</td>
</tr>
<tr>
<td>Reservoir management</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Basic</td>
</tr>
<tr>
<td>BMP (b) evaluation</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>GIS interface</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Open source</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Advantages</td>
<td>Source accounting</td>
<td>Simple or complex setup</td>
<td>Long term and single event simulations</td>
<td>User-friendly</td>
</tr>
<tr>
<td></td>
<td>Combined upland and channel processes</td>
<td>Flexible time scale</td>
<td>Detailed predictions</td>
<td>Continue developments</td>
</tr>
<tr>
<td></td>
<td>Unlimited number of pesticides</td>
<td>Combined upland and channel processes</td>
<td>Interaction between units</td>
<td>Wide range of applications</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Unlimited number of pesticides</td>
<td>Simple or complex setup</td>
<td>Computationally efficient</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Flexible time scale</td>
<td>Suitable for large, complex watersheds</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Easy to link with other MIKE models</td>
<td>Combined upland and channel processes</td>
</tr>
<tr>
<td>Disadvantages</td>
<td>Subunits not linked</td>
<td>Lumped</td>
<td>Data intensive</td>
<td>Numerical instabilities</td>
</tr>
<tr>
<td></td>
<td>Documentation rather limited Watershed limited to 3,000 km²</td>
<td>Extensive calibration</td>
<td>Computationally intensive</td>
<td>Few pesticide applications</td>
</tr>
<tr>
<td></td>
<td>No spatially variable rain</td>
<td>No single event predictions</td>
<td>Numerical instabilities</td>
<td></td>
</tr>
<tr>
<td></td>
<td>No transfer of pollutants to the next day</td>
<td>No groundwater flow simulation</td>
<td>Few pesticide applications</td>
<td></td>
</tr>
<tr>
<td>Reference</td>
<td>Parsons et al., 2004</td>
<td>Johanson et al., 1984</td>
<td>Abbott et al., 1986 a&amp;b</td>
<td>Arnold et al., 1998</td>
</tr>
</tbody>
</table>

References

a: A one-dimensional river model (DHI, 2009)
b: The Universal Soil Loss Equation (section 3.3.1.4)
c: European Soil Erosion Model (Morgan 1993)
d: The Modified Universal Soil Loss Equation (section 3.3.1.4)
e: Groundwater Loading Effects on Agricultural Management Systems (Leonard et al., 1987)
f: Pesticide Root Zone Model (Carsel et al., 1985)
g: A soil-plant-atmosphere model (Hansen 1990)
h: Erosion-Productivity Impact Calculator (Williams 1995)
i: Best Management Practices
The Annualized Agricultural NonPoint Source model or AnnAGNPS, to begin with, was developed based on the single event Agricultural NonPoint Source model (AGNPS) (Young et al., 1987). This was done with the philosophy of maintaining AGNPS’ simplicity while adapting it to continuous long-term simulations. The study area is represented by homogeneous drainage areas or cells. Because of this distributed representation, the study area is said to be limited to 3,000 km² (Bingner et al., 2015). However, Huang and Hong (2010) successfully applied AnnAGNPS for a study area of 14,000 km². A useful feature of AnnAGNPS is the ability to identify the contribution of land or reach components to the output loadings (source accounting) (Bingner et al., 2015). A limitation of these models, however, is the routing of the loads to the watershed outlet before the next day simulation starts, without consideration of the time this may take. This implies that also the fraction of pesticides attached to deposited sediments in the reaches is neglected when moving to the next day (Bingner et al., 2015). AnnAGNPS has a reservoir compound but no management options are available (Table 2).

The Hydrologic Simulation Program FORTRAN, or HSPF (Johanson et al., 1984), secondly, is a modification of the Stanford Watershed model (SWM) (Crawford and Linsley, 1966), probably the first physically based model capable of simulating the entire hydrological cycle at the watershed scale (Pandey et al., 2016). In HSPF, the watershed is subdivided into land segments, based on land use. These non-spatially explicit segments have uniform characteristics and are either pervious or impervious (Borah and Bera, 2003; Jeon et al., 2007; Tuo et al., 2015). Advantages of this tool can be found in Table 2. Limitations are the lumped structure, impeding, for example, the identification of important pesticide sources (Huber et al., 2004). In addition, the tool requires an extensive calibration and is not user-friendly. To end, reservoirs are treated the same as channel reaches and no reservoir management options are available (Borah et al., 2006; Singh et al., 2005).

The European Hydrological System or MIKE SHE, thirdly, uses a distributed structure by dividing the watersheds into rectangular or square grids, each consisting of several horizontal layers (El-Nasr et al., 2005). This structure, combined with detailed process descriptions and multi-dimensional flow equations, makes the developed model computationally and data intensive. Therefore, the tool is more suitable for detailed studies of small watersheds (Borah and Bera, 2003). However, the tool is said to be also applicable at large spatial scales (DHI, 2012). Andersen et al. (2001), for example, applied MIKE SHE to a study area of 375,000 km². An advantage is the simulation of the interaction between spatial units. This is done by routing the output of one unit to the next one downstream, where it is subjected to the processes of that unit, instead of routing it immediately into a reach segment, as is the case with AnnAGNPS and SWAT (Mottes et al., 2014). Another advantage is the broad range of agricultural practices and water control structures that can be simulated (Golmohammadi et al., 2014). Also, flexible reservoir management implementations are possible, by means of user-defined functions in the MIKE 11 module (DHI, 2009). Disadvantages are summarised in Table 2.

The Soil and Water Assessment Tool (SWAT), finally, will be discussed in more detail in the next chapter, as it is used in this study. This choice of using SWAT is justified by its advantages, presented in Table 2 and detailed below, and its agreement with the objectives of this study (section 3.2). A derivative of SWAT, the Soil and Water Integrated Model (SWIM) which has an improvement reservoir module, is not suitable because this tool has no pesticide module and is developed for mesoscale watersheds (Krysanova et al., 1998, 2000).
4 SWAT

4.1 Model description

The Soil and Water Assessment Tool or SWAT is developed in the United States (US) to assess the long-term impact of land use and management on water quantity and quality in large, complex watersheds (Arnold et al., 1998). The history of this development is described by Williams et al. (2008a). The spatial representation of the model consists of spatially explicit subbasins, further subdivided into lumped, non-interacting Hydrologic Response Units (HRUs). Subbasins are created based on the topography such that they represent areas that drain into the same stream segment, i.e. the outlet of the subbasin. The HRUs represent unique combinations of land use, soil and slope within a subbasin. As such, similar fields scattered around a subbasin are lumped together into one homogeneous, non-spatially explicit HRU. The area of an HRU corresponds to the relative importance of the land use, soil and slope combination within the subbasin. The stream network is represented by at least one main channel and one tributary channel per subbasin. In addition, pond, wetlands, depressions and reservoirs may be defined.

Simulations in SWAT consist of two main parts: a land phase and a routing phase. The core behind the land phase simulations is the following water balance, calculated on a daily basis for each HRU:

\[ SW_t = SW_0 + \sum_{i=1}^{t} (P - Q_{surf} - E_a - w_{seep} - Q_{gw}) \]  

Where \( SW_t \) the final soil water content [mm], \( SW_0 \) the initial soil water content on day \( i \) [mm], \( t \) the time [days], \( P \) the precipitation on day \( i \) [mm], \( Q_{surf} \) the amount of runoff on day \( i \) [mm], \( E_a \) the amount of evapotranspiration on day \( i \) [mm], \( w_{seep} \) the total amount of water exiting the bottom of the soil profile on day \( i \) [mm] and \( Q_{gw} \) the amount of baseflow on day \( i \) [mm]. Values are normalised by the area of the HRUs.

A schematic representation of these land phase processes was given earlier (Figure 3). In addition to the processes related to the water balance, the land phase includes specific processes, adapted to the research question. During this phase, the daily loadings of water, nutrients, sediment, pesticides etc. are calculated for each subbasin (as the weighted sums of the loadings from each HRU). In the second phase, which is the routing phase, these loadings are routed via the main channel network to the outlet of the basin. Meanwhile, the principle of mass conservation is applied, taking several sinks and sources into account (e.g. evaporation of water, sedimentation of particles, degradation of pesticides) (Neitsch et al., 2011). An overview of implemented processes related to the water movement during both phases in SWAT is given in Figure 6.

The implementation technique of important processes is indicated in Table 2 and discussed in section 3.3.1. With respect to the pesticide simulations, first, the amount available for transport is calculated considering a certain application efficiency (fraction that reaches the crops), the wash-off from the pesticides on the crops to the soil (only when precipitation exceeds a certain threshold) and degradation processes. Subsequently, pesticides are transported to the channels via runoff and lateral flow (Figures 3 and 6). Pesticide transport via the groundwater is not implemented. During the routing phase, lastly, solid-liquid partitioning, settling and degradation processes are simulated. Extensive theoretical documentation is provided by Neitsch et al. (2011). Practical aspects related to the use of SWAT (input requirements, ArcGIS interface, model setup) will be clarified in chapter 5.
4.2 Advantages and disadvantages

First of all, SWAT is an open source tool and detailed online documentation, user groups, video tutorials, international conferences and a unique literature database (more than 2700 papers) are available. This all makes the tool user-friendly, which can explain, at least partly, the fact that it is one of the best known and most widely used tools to develop water quality models at the watershed scale (Gassmann et al., 2010; Refsgaard et al., 2010; Varga et al., 2016).

Secondly, the tool is continuously improved, supported by the core developmental team and as a response to shortcomings demonstrated by the many users (Arnold et al., 2012a; Bieger et al., 2016). This results in the development of new tools, e.g. GIS interface tools, pre- and post-processing tools and statistical evaluation tools (Gassmann et al., 2010). In addition, a trend to interface SWAT with other environmental or economic models enlarges its application range (Gassman et al., 2007). Moreover, a complete revision of SWAT will be available soon, solving certain limitations of the tool and enhancing its capabilities. Innovations of this revision are the new approach for watershed discretization and a modification of the input files (Bieger et al., 2016).

A third advantage is its comprehensive code. SWAT is proven to be an effective and flexible tool for a wide range of applications, watershed scales and environmental conditions (Gassman et al., 2014; Krysanova and White, 2015; Tuppad et al., 2011). Moreover, the semi-distributed structure makes the model computationally efficient and enables to generate spatially explicit outputs. Finally, the tool is suitable for large, complex watersheds (Gassman et al., 2014).
However, every tool has its shortcomings and these are often linked with its advantages. The constant improvements, for example, have led to a difficult code and a high number of parameters, requiring expertise to run the model and complicating the calibration process (Arnold et al., 2012a; Vigerstol and Aukema, 2011). Additionally, the tool is highly data intensive. Although SWAT is said to run on readily available input data this is not always the case, especially in developing countries. Certainly the data accuracy and precision might be an issue, as expressed by the rule “garbage in is garbage out” (Estrada et al., 2009; Gassman et al., 2007; Querner and Zanen, 2013).

Another limitation is the use of non-interacting HRUs. Because the HRUs are not linked to each other, routing processes of flows and pollutants and pollutant attenuation within the subwatershed are lacking (Arnold et al., 2010; Krysanova and Arnold, 2008). Moreover, the semi-distributed structure impedes to generate spatially explicit outputs at the HRU level (Bieger et al., 2016).

Furthermore, SWAT is said to be a physically based model but also empirical equations like the curve number method are implemented (Bauwe et al., 2016). The curve number method has been applied successfully and enables the adaptation to the study-specific conditions during calibration (Arnold et al., 2012a). On the other hand, this controversial method is not developed for the application at individual HRUs, does not account for all runoff generating processes and causes poor results in some cases (Bieger et al., 2016; Gassman et al., 2007).

Lastly, there are some limitations with respect to the simulation of pesticide dynamics. First of all, pesticide input into the rivers via point sources, drift and groundwater upflow is not taken into account. Especially with respect to point sources this is an important disadvantage, as they can contribute largely to the occurrence of pesticides in surface water (section 2.2). To tackle this issue, Holvoet (2006) and Gevaert et al. (2008) extended the SWAT code to implement point sources and droplet drift. This modification, however, has not been incorporated into the standard SWAT versions (Fohrer et al., 2014). In addition, Fohrer et al. (2014) reports flow partitioning problems and the need to decouple pesticide transport from tile drainage and lateral flow. The last limitation is the fact that SWAT can only route one pesticide at a time (Neitsch et al., 2011).

### 4.3 Applications related to pesticide modelling

As a consequence of SWAT’s advantages and widespread use, the number of SWAT studies is extensive. Overviews are given by Gassmann et al. (2010) and Krysanova and White (2015). Recent studies related to pesticide simulations, more specifically, are summarised in Table 3 and discussed below. This is to illustrate the diversity of SWAT’s applications and to discuss some challenges as well as how the studies handle these.

<table>
<thead>
<tr>
<th>Location</th>
<th>Area [km²]</th>
<th>Analyzed pesticides</th>
<th>Application</th>
<th>Pesticide calibration</th>
<th>$R^2$ of pesticide outlet concentrations for the calibration period</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Germany</td>
<td>50</td>
<td>flufenacet (H), metazachlor (H)</td>
<td>fate and transport</td>
<td>yes (D)</td>
<td>flufenacet: 0.51 (D); metazachlor: 0.62 (D)</td>
<td>Fohrer et al., 2014</td>
</tr>
<tr>
<td>Thailand</td>
<td>77</td>
<td>atrazine (H), chlorothalonil (F), endosulfan (I)</td>
<td>fate and transport</td>
<td>yes (D)</td>
<td>-</td>
<td>Bannewarth et al., 2014</td>
</tr>
<tr>
<td>Thailand</td>
<td>77</td>
<td>chlorothalonil (F), cypermethrin (I)</td>
<td>fate and transport</td>
<td>yes (D)</td>
<td>-</td>
<td>Bannewarth et al., 2016</td>
</tr>
<tr>
<td>France</td>
<td>1,110</td>
<td>metolachlor (H), trifluralin (H)</td>
<td>fate and transport</td>
<td>yes (D)</td>
<td>metolachlor: 0.26 (D), 0.45 (M); trifluralin: 0.02 (D), 0.16 (M)</td>
<td>Bothias et al., 2011</td>
</tr>
<tr>
<td>USA</td>
<td>23,300</td>
<td>chlorpyrifos (I), diazinon (I)</td>
<td>fate and transport</td>
<td>yes (M)</td>
<td>chlorpyrifos: 0.67 (M); diazinon: 0.81 (M)</td>
<td>Ficklin et al., 2013</td>
</tr>
<tr>
<td>USA</td>
<td>?</td>
<td>chlorpyrifos (I), diazinon (I)</td>
<td>BMP (a) comparison</td>
<td>yes (M and Y)</td>
<td>chlorpyrifos: 0.87 (M), 0.96 (Y); diazinon: 0.995 (M), 0.90 (Y)</td>
<td>Zhang and Zhang, 2011</td>
</tr>
<tr>
<td>France</td>
<td>1,230</td>
<td>4 new ‘average active ingredients’</td>
<td>BMP (a) comparison</td>
<td>yes (Y)</td>
<td>-</td>
<td>Lescot et al., 2013</td>
</tr>
<tr>
<td>USA</td>
<td>sum: 53,358</td>
<td>8 herbicides</td>
<td>land use change</td>
<td>no</td>
<td>-</td>
<td>Love et al., 2011</td>
</tr>
<tr>
<td>USA</td>
<td>248</td>
<td>atrazine (H)</td>
<td>climate change</td>
<td>no</td>
<td>0.75 (M)</td>
<td>Ahmadi et al., 2014</td>
</tr>
</tbody>
</table>


a: Best Management Practices
As can be seen in Table 3, a first main application of SWAT is the simulation of pesticide transport and fate. As already mentioned, this can result in valuable information to supplement expensive monitoring data. The capability of SWAT in this respect was positively evaluated by Bannwarth et al. (2014, 2016) and Fohrer et al. (2014). In the study of Bothias et al. (2011), moreover, SWAT was described as a promising tool to provide insights into pesticide dynamics and support water quality management. Pesticide simulations and the partition between the soluble and adsorbed fraction roughly matched the observations for both the calibration and validation period. However, daily and monthly $R^2$ values were rather poor (Table 3). The study of Ficklin et al. (2013) proves that SWAT is also capable of simulating pesticide dynamics at the large watershed scale. The calibration in this study was executed for multiple stations throughout the basin, instead of a calibration at the outlet only. It was shown that, in large watersheds, this improves the reliability of a model to a big extent. A strong agreement between measurements and simulations was obtained, possibly due to the availability of obligatory and detailed pesticide application reports in California.

Once a model’s capability of simulating pesticide dynamics is evaluated successfully, it can be used for scenario analysis. Zhang and Zhang (2011), for example, compared the effectiveness of different best management practices (BMPs) to quantitatively mitigate insecticide pollution. SWAT was used for this research question, being one of the few tools that met the requirements to do so. Although previous studies proved the capability of SWAT to compare BMPs, this study was one of the first to investigate the influence of BMPs on pesticide reduction. Results were assessed as satisfying to support decision making (Table 3). Note that detailed information on application practices was available. Another SWAT based comparison of BMPs to reduce pesticide load was performed by Lescot et al. (2013).

The effects of land use change on pesticide dynamics is another interesting application of SWAT, as described in Love et al. (2011) with a focus on large-scale bioenergy crops. Herbicide concentrations were simulated for 14 different scenarios of bioenergy crop rotations in four large watersheds. Results indicate the increased surface water herbicide concentration over the base scenario and the large differences between the different bioenergy crops. Lastly, SWAT can be used to estimate the influence of climate change on pesticide concentrations. This is done by Ahmadi et al. (2014) for atrazine dynamics over the 21st century.

A challenge that was encountered by multiple of these studies is to obtain reliable data on pesticide practices. Fohrer et al. (2014) stress, on the one hand, the importance of having detailed data on application timing. This is because simulated pesticide concentrations are strongly influenced by the length of the period between application date and the first succeeding rainfall event. On the other hand, they underline the difficulty to obtain these data. To cope with this, the authors recommend to vary the application date throughout the basin. As such, the influence of rainfall patterns is smoothed out and simulations are improved (Winchell et al., 2005). Another method to handle the uncertainty associated with application rate and timing is to consider it as a parameter for calibration, as was done by Bannwarth et al. (2014, 2016). Resulting parameters were applied uniformly throughout the basin. Despite the lack of information on application practices and the short calibration period, simulated daily outlet concentrations matched the observations reasonably well. However, without better application data, the use of the model was said to be restricted to yearly predictions, which can already be useful for management applications according to the authors.
A second challenge for some of the studies was the lack of pesticide concentration data. In the study of Lescot et al. (2013), for example, pesticide concentration data were insufficient to perform monthly calibration and validation. However, the model was still evaluated by sorting both the measurements and simulations to increasing yearly concentration at 15 points. Although differences between monitored and simulated concentrations were observed, these rankings matched well, which proofs the effectiveness of the model to pinpoint risk areas. In the study of Love et al. (2011) concentration data was also insufficient to perform a pesticide calibration. However, flow, runoff and sediment were calibrated successfully and the model was assumed to be accurate enough to support decision making.

In summary, it is clear that SWAT is a popular and useful tool for pesticide simulations at the watershed scale. At this moment, however, these applications are almost completely concentrated in developed countries. Even though SWAT is extensively applied in developing countries, these applications are limited to hydrologic, nutrient or sediment simulations (Bonumá et al., 2015; Dile et al., 2016; Pinto et al., 2013; Strauch et al., 2016). Only three pesticide applications in developing countries were found, simulating pesticide fate in two small watersheds (Bannwarth et al., 2014, 2016; Matamoros, 2004). The reason for this is possibly the lack of reliable data on pesticide practices, which is even in developed countries an issue as is discussed above. In addition, the monitoring of pesticide concentrations, in a spatially and temporally distributed way, is expensive and consequently rare in developing countries. No SWAT studies simulation pesticide dynamics in data scarce conditions at the large watershed scale were found.
5  Case study: application of SWAT for the Guayas River basin

To gain more insight into the potential of the Soil and Water Assessment Tool (SWAT) to simulate pesticide dynamics under data limiting circumstances, SWAT was applied for the Guayas River basin. This application will be described in this chapter. First, general information on the study area will be given. Thereafter, an overview of the available data and the pre-processing of the data will be outlined. Next, the development of the model for the study area will be described. Finally, the hydrological model calibration and evaluation and the pesticide simulations will be discussed.

5.1  Study area

5.1.1  General

The Guayas River basin is the most important watershed in Ecuador, having a drainage area of approximately 34,000 km² and a population of 4.8 million inhabitants (Arias-Hidalgo et al., 2013; Arriaga, 1989; Castro and Andres, 2009). The basin is located in the central, western part of the country (Figure 7-a). The western part of the basin is situated in the coastal area but the eastern part belongs to the Andean region. This implies a wide variation in elevation, going from zero to more than 6000 m above sea level (a.s.l.) (Figure 7-b) (Arias-Hidalgo et al., 2013). However, a large part of the basin has an elevation below 100 m a.s.l. The two main tributaries of the basin are the Daule and Babahoyo River, forming the Guayas River at their confluence. The Guayas is 60 km long, flows through the city Guayaquil and mouths into the Gulf of Guayaquil. In the northern part of the basin a dam is constructed on the Daule River (Figure 7-b, point 1). This dam, named Daule Peripa, is built for hydropower generation, irrigation, drinking water and river control (Arriaga, 1989).

Figure 7: Location of the Guayas River basin in Ecuador (a.). Digital elevation map and river network of the basin (b.). Numbers indicate the Daule Peripa Dam (1), the main rivers, being Daule (2), Vinces (3), Babahoyo (4), Chimbo (5) and Guayas (6), and the Abras de Mantequilla wetland (white circle) (7).
The basin is characterised by a humid tropical climate with a rainy season from December to May (Frappart et al., 2015). During these months, the average total monthly precipitation amounts to 314 mm. Dry season average total monthly precipitation, on the contrary, is limited to 43 mm (calculated based on data from SENAGUA\(^3\)). The precipitation is influenced by orographic effects\(^4\) and increases from west to east. In addition, the El Niño Southern Oscillation causes fluctuations of the yearly rainfall patterns (Borbó-Cordova et al., 2006). During an El Niño event, the discharge of the largest tributary of the Guayas River, being the Daule River, can reach up to 2000 m\(^3\) s\(^{-1}\). Average dry season streamflow of the Daule River, on the contrary, is 178 m\(^3\) s\(^{-1}\) (calculated based on data from INAMHI\(^5\)). The average discharge at the outlet of the basin is 974 m\(^3\) s\(^{-1}\) (Damanik-Ambarita et al., 2016).

Being the most productive agricultural region in Ecuador, the watershed is indispensable for the country’s economy (Frappart et al., 2015). All of the five most produced crops in Ecuador (sugar cane, banana, palm oil, rice and corn) are cultivated on the basin’s many arable lands and plantations (Figure 8). About 70 % of the national crop production arises here. Besides, the region is important for aquaculture and hydropower generation (Arias-Hidalgo et al., 2013; Seo et al., 2010).

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\(^3\) Secretaría Nacional del AGUA (national ministry of water) (http://www.senagua.gov.ec/).

\(^4\) Orographic precipitation is precipitation resulting from moist air flowing over orographic barriers, e.g. mountains (Houze, 2012).

\(^5\) The national meteorological and hydrological institute (http://www.serviciometeorologico.gob.ec/).
5.1.2 Pressures

The intensive human activities (agriculture, fishery, hydropower, industry) within the basin imposes pressures on the aquatic ecosystem. As these activities are promoted by the Ecuadorian government, moreover, the pressures are expected to increase unless measures are taken to stimulate economic growth in a sustainable manner (SENPLADES, 2013; WWAP (UN), 2014). Agricultural intensification, more specifically, results in a high usage of agrochemicals, including pesticides (Borbor-Cordova et al., 2006; Damanik-Ambarita et al., 2016). As discussed in section 2.4, this use has detrimental effects on the aquatic ecosystems and is therefore of concern. For example, the increasing use of extremely and highly toxic pesticides in the basin was reported as being a significant pressure for the ecosystem of the Abras de Mantequilla wetland, which is located in the central part of the basin (white circle on Figure 7-b) (Arias-Hidalgo, 2012). Nonetheless, information on the specific amounts applied in the basin is difficult to obtain (section 5.2.4.2) and only a few studies about the effects of the pesticide use within the basin were found.

5.2 Available data

In this section, the data required to develop and run the hydrological model extended for pesticide modelling will be discussed. Since the quantity of the data is relatively scarce and the accuracy and precision might be assessed as low, special attention will be given to these potential limitations.

5.2.1 Data required to develop the hydrological model

Table 4 presents an overview of the data that were gathered to develop the model. When multiple options were available, a choice (marked in grey) was made based on the year, the resolution and eventual reasons for exclusion (Table 4).

Table 4: Overview of data gathered to setup the hydrological model extended for pollutant fate modelling. Choice is indicated in grey.

<table>
<thead>
<tr>
<th>Type</th>
<th>Format</th>
<th>Resolution/scale</th>
<th>Year</th>
<th>Source</th>
<th>Reasons for exclusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-Digital Elevation Model</td>
<td>IMG</td>
<td>30 m (resampled from 90 m)</td>
<td>2000</td>
<td>SRTM (a)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>TIFF</td>
<td>12.5 m</td>
<td>2006-2011</td>
<td>ALOS PALSAR (b)</td>
<td>Elevation at the outlet contradicts field inspection</td>
</tr>
<tr>
<td>2-Land use</td>
<td>TIFF</td>
<td>9 km</td>
<td>1998-2008</td>
<td>FAO (c)</td>
<td>Outdated</td>
</tr>
<tr>
<td></td>
<td>Shape file</td>
<td>1:250,000</td>
<td>2000</td>
<td>PIGSA program (d)</td>
<td>Multiple landuse types combined in one class</td>
</tr>
<tr>
<td></td>
<td>Shape file</td>
<td>1:100,000</td>
<td>2014</td>
<td>Geoservicios Ecuador, MAGAP (e)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Shape file</td>
<td></td>
<td></td>
<td>IGM (f)</td>
<td>Mismatch spatial scale of data and model</td>
</tr>
<tr>
<td>3-Soil</td>
<td>TIFF</td>
<td>1:5,000,000</td>
<td>1974</td>
<td>FAO (g)</td>
<td>Multiple landuse types combined in one class</td>
</tr>
<tr>
<td></td>
<td>ESRI GRID</td>
<td>1:5,000,000</td>
<td>Update of map from 1971-1981</td>
<td>HWSD (h)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Shape file</td>
<td>1:250,000</td>
<td>2002</td>
<td>PIGSA program (d)</td>
<td>Insufficient availability of soil parameters</td>
</tr>
<tr>
<td>4-River network</td>
<td>Shape file</td>
<td>2002</td>
<td>PIGSA program (d)</td>
<td>Too detailed for intended use (burn in, see section 5.4.1)</td>
<td></td>
</tr>
<tr>
<td>5-River basin polygon</td>
<td>Shape file</td>
<td>2002</td>
<td>PIGSA program (d)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

a: Shuttle Radar Topography Mission (http://www.ambiotek.com/srtm)
b: Advanced Land Observing Satellite Phased Array type L-band Synthetic Aperture Radar (https://www.asf.alaska.edu/sar-data/palsar/)
d: Plan Integral de Gestión Socio-Ambiental de la cuenca del Río Guayas y Península de Santa Elena (socio-environmental management plan for two river basins) (CEDEGE, 2002)
f: Instituto Geográfico Militar (Geographic Military Institute of Ecuador) (http://www.geoportaligm.gob.ec/portal/index.php/geoservicios/)
g: Food and Agriculture Organization of the United Nations (FAO, 1974) (http://www.waterbase.org/download_data.html)
The Digital Elevation Model (DEM), first, is a digital, approximate representation of the elevation of a surface, often stored in a regular grid. As the DEM enables the generation of topographic (e.g. slope) and hydrological (e.g. flow direction) information, it forms an important basis for hydrological studies (Wechsler, 2007). This was also the case in this study, for the reason that the definition of the stream network (e.g. location, channel slope, channel length) and the subbasins (e.g. location, area, slope) were based on the DEM. The DEM used in this study is shown in Figure 7-b. This DEM is a product of the Shuttle Radar Topography Mission (SRTM), using a dual antenna system to sample elevation data (Lillesand et al., 2014). More specifically, the post-processed version 4.1 was used in this study. More information on this version is given by Jarvis et al. (2008). These data were resampled to a resolution of 30 m (bilinear interpolation).

The land use map, secondly, is a hierarchically organised map with 40 different classes, generated based on satellite images (LandSat 8 and RapidEye) and post-processed using Kernel smoothing (MAE - MAGAP, 2015). The agricultural level of the map is shown in Figure 8. The soil map, thirdly, is depicted in Figure 9. The database associated with this map contains most of the soil parameters required by SWAT, contrary to the more recent PIGSA map. The calculation of the required parameters that are not in the database is the topic of section 5.3.2. The river network, finally, is represented on Figures 7 - 10. As no data were available with respect to groundwater parameters, these parameters were calibrated or set to default values.

Figure 9: Soil types within the Guayas River basin.

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7 RapidEye operates at 5 m resolution in five spectral bands (visible, red-edge and near-infrared) (Weichelt et al., 2011).
5.2.2 Meteorological data

An overview of the available meteorological data for the most important weather variables is given in Table 5. The term “reanalysis product” refers to large scale (both spatial and temporal) datasets that are based on the analysis and interpolation of station and/or forecast and/or satellite data (Monteiro et al., 2015). As the amount of satellite and reanalysis data is extensive, the table is not complete but represents a selection of the available data. Below Table 5, the choice of the data for the different weather parameters for use in this study will be discussed. Particular attention is given to the choice of the precipitation data as precipitation is considered to be the driving force of hydrological models (Nossent et al., 2014). The influence of the other weather variables is mainly restricted to the calculation of the reference evapotranspiration (\(E_{T_0} \, [\text{mm day}^{-1}]\)) (Appendix A.1 - A.4) (Neitsch et al., 2011).

Table 5: Overview of available weather data for study area. Grey indicates data that were used for comparison. The final choice is indicated in dark grey.

<table>
<thead>
<tr>
<th>Name</th>
<th>Format</th>
<th>Resolution/number of stations</th>
<th>Period</th>
<th>Source</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - Precipitation</td>
<td>NetCDF</td>
<td>280 km Subdaily, 1948 - present</td>
<td>NCEP (a)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NetCDF</td>
<td>56 km Subdaily, 1979 - 2013</td>
<td>WDEI (b)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HDF</td>
<td>28 km Subdaily, 1998 - 2016</td>
<td>TMPA TRMM (c)</td>
<td>Satellite dataset</td>
<td></td>
</tr>
<tr>
<td></td>
<td>ArcGrid, TIF, NetCDF</td>
<td>28 km Subdaily, 2000 - present</td>
<td>PERSIANN (d)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>GRD</td>
<td>28 km Subdaily, 2002 - present</td>
<td>CMORPH (e)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>TIF</td>
<td>12 km Subdaily, 2015 - present</td>
<td>GPIM (f)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Excel</td>
<td>30 stations Daily, 1963 - 2015</td>
<td>SENAGUA (g)</td>
<td>Gaps, clustered</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>38 km Daily, 1979 - 2014</td>
<td>CSF (h)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>83 km Daily, 1979 - 2016</td>
<td>ERA-Interim (i)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NetCDF</td>
<td>5.5 km Daily, 1981 - 2016</td>
<td>CHIRPS (j)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text, NetCDF</td>
<td>19 km Monthly, 1901 - 2012</td>
<td>CRU TS (k)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>56 km Monthly, 1901 - 2010</td>
<td>GPIC (l)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td>2 - Temperature (min and max)</td>
<td>NetCDF</td>
<td>56 km Subdaily, 1979 - 2013</td>
<td>WDEI (b)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>38 km Daily, 1979 - 2014</td>
<td>CSF (h)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>83 km Daily, 1979 - 2016</td>
<td>ERA-Interim (i)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Excel</td>
<td>20 stations Daily, 1982 - 2015</td>
<td>SENAGUA (g)</td>
<td>Gaps, clustered</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text, NetCDF</td>
<td>19 km Monthly, 1901 - 2012</td>
<td>CRU TS (k)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td>3 - Relative humidity</td>
<td>NetCDF</td>
<td>56 km Subdaily, 1979 - 2013</td>
<td>WDEI (b)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>38 km Daily, 1979 - 2009</td>
<td>CSF (h)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>83 km Daily, 1979 - 2016</td>
<td>ERA-Interim (i)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Excel</td>
<td>16 stations Daily, 1982 - 2015</td>
<td>SENAGUA (g)</td>
<td>Gaps, clustered</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text, NetCDF</td>
<td>19 km Monthly, 1901 - 2012</td>
<td>CRU TS (k)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td>4 - Solar radiation</td>
<td>NetCDF</td>
<td>56 km Subdaily, 1979 - 2013</td>
<td>WDEI (b)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>38 km Daily, 1979 - 2009</td>
<td>CSF (h)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Excel</td>
<td>3 stations Daily, 2003 - 2009</td>
<td>SENAGUA (g)</td>
<td>Gaps, clustered</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text, NetCDF</td>
<td>19 km Monthly, 2012 - 2012</td>
<td>CRU TS (k)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td>5 - Wind speed</td>
<td>NetCDF</td>
<td>56 km Subdaily, 1979 - 2013</td>
<td>WDEI (b)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>38 km Daily, 1979 - 2009</td>
<td>CSF (h)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text</td>
<td>83 km Daily, 1979 - 2016</td>
<td>ERA-Interim (i)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Excel</td>
<td>11 stations Daily, 1987 - 2015</td>
<td>SENAGUA (g)</td>
<td>Gaps, clustered</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Text, NetCDF</td>
<td>19 km Monthly, 2012 - 2012</td>
<td>CRU TS (k)</td>
<td>Reanalysis product</td>
<td></td>
</tr>
<tr>
<td>6 - Potential evapotranspiration</td>
<td>Excel</td>
<td>13 stations Daily, 1972 - 2015</td>
<td>SENAGUA (g)</td>
<td>Gaps, clustered</td>
<td></td>
</tr>
</tbody>
</table>

Source:
- a: National Center for Environmental Prediction (https://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.html)
- b: WATCH Forcing Data methodology applied to ERA-Interim (http://www.eu-watch.org/data_availability)
- d: Precipitation Estimation from Remotely Sensed Information using Artificial Neural Networks (http://chrsdata.eng.uci.edu/)
- e: NOAA CPC Morphing Technique (https://rda.ucar.edu/datasets/ds502.0/#!description)
- g: Secretaria Nacional del Agua (national ministry of water) (http://www.senagua.gov.ec/)
- i: European Centre for Medium-Range Weather Forecasts (ECMWF) Re-Analysis Interim (http://www.ecmwf.int/en/research/climate-reaanalysis/era-interim)
- j: Climate Hazards Group InfraRed Precipitation with Station data (http://chg.ucsb.edu/data/chirps/)
5.2.2.1 Precipitation

Hydrological modelling requires an accurate description of rainfall patterns which are highly spatially variable, especially in the tropics and the presence of orographic effects. Ground stations, however, are not always able to capture this spatial variability (Houze, 2012; Strauch et al., 2012). The data from the SENAGUA ground stations are based on pluviometric or pluviographic precipitation measurements. The location and registration period of the stations within or close to the basin are shown in Figures 10-a and 11 respectively. Figure 10-b indicates the location of the 14 stations for which the percentage of days without data was smaller than 20% for the selected period from 1990 to 2015. This threshold was chosen in order to maximise the data coverage in both time and space. Figure 10-b demonstrates that the study area is not well covered by the selected stations. Especially in the mountainous region stations are scarce. Only two of the selected stations have an elevation higher than 1000 m, although this represents 20% of the study area. For the region above 2000 m, covering 15% of the basin, there is only one station. No metadata were available making it difficult to assess accuracy and precision of the acquired data.

Figure 10: Location of the precipitation stations within or close to the Guayas River basin (a.) and location and name of the 14 selected precipitation stations (b.).
The reanalysis products have a larger spatial coverage than the ground stations data. However, these products are generated with algorithms tested in other regions. Their performance depends on the geographic location and the climatic zone of an area, which makes them possibly less accurate for this study (Essou et al., 2016; Lorenz and Kunstmann, 2012). It is therefore important to compare the reanalysis products with the ground station data before using them (Bitew and Gebremichael, 2011; Dile and Srinivasan, 2014). This was done for four reanalysis products (marked in grey in Table 5 and briefly described in the Appendix B), selected on the basis of the resolution and the period of the datasets. To do so, the following statistics were calculated:

\[
\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{P}_i - P_i)^2}{n}} \tag{5.1}
\]

\[
B = \frac{\sum_{i=1}^{n} \hat{P}_i - P_i}{n} \tag{5.2}
\]

\[
R^2 = 1 - \frac{\sum_{i=1}^{n}(\hat{P}_i - P_i)^2}{\sum_{i=1}^{n}(\bar{P} - P)^2} \tag{5.3}
\]

\[
\rho_s = \frac{\sum_{i=1}^{n}(r_i - \bar{P}) \cdot (s_i - \bar{s})}{\sqrt{\sum_{i=1}^{n}(r_i - \bar{P})^2 \cdot \sum_{i=1}^{n}(s_i - \bar{s})^2}} \tag{5.4}
\]

Where RMSE the Root Mean Squared Error [-], B the bias [mm day\(^{-1}\)], \(R^2\) the coefficient of determination [-], \(\rho_s\) the spearman correlation coefficient [-], \(\hat{P}_i\) the monthly average registered precipitation at station X for month i [mm day\(^{-1}\)], \(P_i\) the monthly average reanalysis precipitation data of cell X where station X is located for month i [mm day\(^{-1}\)], \(n\) the total number of months for which both the station and the reanalysis dataset contain a precipitation value [-], \(\bar{P}\) the average value of the registered precipitation at station X [mm day\(^{-1}\)], \(r_i\) the ranked precipitation at place i for the station X data [mm day\(^{-1}\)], \(s_i\) the ranked precipitation at place i for the reanalysis data of cell X [mm day\(^{-1}\)] and \(\bar{s}\) the average value of the reanalysis precipitation data of cell X [mm day\(^{-1}\)].
These statistics were calculated for each of the 14 selected stations, for which the data were compared with the reanalysis data of the cell where the station is located. This was done on a monthly basis. More specifically, the monthly average of the total daily precipitation [mm day\(^{-1}\)] was used as the many data gaps in the stations dataset did not allow calculating the total monthly precipitation. The statistics were calculated for a period determined by the start date of the reanalysis datasets (the year 1979 or 1981) and the end date of the stations datasets. At the moment of analysis, the stations datasets were only available until 2008, thus the statistics were calculated for the period 1979 (1981) - 2008. The effect of the resolution of the reanalysis products on these statistics was examined but no trend was observed.

The results of this comparison show that the WFDEI dataset corresponds the best with the ground station precipitation data (Appendix C.1). Hence, a choice had to be made between the station and the WFDEI dataset. In Table 6, an overview of the advantages and disadvantages of both sources is given.

Table 6: Advantages and disadvantages of station and reanalysis datasets.

<table>
<thead>
<tr>
<th>Stations</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>More accurate and precise than reanalysis data (?)</td>
<td>Clustered</td>
</tr>
<tr>
<td></td>
<td></td>
<td>No data in mountainous region</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Data gaps</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Only representative for 1 place</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reanalysis products</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 method for the whole period</td>
<td>Limited accuracy and precision (?)</td>
</tr>
<tr>
<td></td>
<td>No data gaps</td>
<td>Accuracy and utility depend on region (Zhang et al., 2014)</td>
</tr>
<tr>
<td></td>
<td>Covering the whole basin</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Representative for the whole grid</td>
<td></td>
</tr>
</tbody>
</table>

The WFDEI dataset was selected as input for the SWAT model based on Table 6 and considering its agreement with the station data. However, a correction factor was applied to adjust the WFDEI dataset to the ground station data. This correction factor was calculated per station and per month separately by means of equation 5.5.

\[
CF_{\text{station } X, \text{ month } j} = \frac{\sum_{i=1}^{n} \bar{Y}_{i, \text{month } j}}{\sum_{i=1}^{n} \sum_{j=1}^{12} \bar{Y}_{i, \text{month } j}} = \frac{\sum_{i=1}^{n} \bar{Y}_{i, \text{month } j}}{\sum_{i=1}^{n} \sum_{j=1}^{12} \bar{Y}_{i, \text{month } j}}
\] (5.5)

Where \(CF_{\text{station } X, \text{ month } j}\) the correction factor for station \(X\) for month \(j\) [-], \(\bar{Y}_{i, \text{month } j}\) the registered monthly average of the total daily precipitation for month \(j\) of year \(i\) at station \(X\) [mm day\(^{-1}\)], \(\bar{Y}_{i, \text{month } j}\) the WFDEI monthly average of the total daily precipitation for month \(j\) of year \(i\) in cell \(X\) (the cell where station \(X\) is located) [mm day\(^{-1}\)] and \(n\) the total number of years for which both the station and the reanalysis dataset contain a precipitation value for month \(j\) [-].

Subsequently, the average of these CF’s was taken (equation 5.6).

\[
CF = \frac{\sum_{i=1}^{14} \sum_{j=1}^{12} CF_{\text{station } i, \text{ month } j}}{14 \times 12}
\] (5.6)

This resulted in a correction factor of 1.32. Consequently, all WFDEI precipitation values were multiplied by 1.32 before using as input to the model. Alternatively, a spatially and/ or temporally variable CF could have been applied as was done by Monteiro et al. (2015). However, as no trend was observed for the CF as a function of elevation, location or time it was decided to apply one constant
The previously mentioned statistics were calculated again for the period of 1990 - 2013, before and after application of the correction factor (Appendix C.2). These statistics show that the bias and the coefficient of determination improve for almost all the stations. The already negative bias for the “La Capilla” station, however, increases (in absolute value).

The many studies found in literature demonstrate the frequent application of reanalysis precipitation products for hydrological modelling (Grusson et al., 2017; Le and Pricope, 2017; Tuo et al., 2016). These studies, on the one hand, recommend the WFDEI dataset but, on the other hand, highlight that its performance is catchment dependent (Monteiro et al., 2015; Nkiaka et al., 2017; Zhang et al., 2014).

### 5.2.2.2 Temperature

With respect to the temperature station data, the stations for which the percentage of gaps was lower than 20 % for the period 1990 - 2015 were selected, as was the case with the precipitation data. For these nine selected stations, the maximal data gap percentage is 7 %. The comparison with the WFDEI data was done again, with the same method as described in the previous section, for the period 1990 - 2013.

As the results indicate (Appendix C.3), the agreement between the WFDEI temperature and the stations temperature is poor. With respect to the minimum temperature, the bias depends strongly on the station and the WFDEI temperature both over- and underestimates the station temperature. The maximum temperature of the WFDEI data is in general an overestimation of the station temperature. The station data indicate that the temperature is rather constant throughout the basin (for regions of the same elevation) but strongly dependent on the elevation. For these reasons, it was chosen to use the station data, however, adjusted to elevation. To do so, the temperature lapse rate was calculated by linear regression between the yearly average temperature registered at a station and the elevation of that station. This resulted in a lapse rate of -5.7 [°C km⁻¹]. It is important to note that no metadata for the temperature records were available. Consequently no information about accuracy and precision of the measurement could be obtained.

To deal with the data gaps, the weather generator function of SWAT was used. This function replaces missing values by values calculated using monthly statistics, assuming a normal distribution and adjusting for dry or wet conditions (Neitsch et al., 2011). The monthly statistics were obtained using the data of the nine selected stations.

### 5.2.2.3 Relative humidity, solar radiation and wind speed

With respect to the remaining weather variables required by SWAT, it was chosen to use the station data. This was under the assumption that the station data are more accurate than the reanalysis data and that it is less important for these weather parameters to capture their spatial variability within the basin (the stations that register these parameters are scarce). In addition, many of the stations have limited registration periods for these parameters. Therefore, the weather generator function was used instead of the registered time series. Thus, monthly statistics were calculated based on the station data and the weather generator was used to calculate the daily values.

---

8 The rate at which air cools with elevation change (Dodson and Marks, 1997).
5.2.2.4 Reference evapotranspiration

Reference evapotranspiration is another parameter provided by SENAGUA. For this parameter, five stations have reasonable registration periods without too many data gaps. These data can be used to validate the reference evapotranspiration simulations of the model (section 5.5.2.4). No actual evapotranspiration measurements were available.

5.2.3 Daule Peripa Dam and lakes

Table 7 presents the data that were available for the Daule Peripa Dam and that were used in this study. SWAT requires more reservoir parameters, including the equilibrium sediment concentration and the hydraulic conductivity of the bottom. These data, however, were not available and default values were used. In addition, daily in- and outflow measurements are only available for a limited period (Table 7).

Table 7: Available data for the Daule Peripa Dam.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Data</th>
<th>Unit</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start operation</td>
<td>1987</td>
<td>-</td>
<td>CELEC (a), 2013</td>
</tr>
<tr>
<td>Maximal surface area max</td>
<td>30,000</td>
<td>ha</td>
<td>CELEC (a), 2013</td>
</tr>
<tr>
<td>Normal surface area</td>
<td>27,000</td>
<td>ha</td>
<td>CELEC (a), 2013</td>
</tr>
<tr>
<td>Maximal volume</td>
<td>6.00E+09</td>
<td>m³</td>
<td>CELEC (a), 2013</td>
</tr>
<tr>
<td>Normal volume</td>
<td>5.40E+09</td>
<td>m³</td>
<td>CELEC (a), 2013</td>
</tr>
<tr>
<td>Daily inflow measurements</td>
<td>Period: 1990 - 2009</td>
<td>-</td>
<td>INAMHI (b)</td>
</tr>
<tr>
<td>Daily outflow measurements</td>
<td>Period: 1990 - 2009</td>
<td>-</td>
<td>INAMHI (b)</td>
</tr>
<tr>
<td>Water level max</td>
<td>88</td>
<td>m</td>
<td>CELEC (a), 2013</td>
</tr>
<tr>
<td>Water level min</td>
<td>70</td>
<td>m</td>
<td>CELEC (a), 2013</td>
</tr>
</tbody>
</table>

a: Corporacion Electrica del Ecuador (Electrical organisation of Ecuador) [https://www.celec.gob.ec/]
b: Instituto Nacional de Meteorologia e Hidrologia (national meteorological and hydrological institute) [http://www.serviciometeorologico.gob.ec/]

Besides the dam, many natural lakes are present in the basin (Figures 7 - 10) for which no data (e.g. area and volume) were available. Only for the Abras de Mantequilla wetland (wetland located in the central part of the basin, white circle on Figure 7-b), depth, volume and area measurements were available from a local topographic survey (Arias-Hidalgo, 2012).

5.2.4 Pesticides application data

5.2.4.1 Pesticides choice

Numerous pesticides are applied within the basin, however, only two pesticides were selected to simulate the dynamics for. Pendimethalin, first, is a dinitroaniline herbicide. It controls broadleaf and grassy weeds by inhibiting cell division. This herbicide is characterised by a rather low solubility. It has a low acute toxicity but may have adverse chronic effects on (semi-) aquatic plants, invertebrates, fish and birds (Peterson et al., 2010; US EPA, 1997). Fenpropimorph, secondly, is a widely used morpholine fungicide, e.g. to control the Sigatoka disease in bananas. It inhibits the ergosterol biosynthesis and is classified in the European Union pesticide database as toxic to aquatic life with long lasting effects (European Union, 1995; US EPA, 2006).

In the first place, this selection was based on prior estimated importance (risk). This risk was estimated in consultation with local river managers and farmers. Additionally, the analysis results of samples collected during the summer of 2016 gave an indication of which pesticides are both frequently applied throughout the basin and have the characteristics (e.g. solubility and decay rate) to persist in the water phase. During this campaign, water samples were taken at 181 locations distributed throughout the Guayas River basin and collected in a dark glass bottle (1 L). These
samples were vacuum filtered and subsequently passed through an activated SEP-PACK filter in order to sorb the pesticides. The SEP-PACK filters were then stored at -21 °C and transported to Belgium. Once in Belgium, the pesticides were extracted using 10 mL of hexane, from which 2 mL were used for GC-ECD (gas chromatography coupled with electron capture detector) analysis. Another 5 mL of extract were evaporated and 1 mL acetonitrile was added. This solution was 10 times diluted with water and 2 mL were used for LC-MSMS (liquid chromatography-tandem mass spectrometry) analysis. As such, the samples were analysed for 91 pesticides from which 20 pesticides were detected. At 108 of the 181 locations one or more pesticides were found. Six pesticides (cadusafos (62), butachlor (21), pendimethalin (21), fenpropimorph (15), malathion (12) and pyrimethalin (11)) were detected (concentration above detection limit) at multiple locations (> 6). The number of locations where the pesticides were detected are given between brackets. The maximum number of pesticides that were detected at one location is six. This location, situated in a rice cultivation region, is indicated with a black circle on Figure 12. The locations where pendimethalin and fenpropimorph were detected are also shown in this figure, with an indication of the measured concentrations. The maximum concentration that was measured was 2 µg L⁻¹ for the pesticide butachlor.

The second criterion for the pesticide selection was the availability of application data. These data are scarce (see below) and for only two (pendimethalin and fenpropimorph) of the six abundant pesticides the available application data were sufficient to be used as input data.
5.2.4.2 Application data

The required detailed information (application rate (AR [L product or kg of active ingredient ha\(^{-1}\)]) and application timing) for the selected pesticides was extensively searched in literature. In addition, national (Agrocalidad) and international (Homologa) databases of registered products were explored and agricultural guidelines were sought for. Furthermore, several farmers were interviewed for big banana, corn, rice and sugar cane farms (one interview for each crop). These crops represent four of the five most cultivated crops within the basin. Altogether, this resulted in the data presented in Tables 8 and 9.

Table 8: Application data for pendimethalin. AR: application rate, AI: active ingredient.

<table>
<thead>
<tr>
<th>Crops</th>
<th>Product</th>
<th>Application timing</th>
<th>AR</th>
<th>Unit</th>
<th>Source</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corn</td>
<td>Gramilaq</td>
<td>1 - 2 days after seeding: end of December and end of June</td>
<td>2</td>
<td>L product ha(^{-1})</td>
<td>Plan Agripac (c) + interview farmer</td>
<td>Interview at a farm of 25 ha near Balzar</td>
</tr>
<tr>
<td>Rice</td>
<td>?</td>
<td>8th of October</td>
<td>0.1</td>
<td>kg AI ha(^{-1})</td>
<td>Interview farmer of Guayas</td>
<td>The AR in Los Rios is twice as big as the AR in Guayas</td>
</tr>
<tr>
<td>Rice</td>
<td>Various products (e.g. Prowl top)</td>
<td>?</td>
<td>3</td>
<td>L product ha(^{-1})</td>
<td>MAGAP and Agrocalidad (2016) (a+b)</td>
<td>Recommended dosis</td>
</tr>
<tr>
<td>Sugar cane</td>
<td>Pendimethalin 40EC</td>
<td>Month 1, 6, 7, 8, 9, 10, 11, 12</td>
<td>3</td>
<td>L product ha(^{-1})</td>
<td>Interview farmer</td>
<td>Interview at a big industrial farm (16,500 ha)</td>
</tr>
<tr>
<td>Sugar cane</td>
<td>Various products (e.g. Prowl top)</td>
<td>?</td>
<td>3</td>
<td>L product ha(^{-1})</td>
<td>MAGAP and Agrocalidad (2016) (a+b)</td>
<td>Recommended dosis</td>
</tr>
<tr>
<td>?</td>
<td>Gramilaq</td>
<td>?</td>
<td>3</td>
<td>L product ha(^{-1})</td>
<td>MAGAP and Agrocalidad (2016) (a+b)</td>
<td>Recommended dosis</td>
</tr>
</tbody>
</table>

Table 9: Application data for fenpropimorph. AR: application rate.

<table>
<thead>
<tr>
<th>Crops</th>
<th>Product</th>
<th>Application timing</th>
<th>AR</th>
<th>Unit</th>
<th>Source</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Banana</td>
<td>Volley</td>
<td>week 1, 6, 17, 23, 25</td>
<td>?</td>
<td>(a)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Banana</td>
<td>Volley</td>
<td>?</td>
<td>0.5</td>
<td>L product ha(^{-1})</td>
<td>MAGAP and Agrocalidad (2016) (b+c)</td>
<td>Recommended dosis</td>
</tr>
<tr>
<td>Corn</td>
<td>?</td>
<td>17th of July</td>
<td>?</td>
<td>0.5</td>
<td>MAGAP and Agrocalidad (2016) (b+c)</td>
<td>recommended dosis</td>
</tr>
</tbody>
</table>

As can be seen in Tables 8 and 9, the available application data are scarce and not spatially distributed. Moreover, no data were found in the literature and the application timing and AR do not always originate from the same source. For banana, the most recent timing information dates from 2011. However, it was confirmed by personal communication that the product Volley is still being used. In section 5.5.3.1 will be explained which assumptions were made to use the limited application data as input to the model. With respect to the fifth of the five most produced crops, being cocoa, no application plans were available, as the pest control for these plantations is mainly mechanical and pesticides are applied during specific events only (personal communication).

5.2.5 Calibration data

Although the developed model is a mechanistic model, with physically based parameters, it was necessary to do a streamflow calibration in order to reproduce the measured streamflow dynamics. This is because, especially considering the data limitations encountered during this study, information on many parameters (e.g. groundwater parameters) is not available. Additionally, the model contains empirical components (e.g. the curve number method). As will be described, the data availability limits the calibration to a streamflow calibration.
5.2.5.1 Streamflow

With respect to streamflow (Q [m³ s⁻¹]), data for 17 stations were obtained from INAMHI⁹. At these stations, water levels (h [m]) are measured daily using limnimeters or limnigraphs. Subsequently, streamflows are estimated by means of Q,h-relationships. As these relationships may change because of sedimentation or river bank erosion, they should be established regularly (Braca, 2008). The location and registration period of these stations are shown in Figures 13-a and 14 respectively.

Figure 13-b shows the location of the five stations for which the percentage of days without data was smaller than 20 % for the selected period from 1990 to 2014. The threshold of 20 % was chosen in order to maximise the data coverage both in time and space. The data from these selected stations were used to calibrate the streamflow. As can be seen on Figure 13-b, these stations are rather well distributed throughout the basin. An important limitation, however, is the lack of a station at the outlet of the basin. In addition, no station on the Chimbo River is present and the station on the Babahoyo River (the “Zapotal en Lechugal” station) is located quite far upstream. Even more, a number of gaps are present in the time series, making it difficult to assess the performance of the simulated flows for those periods. To end, the Q,h-relationships that were used to estimate the flow might be outdated, raising questions about the accuracy and the precision of the data (personal communication).

Figure 13: Location of streamflow stations within the Guayas River basin and indication of the Babahoyo (1) and Chimbo (2) Rivers (a.). Location and name of the five selected streamflow stations (b.).

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⁹ The national meteorological and hydrological institute (http://www.serviciometeorologico.gob.ec/).
Figure 14: Overview of the registration period and data gaps for the streamflow stations. Based on this, the Baba dam, Daule en La Capilla, Quevedo en Quevedo, Vinces en Vinces and Zapotal en Lechugal stations were selected for further use.

### 5.2.5.2 Sediment yield

With respect to sediment yield, on which an important fraction of the pesticides can be adsorbed (section 2.2), no daily or monthly measurements were available. This impeded to do a sediment calibration. Data that were available are presented in Table 10.

<table>
<thead>
<tr>
<th>Station</th>
<th>Sediment production [tons year(^{-1})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Daule en La capilla</td>
<td>4,900,000</td>
</tr>
<tr>
<td>Baba dam</td>
<td>155,000</td>
</tr>
<tr>
<td>Quevedo en Quevedo</td>
<td>880,000</td>
</tr>
<tr>
<td>Vinces en Vinces</td>
<td>1,600,000</td>
</tr>
<tr>
<td>Zapotal en Lechugal</td>
<td>1,330,000</td>
</tr>
</tbody>
</table>

### 5.2.5.3 Pesticides

Only the surface water pesticide concentration data from the previous mentioned sampling campaign in 2016 (section 5.2.4.1) were available for the pesticides of interest. During this campaign, each site was only sampled once. Consequently, it is currently not possible to calibrate pesticide concentrations. For this reason and because of the uncertainty associated with the pesticide application data, the use of the pesticide simulations is limited to a system analysis.

### 5.3 Data pre-processing

The next step, before developing the model, is the processing of the data. This was done using ArcMap and Matlab. The shape file of the river network was transformed from the original polygons to one single line at the center of the river. In addition, the lakes were removed and the placement with respect to the DEM was optimised, prior to using the file for burn in (section 5.4.1). All the shape files were projected to the same projection (WGS1984 UTM Zone 17M South) and were clipped with the contour of the river basin. Furthermore, the required SWAT input files (e.g. daily precipitation, weather statistics, location of the streamflow stations) were generated. The recategorisation of the land use categories and the calculation of the soil parameters, finally, will be discussed in more detail in the next two sections.
5.3.1 Land use reclassification

SWAT includes an extensive land cover database, containing the parameters needed for e.g. soil erosion and transpiration calculations (Arnold et al., 2012b). To make use of database, the categories of the land use map should be linked to the categories of the database. This was done by means of a “look up table”, illustrated in Figure 15. It is important to note that only the agricultural land use categories that will be included into the model are shown in the look up table on this figure. Which categories that are included depends on the threshold value for land use during the Hydrologic Response Unit (HRU) definition (section 5.4.2). In addition, urban land use was linked to the category URBN in the SWAT urban database. A final remark is that categories that were not available in the ArcSWAT database (e.g. TUHB which is herbaceous toendra) come from the more extensive database of the MapWindow-SWAT interface (MWSWAT) (http://swat.tamu.edu/software/mwswat/).

Figure 15: Illustration of the land use reclassification.

5.3.2 Soil parameters

As the soil database of SWAT is only applicable for soils in the United States, a new user defined database was created for the soil classes within the basin (Figure 9). An overview of the methods used to obtain the required soil parameters for each of these classes is given in Table 11. Studies that used similar methods are Nielsen et al. (2013) and Stehr et al. (2008). Detailed information on the required parameters can be found in Arnold et al. (2012).
5.4 Model development

Once the data were pre-processed, they could be used to develop a model of the Guayas River basin (Figure 16). The philosophy followed during this step is that there is no point in developing a spatially detailed model if the spatial resolution of the available data, e.g. soil map and precipitation stations, does not support this. Therefore, it was chosen to develop a rather coarse model that can eventually be refined in the future. As such, this enables to learn on which steps of the development phase future model refinement should focus. The model was developed with the ArcGIS interface of SWAT. More specifically, the ArcSWAT version 2012 was used, downloadable at http://swat.tamu.edu/software/arcswat/. A description of SWAT was given in section 4.1.

Figure 16: Illustration of the model setup in ArcSWAT. Left: layers used for the model development. Middle: resulting model with delineated subbasins and river network. Indication of the streamflow stations (white dots) and Daule Peripa Reservoir (green dot). Right: further subdivision of subbasin 1 into Hydrological Respons Units (HRUs) with indication of land use/ soil/ slope classes.

Below, the definition of the stream network and the delineation of the watershed into subbasins will be discussed. Thereafter, the partitioning of the subbasins into Hydrologic Response Units (HRUs) will be outlined. To end, additional model settings will be discussed.

5.4.1 Watershed delineation

The first step of the model development comprises the definition of the river network, which was done based on the DEM (using the eight directional flow model (Jenson and Domingue, 1988)). However, to improve this process – especially near the outlet, where the basin is flat (Figure 7-b) – the edited shapefile of the river network was “burned” into the DEM. This refers to the small
reduction of the elevation of the DEM cells overlapping with the stream network and is recommended by Luo et al. (2011). Important during this step is the choice of the threshold drainage area (TDA). This is the minimum drainage area required to form the beginning of a stream (Omran et al., 2016). As this threshold initiates streamflow routing, it determines the degree of detail of the delineated network and thus the degree of detail of the streamflow and pesticide simulations. In addition, this choice influences the amount of subbasins that will be created during the second step. To end, it affects the spatial resolution of the input data, e.g. precipitation data (one value per subbasin) and pesticide application data (one value per HRU). However, reported recommendations with respect to this choice are limited as the right choice is dependent on the study area and the resolution of the available data (Thompson et al., 2001). Nevertheless, the suggestions of Jha et al. (2004) were followed and a TDA of 3 % (102,000 ha) of the total watershed area was chosen. The resulting network is coarse (Figure 16) and does not include all the locations where samples were taken during the campaign of 2016 (section 5.2.4.1). Especially the Babahoyo River is shorter in the model than in reality. However, the major portion of the non-included part of the Babahoyo River is situated in the mountainous region where agricultural practices are rare (Figure 8). The implications of this missing part with respect to the objective to simulate pesticide dynamics can thus be assumed to be limited. Additionally, it was verified that the main rivers and the selected streamflow stations were included into the delineated network.

In a second step, the watershed was delineated into subbasins based on both the DEM and the delineated stream network. For every river branch another subbasin was created. Subsequently, a smaller TDA, chosen in step one, results in a larger amount of subbasins and thus allows more spatial variation into the model. In addition, at each of the five selected streamflow stations (section 5.2.5.1) the interface defines a new subbasin. This is done in order to enable the comparison of the simulated flow with the registered discharge. Finally, an extra subbasin was created at the location of the Daule Peripa Reservoir. As such, the TDA of 3 % resulted in 29 subbasins (Figure 16). The influence of the watershed subdivision on the simulations will be discussed in section 6.2.2.

5.4.2 HRU definition

The partitioning of the subbasins into HRUs is based on the land use, soil and slope types. With respect to the slope, it was decided to include only two slope classes in order to avoid the generation of too many HRUs. As the slope within the basin has no bimodal but an exponential decaying distribution, where weak slopes are the most abundant, the limit between the two classes was arbitrarily set at 10 %. As already explained (section 4.1), every HRU represents the total area of a certain combination of land use, soil and slope type within a subbasin. However, not every combination results in a HRU. Only the land use, soil and slope types for which the percentage area within the subbasin is above a certain threshold are included into the model. These thresholds were chosen to be 5 % for land use and 20 % for soil and slope, as suggested in the SWAT tutorial. Subsequently, land use, considered to be of major importance for this study, is represented by the model with more detail than soil and slope. The higher threshold for soil type is justified by the low spatial resolution of the soil map and the limited availability of the required soil parameters. With this thresholds, 268 HRUs were obtained. The HRUs for subbasin one are listed in Figure 16. The impact of the threshold choice on water quality simulations prediction is discussed by Her et al. (2015).
5.4.3 Additional settings
In this section, additional settings with respect to the model setup will be discussed. Elevation bands, first, were included in order to adjust the temperature records to variation in elevation (section 5.2.2.2). Thus, five equally represented elevation bands were defined for each subbasin. The lakes, secondly, were taken into account as they affect streamflow routing and pesticide transport and fate, e.g. pesticide loss via sedimentation and transformation processes (Luo and Zhang, 2009). They were represented as “ponds” in the model. These are conceptual water bodies, one per subbasin, that aggregate the lakes in that subbasin (Neitsch et al., 2011). The total area of lakes per subbasin was obtained from the river basin map. The volume of the lakes was estimated using a volume-area ratio of 2 m, which is in agreement with the data from the Abras de Mantequilla wetland survey (Arias-Hidalgo, 2012). It should be noted the area and volume of these lakes are in reality not constant throughout the year that, as they are natural and temporary. With respect to the operation of the Daule-Peripa reservoir, thirdly, it was chosen to use the available daily outflow measurements (Table 7) to simulate the daily reservoir outflow volume. To end, the (surface) runoff method was set to the SCS curve number method (section 3.3.1.2) and for streamflow routing the Manning equation together with the variable storage routing method, a hydrologic routing model (section 3.3.1.3), was chosen (Manning, 1891; Williams, 1969). Manning’s n values were assigned per subbasin according to Chow (1959) and using the information on the channel shape and the pool/ riffle class as noted during the sampling campaign of 2016. Accordingly, the Manning’s n value for the main channel amounts to 0.03 (straight channel, absent pool-riffle pattern), 0.035 (straight, poorly developed pool-riffle pattern), 0.045 (winding, moderately developed pool-riffle pattern) or 0.07 (winding, well developed pool-riffle pattern). With respect to the tributary channels, the Manning’s n value of the main channel is raised by 0.005 to account for an increase in friction by the presence of e.g more rocks and vegetation.

5.5 Model calibration and simulations
After development, the model was run on a daily time step for the period 1990 – 2009. The end of this period was constrained by the availability of the discharge measurements at the outlet of the Daule-Peripa dam (Table 7 and section 5.4.3). A warm-up period of three years was used to estimate initial conditions for soil water and groundwater storage as recommended by Malone et al. (2015). The remaining period was divided by two, resulting in an eight year calibration period (1993 – 2000) and a nine year validation period (2001 – 2009) (split sample methodology) (Klemeš, 1986). First, the model was calibrated manually for streamflow. Subsequently, the calibrated model was evaluated. Thereafter, simulations for the two selected pesticides and a system analysis were done.

5.5.1 Streamflow calibration approach
This section will describe the approach used for the manual calibration of the streamflow simulations. During calibration, parameters values are adjusted within physically realistic ranges to closely match simulations and observations (Zeckoski et al., 2015). The first section will give general information and will discuss the choice of the objective function. The next section will give information on the parameters that were calibrated. In the third section will be explained how the calibration was performed using multiple stations throughout the basin. Thereafter, the different steps of the calibration procedure will be outlined. To end, the criteria to evaluate the performance of the calibrated model will be given.
5.5.1.1 Calibration period and objective function

Streamflow calibration was done for the period 1993 – 2000, which is longer than the recommended minimum of five years and includes dry (e.g. 1996) and wet years (e.g. 1997 – 1998 associated with an El Niño event) (Gan et al., 1997). This El Niño event results in the occurrence of very high peak flows, which are recommended to be included in the calibration period (Gan et al., 1997; Kannan et al., 2007; Van Liew and Garbrecht, 2003).

The calibration was performed on a monthly basis using the monthly average of the daily observed and simulated streamflows. The simulated flows refer to the flows calculated at the outlet of each subbasin. It was not possible to use the monthly accumulated streamflow due to the data gaps in the streamflow observation data. It was chosen to calibrate manually as this allows to get a better understanding of the catchment functioning and the effect of parameter values. Therefore, visual inspection, by means of daily and monthly time series and scatter plots, was used to achieve this understanding and to facilitate the calibration process. The goal of the calibration was to reconstitute the dynamics of the registered streamflow (peak flow and baseflow volume, timing, form of the recession curve) as all these elements seem important with respect to the simulation of pesticide dynamics. Because the Nash-Sutcliffe efficiency (NSE) (equation 5.7) was positively evaluated to do so, it was selected as objective function (Servat and Dezetter, 1991). Moreover, it is commonly used and therefore allows comparison with other models (Moriasi et al., 2007). Additionally, this objective function is recommended by several authors (Legates and McCabe, 1999; Moriasi et al., 2007).

\[
\text{NSE} = 1 - \frac{\sum_{i=1}^{n}(Q_{i}^{\text{obs}} - Q_{i}^{\text{sim}})^2}{\sum_{i=1}^{n}(Q_{i}^{\text{obs}} - Q_{\text{obs}}\bar{\bar})^2}
\]

(5.7)

Where NSE the Nash-Sutcliffe efficiency [-], \(Q_{i}^{\text{obs}}\) the observed streamflow \([m^3 \cdot s^{-1}]\), \(Q_{i}^{\text{sim}}\) the simulated streamflow \([m^3 \cdot s^{-1}]\), \(Q_{\text{obs}}\bar{\bar}\) the average value of the observed streamflow \([m^3 \cdot s^{-1}]\) and \(n\) the total number of observations [-].

NSE varies from \(-\infty\) to 1, where 1 indicates a perfect fit and negative values indicate that the average value of the observed streamflow is a better prediction than the one of the model. A disadvantage of NSE is that it gives more weight to higher flows compared to lower flows due to the use of squared errors. In addition, these squared errors make the function relatively unsensitive towards systematic over- or underpredictions. Lastly, when comparing NSE values of models for different watersheds it is important to note that the denominator in the NSE equation is larger for watersheds with higher dynamics, which makes it easier to obtain high NSE values (Krause et al., 2005).

To avoid systematic over- or underpredictions of the model, the percent bias (PBIAS) (equation 5.8) was used as a second criterion during manual calibration and parameters that maximise NSE while minimising PBIAS were sought for. This statistic is recommended by Moriasi et al. (2015) due to its ability to estimate how well the model reproduces average streamflow magnitudes. In addition, it is commonly used and consequently enables comparison with other models.

\[
\text{PBIAS} [\%] = \frac{\sum_{i=1}^{n}(\bar{Q}_{i} - Q_{i}) \times 100}{\sum_{i=1}^{n} Q_{i}}
\]

(5.8)

Where PBIAS the percent bias [\%], \(\bar{Q}_{i}\) the observed streamflow \([m^3 \cdot s^{-1}]\), \(Q_{i}\) the simulated streamflow \([m^3 \cdot s^{-1}]\) and \(n\) the total number of observations [-].
5.5.1.2 Calibration parameters

A list of 11 parameters relevant to streamflow calibration was composed based on a number of pilot runs and the literature (Abbaspour et al., 2007, 2015; David, 2014; Holvoet, 2006; Neitsch et al., 2002; Santhi et al., 2001; Shen et al., 2012a; Van Liew et al., 2005) (Table 12). For each of these parameters the initial value, being a default value or based on pilot runs, was changed by 50 % (taking into account the permitted range of parameter values (Table 12) and the effect on the streamflow simulations was examined. This was to get an estimation of the sensitivity of the streamflow output towards these parameters. Subsequently, the seven most influential parameters were selected to calibrate the model (Table 12). This selection consists of four groundwater parameters (ALPHA_BF, GW_DELAY, GW_REVAP, GWQMN), one parameter influencing actual evapotranspiration (AWC), one governing streamflow routing (CH_K2) and a last parameter influencing runoff (CN2). In addition to these parameters, the effect of including temperature elevation bands (section 5.2.2.2) on the model performance was investigated. A brief description of each of the parameters is given below Table 12 and more information can be found in Arnold et al. (2012).

Table 12: Parameters selected for streamflow calibration based on pilot runs and literature (Abbaspour et al., 2007, 2015; Holvoet, 2006; Neitsch et al., 2002; Santhi et al., 2001; Shen et al., 2012; Van Liew et al., 2005). Parameters indicated in grey were optimised during streamflow calibration. Range: range of possible parameter values as implemented in SWAT. Initial value: default value or based on pilot runs.

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Range</th>
<th>Initial value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>AWC(n)</td>
<td>Available water capacity of soil layer n</td>
<td>0 - 1</td>
<td>(a)</td>
<td>mm H2O mm soil⁻¹</td>
</tr>
<tr>
<td>ALPHA_BF</td>
<td>Baseflow alpha factor</td>
<td>0 - 1</td>
<td>0.02</td>
<td>days⁻¹</td>
</tr>
<tr>
<td>CH_K1</td>
<td>Effective hydraulic conductivity in tributary channel alluvium</td>
<td>-0.01 - 1</td>
<td>0</td>
<td>mm h⁻¹</td>
</tr>
<tr>
<td>CH_K2</td>
<td>Effective hydraulic conductivity in main channel alluvium</td>
<td>0 - 300</td>
<td>10</td>
<td>mm h⁻¹</td>
</tr>
<tr>
<td>CN2</td>
<td>SCS runoff curve number for moisture condition II</td>
<td>35 - 98</td>
<td>(b)</td>
<td></td>
</tr>
<tr>
<td>ESCO</td>
<td>Soil evaporation compensation factor</td>
<td>0 - 1</td>
<td>0.85</td>
<td></td>
</tr>
<tr>
<td>GW_DELAY</td>
<td>Groundwater delay time</td>
<td>0 - 500</td>
<td>62</td>
<td>days</td>
</tr>
<tr>
<td>GW_REVAP</td>
<td>Groundwater &quot;revap&quot; coefficient</td>
<td>0.02 - 0.2</td>
<td>0.04</td>
<td></td>
</tr>
<tr>
<td>GWQMN</td>
<td>Threshold depth of water in the shallow aquifer required for return flow to occur</td>
<td>0 - 5000</td>
<td>1000</td>
<td>mm H2O</td>
</tr>
<tr>
<td>REVAPMN</td>
<td>Threshold depth of water in the shallow aquifer required for &quot;revap&quot; or percolation to the deep aquifer to occur</td>
<td>0 - 1000</td>
<td>1</td>
<td>mm H2O</td>
</tr>
<tr>
<td>SURLAG</td>
<td>Surface runoff lag coefficient</td>
<td>1 - 24</td>
<td>8</td>
<td></td>
</tr>
</tbody>
</table>

(a) Value that was estimated for the different soil types using a pedotransfer function (Table 12).
(b) Determined in function of land cover and soil type according to Cronshey (1986).

The baseflow alpha factor (ALPHA_BF), first, represents the rate of baseflow response on a changing groundwater table and influences the shape of the recession curve. GW_delay, secondly, is the time required for the water to pass from the subsurface to the shallow aquifer. A lower value, indicating a fast response, brings more seasonal variations into the baseflow. GW_REVAP, further, determines the maximum amount of water from the shallow aquifer that can re-enter the unsaturated zone via capillary fringe or uptake by deep roots ("revap"). As a larger value results in more "revap", the associated baseflow will be lower. GWQMN, the last baseflow parameter, defines when groundwater will contribute to the streamflow or, in other words, when baseflow will occur. Consequently, a larger threshold value limits the baseflow component. The available water capacity (AWC), additionally, influences the amount of water that can be taken up by plants and thus can be transpired. As such, a higher AWC results in more actual evapotranspiration and less river discharge. The curve number (CN2), further, directly affects the amount of runoff. As the retention parameter (equation 3.1) is inversely related to the curve number, a larger CN2 leads to more runoff.
The effective hydraulic conductivity of the main channel (CH_K2), lastly, governs the loss of water out of the streambed to the subsurface of the channel. By increasing this parameter the simulated flow is lagged, the baseflow is increased and streamflow fluctuations are dampened. However, this value should only be greater than zero for ephemeral streams, as perennial streams have a continue groundwater contribution which compensates for the channel losses (Neitsch et al., 2011).

5.5.1.3 Multi-site calibration
Streamflow calibration is often done based on observations at the outlet of the basin (Krause et al., 2005). However, the reliability of distributed large watershed scale models improves by calibrating at multiple site throughout the basin (Ficklin et al., 2013). Such a multi-site approach was used for this reason. In addition, no outlet station is available for the Guayas River basin. To do so, the delineated subbasins were subdivided into three regions associated with the drainage area of the three main rivers (Figure 17). The drainage area of the Chimbo River, where no station is located, was joint with the adjacent drainage area of the Babahoyo River (region 3). The subbasin of the Guayas River was added to region 1 that has the most downstream station and the largest river of the three regions. Within each of these regions, the same parameter values for the different subbasins were used. In a first step, the calibration was done for region 1, using the observations at the “Daule en la Capila” station (Figure 17) and using the initial parameter values from Table 12. This region was selected because it delivers the largest average flow to the outlet.

![Figure 17: Subdivision of the subbasins into three regions with indication of the names of the streamflow stations used during model calibration and evaluation. Numbers indicate the main rivers, being Daule (1), Vinces (2), Babahoyo (3), Chimbo (4) and Guayas (5).](image)

In a second step, the optimised values from the first step were used as initial values to calibrate for the region associated with the Vinces River (region 2), while keeping them constant for the subbasins of region 1. For this second calibration, the “Vinces en Vinces” station (Figure 17) was chosen for three reasons. First, it allows to consider the largest area possible during the calibration. Secondly, the discharge at this station is larger than at the two stations further upstream. A third reason is associated with the objective to simulate pesticide dynamics. As the region between the “Vinces en Vinces” and the “Quevedo en Quevedo” station is the main corn cultivation region, it is important to
simulate the discharge at the “Vinces en Vinces” station correctly. Agriculture upstream of the “Quevedo en Quevedo” station is less intensive and mainly consists of oil palm and cocoa plantations for which no pesticide application is considered. However, there are also some banana, corn and rice fields upstream of the “Quevedo en Quevedo” station. In addition, it is important to keep in mind that errors in the simulated flows at upstream subbasins might be propagated to downstream subbasins. Moreover, the spatial variability of the calibration parameters between the up- and downstream regions is not considered using this approach.

In a third step, only two simulations were run. For the first simulation, the optimised values from step 1 were used for the subbasins of region 1 and 3, while the optimised values from step 2 were used for region 2. For the second simulation, the optimised values from step 2 were used for region 3. The parameter set being superior with respect to the objective functions at the “Zapotal en Lechugal” station (Figure 17) was selected for region 3. The reason that no third calibration was done for this region is the location of the “Zapotal en Lechugal” station. As this station is located quite far upstream, such a calibration could only consider a small, upstream fraction of region 3, contrary to the calibration for the two other regions (Figure 17). Therefore, the two parameter sets from region 1 and 2 were expected to be more representative than a parameter set obtained from a third calibration. Whether this approach to extrapolate spatially lumped parameters from one region to another is legitimate will be pointed out by the evaluation statistics for the “Zapotal en Lechugal” station (section 5.5.2.1). The multi-site approach will be commented in the discussion and suggestions for improvement will be given (section 6.2.3).

5.5.1.4 Calibration steps
The manual calibration was performed in different steps. First, the water balance was inspected as it is crucial for streamflow simulations to correctly balance the water among the hydrological components (Neitsch et al., 2002). However, with respect to the Guayas River basin the available hydrological data are limited to the precipitation, reference evapotranspiration and total streamflow. Consequently, parameters influencing the actual evapotranspiration (e.g. AWC, ESCO (Table 12)) could only be optimised by inspecting the effect on streamflow. Related to the reference evapotranspiration, three calculation methods (Appendix A.2 – A.4) were tested for the calibration period. The method revealing the smallest average difference between the simulated and registered yearly total reference evapotranspiration was selected (Hargreaves method, section 5.5.2.4). The next two steps were performed for each of the three regions (section 5.5.1.3) separately. The second step is used to get a first estimation of the parameter values. This is done by minimising the difference between yearly average simulated and observed streamflow. In a last step, the model is calibrated on a monthly basis. Parameter values are changed one by one to optimise the objective functions, guided by the calculated statistics (NSE and PBIAS), visual inspection of monthly and daily time series and the knowledge on the effect of the parameters (section 5.5.1.2).

5.5.1.5 Evaluation criteria
In order to evaluate the calibrated model, NSE (equation 5.7) and PBIAS (equation 5.8) were calculated both on a daily and a monthly basis for the calibration (1993 – 2000) and validation (2001 – 2009) period for each of the five selected stations (Figure 13-b). These daily and monthly NSE and PBIAS values were compared with the values for watershed scale models recommended by Moriasi et al. (2015), which are based on a meta-analysis of performance data reported in recent literature. As such, model performance was classified as “very good”, “good” and “satisfactory” when daily or
monthly NSE values exceeded 0.80, 0.70 and 0.50 respectively. With respect to daily and monthly PBIAS, the model was rated as “very good”, “good” and “satisfactory” for values smaller than or equal to 5 %, 10 %, and 15 % respectively. When the model performance was appointed a different rating based on the two statistics, the most conservative rating was used. In any case, NSE values below 0.0 and PBIAS values above 30 % are reported to indicate unacceptable model performance (Moriasi et al., 2015).

In addition to the statistics, scatter plots and daily and monthly time series were used as visual inspection, graphical performance measurements being an important validation supplement (Daggupati et al., 2015). The time series enable to (subjectively) evaluate the timing and magnitude of the simulated peak flows and the shape of the recession curve. This all was done for the five selected streamflow stations. To end, the average simulated discharge at the outlet of the basin was inspected and compared with the reported value. With respect to the non-selected stations, no evaluation statistics were calculated because of the presence of many data gaps (Figure 14). In addition, these stations were not included in the model during the watershed delineation and thus no streamflow simulations were available at the location of these stations.

5.5.2 Hydrological model performance and simulations
The calibrated parameters values resulting from the manual streamflow calibration are given in Appendix D and will be discussed in section 6.2.3. Below, the calibrated model will be evaluated using the approach outlined in the previous section. First, the evaluation statistics will be discussed for all stations and for both periods. Secondly, the graphical evaluation will be illustrated for the “Daule en la Capilla” station. Thereafter, the streamflow simulations at the outlet of the basin will be shortly addressed. To end, the water balance and sediment yield, simulated using the calibrated model, will be commented.

5.5.2.1 Statistical evaluation
Table 13 and 14 summarise the evaluation criteria for the calibration period and validation period respectively. As can be seen, the model performance on a daily basis, on the one hand, is classified as unsatisfactory for all the stations except for “Daule en La Capilla” during the calibration period and “Vinces en Vinces” during the validation period. The model performance on a monthly basis, on the other hand, is very good during the calibration period for “Daule en La Capilla” and “Quevedo en Quevedo”. The performance is classified as satisfactory for “Baba dam” and “Vinces en Vinces” and unsatisfactory for “Zapotal en Lechugal” for the calibration period. The performance during validation is rated as very good for “Vinces en Vinces” and “Zapotal en Lechugal”, as good for “Daule en La Capilla” and as unsatisfactory for “Baba dam” and “Quevedo en Quevedo”. Besides, it has to be noted that the difference in average registered streamflow during the calibration and validation period (Tables 13 and 14) is explained by the occurrence of an El Niño event during the calibration period.
Interesting features appear when calculating the monthly statistics for low and high flow periods separately, with the average registered flow during the calibration or validation period as a threshold (Appendix E). First of all, the fact that these statistics are worse than the overall statistics demonstrates that errors during low and high flow periods are compensated in the evaluation metrics. In addition, PBIAS values are remarkably higher in absolute value during low flow than high flow periods. Reasons for this are the smaller denominator for low flow periods (equation 5.8) and the fact that the baseflow is underestimated at some stations (see below). Moreover, the unexpected trend of better overall validation than calibration statistics that is observed for “Vinces en Vinces” and “Zapotal en Lechugal” (Tables 13 and 14), is only true for high flow periods. For low flow periods, the NSE and PBIAS values are better than validation for virtually all stations (Appendix E). To end, it has to be noted that the threshold that separates low and high flows differs for both periods.

### 5.5.2.2 Graphical evaluation

Daily and monthly time series and scatter plots for the five stations and the two periods are given in Appendix F.1 – F.4 and G.1 – G.4 respectively. In this section, the evaluation of the streamflow simulations using these plots will be illustrated for the “Daule en La Capilla” station. To facilitate this, the monthly time series for this station are also shown in Figures 18 and 19. Visual inspection of Figure 18 learns that the simulated streamflow follows the observed trends quite well. This agrees with the ratings based on the monthly statistics (very good) (Table 13) and the scatter plot with 0.999 as slope of the regression line (Figure G.3.2). However, the scatter plot indicates an underestimation when the streamflow is below 300 m³ s⁻¹, which can also be observed on the time series. This underestimation during low flow periods is also observed at other stations, especially at the “Baba

### Table 13: Evaluation criteria with indication of model performance according to Moriasi et al. (2015) and average registered streamflows (Qav: whole period, dry: dry season, rainy: rainy season) for the calibration period (1993 – 2000). The stations for which manual calibration was done are indicated in grey. NSE: Nash-Sutcliffe efficiency (equation 5.7), PBIAS: percent bias (equation 5.8).

<table>
<thead>
<tr>
<th>Station</th>
<th>NSE daily</th>
<th>PBIAS daily [%]</th>
<th>NSE monthly</th>
<th>PBIAS monthly [%]</th>
<th>Qav [m³ s⁻¹]</th>
<th>Qav dry [m³ s⁻¹]</th>
<th>Qav rainy [m³ s⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baba dam</td>
<td>0.26 (US)</td>
<td>15 (S)</td>
<td>0.71 (G)</td>
<td>14 (S)</td>
<td>126</td>
<td>57</td>
<td>195</td>
</tr>
<tr>
<td>Daule en La Capilla</td>
<td>0.52 (S)</td>
<td>-1 (VG)</td>
<td>0.82 (VG)</td>
<td>-1 (VG)</td>
<td>412</td>
<td>256</td>
<td>561</td>
</tr>
<tr>
<td>Quevedo en Quevedo</td>
<td>0.35 (US)</td>
<td>4 (VG)</td>
<td>0.80 (VG)</td>
<td>4 (VG)</td>
<td>260</td>
<td>93</td>
<td>431</td>
</tr>
<tr>
<td>Vinces en Vinces</td>
<td>0.29 (US)</td>
<td>-15 (S)</td>
<td>0.62 (S)</td>
<td>-14 (S)</td>
<td>267</td>
<td>120</td>
<td>412</td>
</tr>
<tr>
<td>Zapotal en Lechugal</td>
<td>0.44 (US)</td>
<td>16 (US)</td>
<td>0.80 (VG)</td>
<td>16 (US)</td>
<td>235</td>
<td>91</td>
<td>379</td>
</tr>
</tbody>
</table>

VG: very good, G: good, S: satisfactory, US: unsatisfactory

### Table 14: Evaluation criteria with indication of model performance according to Moriasi et al. (2015) and average registered streamflows (Qav: whole period, dry: dry season, rainy: rainy season) for the validation period (2001 – 2009). The stations for which manual calibration was done are indicated in grey. NSE: Nash-Sutcliffe efficiency (equation 5.7), PBIAS: percent bias (equation 5.8).

<table>
<thead>
<tr>
<th>Station</th>
<th>NSE daily</th>
<th>PBIAS daily [%]</th>
<th>NSE monthly</th>
<th>PBIAS monthly [%]</th>
<th>Qav [m³ s⁻¹]</th>
<th>Qav dry [m³ s⁻¹]</th>
<th>Qav rainy [m³ s⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baba dam</td>
<td>0.29 (US)</td>
<td>19 (US)</td>
<td>0.79 (G)</td>
<td>19 (US)</td>
<td>91</td>
<td>27</td>
<td>155</td>
</tr>
<tr>
<td>Daule en La Capilla</td>
<td>0.45 (US)</td>
<td>-1 (VG)</td>
<td>0.70 (G)</td>
<td>-2 (VG)</td>
<td>220</td>
<td>113</td>
<td>328</td>
</tr>
<tr>
<td>Quevedo en Quevedo</td>
<td>0.38 (US)</td>
<td>21 (US)</td>
<td>0.68 (S)</td>
<td>20 (US)</td>
<td>199</td>
<td>46</td>
<td>357</td>
</tr>
<tr>
<td>Vinces en Vinces</td>
<td>0.61 (S)</td>
<td>6 (G)</td>
<td>0.87 (VG)</td>
<td>5 (VG)</td>
<td>185</td>
<td>51</td>
<td>312</td>
</tr>
<tr>
<td>Zapotal en Lechugal</td>
<td>0.41 (US)</td>
<td>-2 (VG)</td>
<td>0.83 (VG)</td>
<td>-2 (VG)</td>
<td>128</td>
<td>26</td>
<td>230</td>
</tr>
</tbody>
</table>

VG: very good, G: good, S: satisfactory, US: unsatisfactory
Despite this underestimation, PBIAS values for the “Daule en La Capilla” station are negative, which can be explained by the overestimated peak flow in 1998 (Figure 18). During other years, the peak flow volume agrees quite well with the observations (in 1995, 1996) or is underestimated (e.g. in 1993). The overestimation of the peak flow during the 1998 El Niño event and the underestimation of peak flows during the other calibration years are observed at all other stations (Appendix F.3). When the statistics (NSE and PBIAS) are calculated for low and high flow periods separately (Table E.1), the underestimation of the baseflow at “Daule en La Capilla” and “Baba dam” is confirmed by the highly positive PBIAS values. In addition, the NSE values at these stations indicate better performance during high flow periods. A last remark with respect to the monthly time series for the calibration period is that the slope of the recession curve is sometimes not steep enough (e.g. in 1998).

The observed trends (underestimation of the baseflow and lag of the recession curve) are accentuated during the validation period (Figure 19). Also here, the performance is better during high flow periods (Table E.2). Despite the underestimation of the baseflow, the overall PBIAS is again negative because of the overestimated peak flows. The overestimated peak flows are not observed at other stations, where, on the contrary, the peak flow is often underestimated, e.g. at “Quevedo en Quevedo” (Figure F.4.3). Neither the lag of the recession curve is observed for the other stations, only at the “Zapotal en Lechugal” station the slope of the recession curve is also slightly too weak (Figure F.4.5). These differences in simulation trends can be explained by the fact that the other three stations are located in region 2, for which other parameters values were used (Appendix D). The higher baseflow alpha factor causes a different shape of the recession curve and the lower curve number value results in less runoff and thus lower peak flow volumes.
Figure 19: Monthly time series for the “Daule en la Capilla” station during the validation period (2001 – 2009).

5.5.2.3 Streamflow at the outlet of the basin

As already mentioned, the reported average discharge at the outlet of the basin is 974 m$^3$ s$^{-1}$. As not more information is available, only the average simulated discharge at the outlet can be compared with this reported value. The average simulated discharge at the outlet is 1353 m$^3$ s$^{-1}$, 770 m$^3$ s$^{-1}$ and 1045 m$^3$ s$^{-1}$ for the calibration, the validation and the whole simulation period respectively. Especially the simulated average for the whole simulation period is close to the reported value. This gives an indication that the order of magnitude of the simulated flow at the tributary of the Guayas where no station is located (i.e. the Chimbo River) is realistic.

5.5.2.4 Water balance and sediment yield

Table 15 presents the yearly simulated amount of the different hydrologic components, averaged over the simulation period. The total water yield, i.e. the total amount of water contributing to the streamflow, is equal to the sum of the (surface) runoff, the lateral flow and the groundwater flow. The total precipitation is equal to the sum of the runoff, the lateral flow, the total recharge of the aquifers and the actual evapotranspiration. The total aquifer recharge differs from the groundwater flow as the groundwater table can deviate between the start and the end of a simulated year. A second reason is the fact that the model considers the water that enters the deep aquifer as lost from the watershed (Neitsch et al., 2011).

Table 15: Simulated average yearly water balance for the period 1993 – 2009. Values are normalised by the area of the watershed.

<table>
<thead>
<tr>
<th>Hydrological component</th>
<th>Depth [mm year$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Precipitation</td>
<td>2097</td>
</tr>
<tr>
<td>Surface runoff</td>
<td>536</td>
</tr>
<tr>
<td>Lateral flow</td>
<td>183</td>
</tr>
<tr>
<td>Groundwater flow (shallow and deep aquifer)</td>
<td>311</td>
</tr>
<tr>
<td>Total water yield</td>
<td>1030</td>
</tr>
<tr>
<td>Reference evapotranspiration</td>
<td>1495</td>
</tr>
<tr>
<td>Actual evapotranspiration</td>
<td>919</td>
</tr>
<tr>
<td>Total aquifer recharge (shallow and deep aquifer)</td>
<td>455</td>
</tr>
</tbody>
</table>
As already mentioned, only the total streamflow and the reference evapotranspiration can be compared with observed values (section 5.5.1.4). With respect to the reference evapotranspiration, the difference between the registered and simulated yearly total reference evapotranspiration, averaged over the calibration period and for the five stations and normalised for the average registered reference evapotranspiration (1217 mm), is 38 %, 24 % and -21 % for simulations using the Penman-Monteith, Priestley-Taylor and Hargreaves method respectively. Based on this, the temperature-based Hargreaves method was selected. The reference evapotranspiration is overestimated by this method, contrary to the two other methods.

The simulated yearly average sediment yield, to end, amounts to 230,000,000 tons sediment year\(^{-1}\) for the whole basin. This is much more than the maximal reported value, which is 4,900,000 tons sediment year\(^{-1}\) at the “Daule en La Capilla” station (section 5.2.5.2). However, as the available sediment data were limited and no sediment calibration was possible, this potential overestimation of the sediment yield was not further adjusted.

5.5.3 Pesticide simulations

The evaluated hydrological model was used to run simulations for two pesticides. The aim of these simulations is to obtain an insight into the system dynamics and model functioning. In this section, the assumptions made to deal with the limited application data will be listed. Thereafter, details about implementing the pesticide application and running the model will be given. Thirdly, a selection of the simulations will be analysed in detail. Lastly, the agreement of the pesticide simulations results with the outcome of the sampling campaign will be discussed. A short description of the implementation of pesticide specific processes was given in section 4.1.

5.5.3.1 Input data assumptions

As the available information on pesticide application practices in the Guayas River basin is limited (section 5.2.4.2), four major assumptions were made:

1. Each farmer has the same practices as the farmer that was interviewed. As no information could be gathered with respect to the practices on small farms, no distinction was made between small and big farms. In addition, the application rates (AR) from the interviews were considered to be the effectively applied rates.

2. The farmers comply with the recommended AR. This assumption applies only with respect to the crops (banana and rice) for which no other than the recommended AR was available.

3. There is no spatial variability in application practices for banana and sugar cane. For rice, the spatial variability was limited to a distinction between the provinces Guayas and Los Rios. For corn, spatial variability with respect to the cultivation cycles was taken into account (see below).

4. The pesticides were applied only to the crops reported in Tables 8 and 9.

Because the application timing is not as explicit as required, the first day of the week was taken when the application timing is expressed in weeks (banana). For corn, moreover, the seeding timing was assumed to be on the 20\(^{th}\) of the given months and the pesticide application was assumed to be two days after the seeding. In the case of sugar cane, the 15\(^{th}\) day of the given months was taken.
To recalculate the AR, which is given in litres of commercial product per hectare, to kg of active ingredient (AI) per hectare, equation 5.9 and the concentrations given in Table 16 were used. This resulted in the AR presented in Table 17.

\[
\text{AR} \left[ \frac{\text{kg AI}}{\text{ha}} \right] = \text{AR} \left[ \frac{\text{L product}}{\text{ha}} \right] \times \text{concentration} \left[ \frac{\text{g AI}}{\text{L product}} \right] \times 0.001 \left[ \frac{\text{kg}}{\text{g}} \right]
\]  
(5.9)

Table 16: Concentrations of active ingredient (AI) in commercial pesticide products (MAGAP and Agrocalidad (2016)).

<table>
<thead>
<tr>
<th>Product</th>
<th>Concentration [g AI L product⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volley</td>
<td>880</td>
</tr>
<tr>
<td>Gramilaq 400 EC</td>
<td>400</td>
</tr>
</tbody>
</table>

Table 17: Pesticide application timing, application rates (AR), cultivation area and slope classes for the different crops for which pesticide application was implemented. P: pendimethalin, AI: active ingredient, F: fenpropimorph.

<table>
<thead>
<tr>
<th>Land use</th>
<th>Timing P</th>
<th>AR P [kg AI ha⁻¹]</th>
<th>Timing F</th>
<th>AR F [kg AI ha⁻¹]</th>
<th>Area [km²]</th>
<th>Slope class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Banana</td>
<td>-</td>
<td>-</td>
<td>29/12 – 4/1, 2 – 8/2, 20 – 26/4, 1 – 7/6, 15 – 21/6</td>
<td>-</td>
<td>0.44</td>
<td>801</td>
</tr>
<tr>
<td>Corn</td>
<td>22 – 28/6, 22 – 28/12</td>
<td>0.8</td>
<td>17 – 23/7</td>
<td>-</td>
<td>2,925</td>
<td>90 % &lt; 10 %</td>
</tr>
<tr>
<td>Rice</td>
<td>8 – 14/10</td>
<td>0.1 or 0.2</td>
<td>-</td>
<td>-</td>
<td>3,033</td>
<td>Always &lt; 10 %</td>
</tr>
<tr>
<td>Sugar cane</td>
<td>15 – 21/1, 15 – 21/6, 15 – 21/7, 15 – 21/8, 15 – 21/9, 15 – 21/10, 15 – 21/11, 15 – 21/12</td>
<td>1.2</td>
<td>-</td>
<td>-</td>
<td>543</td>
<td>60 % &lt; 10 %</td>
</tr>
</tbody>
</table>

A second aspect related to the AR is the fact that multiple days are needed for one farm to apply the doses. Especially when no machines are used, this task can take up to one week (information from farmers). To approximate this in the model, which only considers pesticide application at the HRU level, the AR were divided by seven and applied during seven successive days, starting on the dates mentioned above. In the meantime, this allows to add variation in application timing between the different farms of the same HRU into the model. Table 17 presents the timing as implemented in the model.

Concerning the cultivation cycles of corn and rice, the harvest frequency depends on the availability of irrigation equipment, in contrast to banana and sugar cane. Without irrigation these crops can only be grown during the rainy season and, consequently, only during the rainy season pesticides will be applied. With irrigation equipment, which is the case for the farms where the information was gathered, pesticides might be applied in both seasons. This is the case for pendimethalin on corn fields (Table 17). In order to have an estimation of the area of corn fields equipped with irrigation, the comparison was made between dry and rainy season corn productivity [tons] as reported by Castillo (2013) for the period 2009 - 2012 and for three provinces. If one assumes the productivity per unit of area to be constant, the percentage of area with irrigation is obtained by dividing the dry season productivity by the rainy season productivity. This resulted in 14, 25 and 3 % of the corn area for the Guayas, Los Rios and Manabi province respectively. The HRUs of the model for which the application of pendimethalin was implemented twice per year were selected based on these percentages per province. On rice fields, in contrast, pendimethalin is, according to the available data, only applied during the rainy season – even for farms with irrigation equipment.
5.5.3.2 Methodology

The pesticide application was implemented in the model as a “management operation” for each of the crops listed in Table 17. More specifically, the AR, the active ingredient and the date of application were written to the model input files of all HRUs that have one of these crops as land use. Meanwhile, the spatial variation for corn (one or two cultivation cycles) and in AR for rice (the AR in Los Rios is twice the amount of the one in Guayas) was taken into account. Important in this respect is that SWAT provides two methods to schedule management operations, either by a heat index or by dates. The heat index, which is the default method, is calculated by summing the heat units of every day. Daily heat units are equal to the difference between the average daily temperature and a crop-specific base temperature. As such, operations, e.g. planting and harvesting, are defined as a function of these accumulated heat units (Neitsch et al., 2011). This default method was used during the calibration of the hydrological model. However, as the application data for the pesticides are expressed in days, the second method was chosen for the pesticide simulations i.e. the scheduling by dates. Unfortunately, SWAT allows the use of only one method for all the operations within one HRU. Therefore, also the planting and harvest timing needed to be rescheduled by date for the HRUs for which pesticide application was considered. As this influences the evapotranspiration calculations and potentially the streamflow simulations, the monthly NSE and PBIAS for streamflow were examined for the model extended for pesticide simulations.

Pesticide properties needed for the simulations of the land use phase and transport of the pesticides were taken from the SWAT database or online databases for pendimethalin and fenpropimorph respectively (Table 18). Default parameters values were used for the routing of the pesticides.

Table 18: Pesticide properties for fenpropimorph (F) and pendimethalin (P) as implemented in the model.

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>P (a)</th>
<th>F (b)</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>SKOC</td>
<td>Soil adsorption coefficient normalized for soil organic carbon content</td>
<td>5000</td>
<td>2401</td>
<td>(mg kg⁻¹)(mg L⁻¹)⁻¹</td>
</tr>
<tr>
<td>WOF</td>
<td>Fraction of the pesticide on the foliage that is washed-off</td>
<td>0.4</td>
<td>0.4</td>
<td>-</td>
</tr>
<tr>
<td>HLIFE_F</td>
<td>Degradation half-life of the pesticide on the foliage</td>
<td>30</td>
<td>2</td>
<td>days</td>
</tr>
<tr>
<td>HLIFE_S</td>
<td>Degradation half-life of the pesticide in the soil</td>
<td>90</td>
<td>26</td>
<td>days</td>
</tr>
<tr>
<td>AP_EP</td>
<td>Application efficiency</td>
<td>0.75</td>
<td>0.75</td>
<td>-</td>
</tr>
<tr>
<td>WSOIL</td>
<td>Solubility of the pesticide in water</td>
<td>0.28</td>
<td>4.32</td>
<td>mg L⁻¹</td>
</tr>
</tbody>
</table>

(a): Source: SWAT pesticide database

To end, it should be noted that no difference was made between corn and sweet corn with respect to the pesticide practices. In addition, the use of sugar cane as crop for the more general “industrial semi-permanent crops” class of the land use map (look up table on Figure 15) implies that pesticide application for sugar cane occurred both on the sugar cane fields in the south of the basin (shown in Figure 8) and on the industrial crop fields, which are located upstream of the “Zapotal en Lechugal” station and are not shown in Figure 8. The total area on which pesticides were applied are given in Table 17.

Once the pesticide application was implemented, several simulations were run in order to obtain insight into the pesticide dynamics (temporal and spatial variation), the importance of the different crops and the influence of pesticide practices (AR), system characteristics (presence of lakes) and pesticide properties. As the hydrological model performance was rated as unsatisfactory on a daily basis, the model was run using a monthly time step. Simulations were done for the year 2009, assuming that this year represents normal conditions with respect to pesticide transport and fate, as the average daily precipitation during this year (4 mm day⁻¹) is the median value of the yearly
averages of the daily precipitation during the nine validation years. The pesticide output of a subbasin, given in total mass of dissolved pesticides transported with the streamflow, was recalculated to concentration using the streamflow simulations (equation 5.10).

\[ C = \frac{M}{Q \cdot S} \]  

(5.10)

Where \( C \) the average pesticide concentration at the outlet of a subbasin for a given month \([\text{mg} \, \text{m}^{-3}]\) or \([\mu \text{g} \, \text{L}^{-1}]\), \( M \) the total simulated dissolved pesticide mass at that subbasin’s outlet during that month \([\text{mg} \, \text{month}^{-1}]\), \( Q \) the average monthly streamflow at the subbasin’s outlet during the month \([\text{m}^3 \, \text{s}^{-1}]\) and \( S \) the number of seconds in that month \([\text{s} \, \text{month}^{-1}]\).

5.5.3.3 Analysis of the pesticide simulations

In this section four pesticide simulations will be discussed in detail. Three simulations were run considering pendimethalin application practices (Table 17) at corn fields (simulation 1), at corn and rice fields (simulation 2) and at corn, rice and sugar cane fields (simulation 3). Thereafter, the model was run for fenpropimorph application practices at banana and corn fields (simulation 4). As there are 29 subbasins (Figure 16), 29 pesticide concentrations were obtained per month for each of these simulations. The analysis focussed on the simulations at three streamflow stations (“Daule en La Capilla”, “Vinces en Vinces” and “Zapotal en Lechugal”) (Figure 21) and the outlet of the watershed. In addition, the spatial variation between the 29 simulations was examined for the month during which the concentration was maximal for most of the subbasins. The discussion of the four simulations will focus on the explanation of observed trends, e.g. seasonal variation. Moreover, for simulation 3 and 4 the recalculated monthly PBIAS and NSE values for the models extended with the pesticide application practices will be compared to the original values. This is because the change in management scheduling method can influence the streamflow simulations (section 5.5.3.2). The last paragraph of this section will shortly describe the outcomes of additional simulations.

Simulation 1, for which pendimethalin application at corn farms was implemented, demonstrates the importance of runoff as transport route, the difference in simulation trends between pesticide mass and concentration, and the low pesticide transport during the dry season. To illustrate this, the simulations at the “Vinces en Vinces” station, located downstream of the main corn cultivation region (Figure 21), are depicted in Figure 20. On this figure the relationship between simulated runoff and transported pesticide mass becomes clear. The absence of a mass peak in May can be explained by the long time interval after application and the transport of the pesticide to the rivers during the preceding months. The decline in concentration in February and the small concentration peak in May are due to an increase or decrease in streamflow, and associated dilution or upconcentration effects (Figure 20-b,d). A last remark with respect to Figure 20 is that the application during the dry season does not cause an increase in surface water pesticide concentrations, explained by the absence of the wash-off from the pesticides on the crops to the soil (which occurs only when the precipitation exceeds a certain threshold, section 4.1) and the low runoff and lateral flow rates.

The simulated concentrations for the different subbasins are maximal in February or March, when precipitation and runoff are maximal. Peak concentrations occur earlier in subbasins located in the eastern part of the basin, where the rainy season starts earlier. The highest concentrations occur downstream of the main corn cultivation region and are subsequently diluted (Figure 21). The maximal concentration was simulated at “Vinces en Vinces”.

50
Figure 20: Monthly average precipitation, runoff and lateral flow normalised by the subbasin area (a.), monthly average streamflow (b.), total dissolved pendimethalin mass transported with streamflow and indication of application rate, where dotted line indicates that the application occurs only at a fraction of the HRUs (c.), and calculated monthly average pendimethalin concentrations (d.) at the “Vinces en Vinces” station for simulation 1.

Figure 21: Location of the five streamflow stations and indication of simulated pendimethalin concentration range (diamonds, green: low, yellow: moderate, red: high concentration) for simulation 1 (March 2009). Numbers indicate the Daule Peripa Dam (1) and the main rivers, being Daule (2), Vinces (3), Babahoyo (4), Chimbo (5) and Guayas (6).
For a second simulation, the pendimethalin application at rice and corn fields was considered. However, no difference in pesticide concentrations was observed compared to simulation 1 (figure not shown). This learns that, according to the simulations, the contribution of pesticide practices at rice fields to the pendimethalin input into the rivers is negligible. This has several reasons. First, the AR is low compared to the other crops and the application occurs during the dry season (Table 17). In addition, rice is always cultivated in flat areas and consequently all rice HRUs have a slope class lower than 10 %, which implies low runoff rates.

Simulation 3, for which pendimethalin application at corn, rice and sugar cane fields is implemented, demonstrates that pesticide practices at sugar cane farms, in contrast to the rice farms, have major but localised contributions to the pesticide input into the rivers. These are explained by the high AR and application frequency, and the large fraction of HRUs with a slope above 10 % (40 % in area), implying high runoff rates (Table 17). Consequently, there is no influence of the sugar cane practices on the simulation pesticide concentration in the Daule and Vinces Rivers, due to the absence of sugar cane fields in the drainage area of these rivers (Figure 21). At the “Zapotal en Lechugal” station, in contrast, the strong influence of the sugar cane practices becomes clear (Figure 22). This is explained by the industrial semi-permanent crop fields, located upstream of “Zapotal en Lechugal” and implemented as sugar cane into the model (not shown in Figure 21, see previous section). The simulated concentrations at this station are many times higher compared to simulation 1 (only application on corn fields), e.g. 140 times higher for July. Interestingly, an enormous concentration peak appears in December at this station (Figure 22-d), originating from sugar cane practices. This peak cannot be explained by an increase in runoff, even more, the simulated runoff for this subbasin is equal to zero from July onwards. The lateral flow, however, increases slightly (7 times higher with respect to the previous month, not visible on Figure 22). The precipitation, on the contrary, increases strongly in December and explains the difference in transported pesticide mass compared to the previous months. The reason that the transported mass was negligible during the previous months is that the precipitation threshold (2.54 mm day$^{-1}$) for the simulation of wash-off was never exceeded during these months. As no pendimethalin was present on the soil, except for the fraction that immediately reached the soil during application, no pendimethalin could be transported to the rivers. When the threshold was exceeded in December, the accumulated amount of pendimethalin present on the crops was washed-off and transported to the river by lateral flow. Because the streamflow in December is low, this mass was not diluted, resulting in a very high concentration. When the same simulation was done for 2008, this December peak was not observed. This is explained by the fact that 2008 is a wetter year than 2009, exceeding the threshold for wash-off during most of the months. Whether this is realistic will be discussed in section 6.1.2.

When comparing the simulations at the different subbasins of the Babahoyo River, the simulated concentrations gradually decrease from upstream to downstream because of dilution, degradation and diffusion processes. However, the very high December peak is still visible at the outlet of the watershed. The simulated concentrations were maximal in February for all subbasins, except for the Babahoyo River (as discussed). The largest concentrations were observed downstream of the two sugar cane cultivation regions (Babahoyo and Chimbo Rivers).

With respect to the calculation of the monthly NSE and PBIAS values, to end, the maximal deviation of NSE, compared to NSE calculated for the calibrated hydrological model for the year 2009, is 0.01. The maximal deviation of the PBIAS values is 1 %.
Figure 22: Monthly average precipitation, runoff and lateral flow normalised by the subbasin area (a.), monthly average streamflow (b.), total dissolved pendimethalin mass transported with streamflow and indication of application rate, where dotted lines indicate that the application occurs only at a fraction of the HRUs (c.), and calculated monthly average pendimethalin concentrations (d.) at the “Zapotal en Lechugal” station for simulation 3.

Related to simulation 4, implementing the fenpropimorph application practices at banana and corn farms as given in Table 17, several aspects will be discussed, being the difference in contribution of pesticide transport to the rivers between banana and corn farms, the correlation between runoff and simulated pesticide mass, the comparison with the pendimethalin concentrations and the transport of the pesticides to the outlet of the river basin.

The contribution of corn farms practices to the river pesticide concentrations, on the one hand, is negligible. This is observed at the “Daule en La capilla” and “Zapotal en Lechugal” stations, located on rivers that do not have banana farms in their catchment (Figure 21). The reason for the negligible contribution is that fenpropimorph is – according to the available data – applied during the dry season on corn fields, during which there is no wash-off and runoff and lateral flow are low. More upstream on the Daule River, however, a low peak is simulated for December. Thus, the beginning of the rainy season induces the transport of the remainder of the fenpropimorph applied in July to the rivers. The pesticide practices at banana plantations, on the other hand, have a larger contribution. This is observed at “Vinces en Vinces”. Again, a relationship between runoff and simulated pesticide mass is observed (Figure 23-a,c), being, however, less pronounced than was the case with simulation 1 (Figure 20). This is explained by the distance between the banana plantations, located upstream of “Quevedo en Quevedo”, and the “Vinces en Vinces” station (Figure 21). More specifically, the precipitation and runoff are maximal in February for the subbasin where the banana farms are located, which explains the occurrence of a pesticide mass peak in February and not in March (Figure 23-c). The small concentration peak in May is due to the decline in streamflow, confirmed by the absence of a mass peak. The pesticides applied during the dry season are not transported to the rivers because of the low precipitation, lateral flow and runoff (Figure 23-a,c).
As was the case with pendimethalin, the application during the dry season does not cause an increase in pesticide concentration. In addition, the fenpropimorph application practices have a smaller contribution to surface water pesticide concentration compared to pendimethalin. This is due to the location of the banana fields further from the station and their smaller area (Table 17). It is not because of the pesticide properties, as pendimethalin has a higher soil adsorption coefficient than fenpropimorph, and thus has a lower tendency to be dissolved into the water phase (Table 18).

The simulated fenpropimorph concentrations at the outlet of the Guayas River basin (Figure 24) are the result of the fenpropimorph transport via the Vinces, Babahoyo (transport from more downstream than “Zapotal en Lechugal”) and Chimbo Rivers, all coming from banana plantations except for the minor peak in November. This November peak results from the application at sweet corn farms and the subsequent transport via the Chimbo River. The fact that fenpropimorph is already mobile in November is due to the location of these corn field in the Andes region where precipitation is higher because of orographic effects. The concentrations at the outlet are due to transport from upstream subbasins, being the reason that the concentrations not fully correspond with the runoff simulated for the outlet’s subbasin. For all subbasins, the simulated concentrations are maximal during February, except for the minor December peaks at some locations along the Daule River. The simulated February concentrations are the highest upstream of the Vinces River and downstream of the Babahoyo River, associated with the location of the banana plantations.

With respect to NSE and PBIAS, the deviations were larger than was the case with the model extended for pendimethalin application (simulation 3). The monthly NSE and PBIAS values changed maximally by 0.03 and 2 % respectively.
Subsequent simulations consider a change in AR, a change in the fraction of the subbasins that drains into a lake and a change in pesticide properties. Changing the AR, first, resulted in a proportional change in simulated concentrations for the subbasins located near the agricultural areas. The effect was less pronounced for more downstream subbasins. Increasing the fraction of the subbasins that drains into a lake, secondly, decreased the simulated concentration at some of the subbasins, while having a negligible effect on the simulated streamflow. This decrease is due to the retention and degradation of the fraction of the pesticides that is not transported to the rivers but to the lakes. The fact that this effect was not observed everywhere is because the lakes are only implemented for a few subbasins. With respect to the pesticide properties, lastly, the effect of the soil adsorption coefficient normalised for soil organic carbon content (SKOC), the degradation half-life of the pesticide on the foliage (HLIFE_F) and in the soil (HLIFE_S) and the solubility of the pesticide in water (WSOL) was tested. As expected, a doubled SKOC resulted in lower concentrations. The simulated concentrations halved at some subbasins but the effect at other subbasins was less pronounced. When a negligible degradation during the land phase was considered, by setting the half-lives to 1000, the maximal simulated concentrations increased by up to three (pendimethalin) and seven (fenpropimorph) times. Logically, the effect of ignoring the land phase degradation is more pronounced when the time lag between pesticide application and pesticide transport is larger. Halving the water solubility had no effect, indicating that the concentration of the pesticides during the land phase did not reach the solubility limit.

5.5.3.4 Comparison with the results of the sampling campaign

The comparison of the model outcome with the measured concentrations should be done with care, as the year is different (2009 versus 2016). Moreover, Figure 21 depicts the simulated concentrations during the wet season while the sampling campaign was done during the summer (Figure 12) (section 5.2.4.1). In addition, the locations of the sampling campaign not always agree with those of the simulations and the sampling density along the Vinces River was low. Nevertheless, the fact that simulated pendimethalin concentrations during the dry season are not zero for the Daule River, in
contrast to the Babahoyo and Chimbo Rivers, indicates a certain agreement with the many pendimethalin detections for the downstream region of the Daule River (Figure 12). The high measured pendimethalin concentration sampled at the Babahoyo River (black circle on Figure 12) was, however, not observed for the simulations. As this sample was taken in a rice cultivation region, this might indicate that the simulation underestimate the contribution of the pesticide application at rice farms. With respect to fenpropimorph, the many detections in the upstream region of the Daule River (Figure 12) do not agree with the simulated concentrations in the Daule River that are zero (simulation 4). This might indicate that the available data about the timing of fenpropimorph application at corn fields (only during the dry season when pesticide transport is negligible) is not correct. Another plausible explanation is that fenpropimorph is also applied for other crops than banana and corn, which is suggested by the two highest measured concentrations, both sampled in the vicinity of cocoa farms (red crosses on Figure 12). To end, both the simulated and the measured concentrations are higher for pendimethalin than fenpropimorph.
6 Discussion

In this chapter, four aspects will be discussed. First, model calibration and pesticide simulation results will be commented. In a second section, the methodology used to apply the Soil and Water Assessment Tool (SWAT) for the case study will be discussed and suggestions for improvement will be formulated. Thirdly, an evaluation of SWAT and future perspectives for the Guayas River basin will be given. Lastly, implications of the pesticide simulations analysis for river management within the Guayas River basin will be formulated.

6.1 Model outcome

6.1.1 Model performance

The evaluation of the hydrological model performance will be analysed in more detail in this section. On a daily basis, first, low Nash-Sutcliffe efficiency (NSE) values were obtained (Tables 13 and 14). This can be due to data limitations, e.g. low resolution of the soil map and potentially low daily accuracy of the WFDEI dataset (section 6.2.1). Another reason might be the level of detail of the model structure, however, the effect on streamflow simulations is expected to be small (section 6.2.2). Furthermore, the calibration was done on a monthly basis and probably with a too limited spatial variability to have a good daily model performance (section 6.2.3).

The monthly performance of the model, secondly, is satisfactory or better for most of the stations (Tables 13 and 14), possibly due to a good monthly performance of the WFDEI dataset. It should be noted, however, that the use of this dataset forms a plausible reason for the overestimated streamflow during the 1998 El Niño event at all stations (Appendix F.3). Indeed, the average daily corrected WFDEI precipitation during this year (12.6 mm day$^{-1}$) is twice as much compared to the stations (5.9 mm day$^{-1}$). The high positive percent bias (PBIAS) values that were obtained at some stations indicate an underestimation of the streamflow. There was an underestimation of the baseflow (“Baba Dam”), the peak flows (“Zapotal en Lechugal”) or both (“Quevedo en Quevedo”) (Appendix E) which indicates some shortcomings of the model, e.g. inadequate simulation of the groundwater processes at the “Baba Dam” station. However, it is important to remember that no information was available about the accuracy of the streamflow measurements and measurement errors might also contribute to the high PBIAS values (David, 2014). The increasing trend of the streamflow registered at the “Quevedo en Quevedo” station, for example, might indicate inaccurate measurements (e.g. outdated Q,h-relationships). In addition, the effect of the data gaps in the registered streamflow dataset on the streamflow statistics could be questioned. However, no trend was observed when plotting the statistics as a function of the data gap percentage. Lastly, a better balance between the NSE and PBIAS values during calibration might reduce the high PBIAS values.

When comparing the monthly statistics between the calibration and validation period, it is remarkable that, first, the statistics are not always better during calibration than validation, contrary to the expectations (Moriasi et al., 2007). Even more, the validation ratings for the “Vinces en Vinces” station and “Zapotal en Lechugal” station are the same or better (up to three classes) than the calibration ratings. This might be because of errors in the registered streamflow data during the calibration period. The validation ratings for the “Baba dam” and “Daule en La Capilla” stations, on the contrary, are equal to or one class worse than the calibration ratings. The trend between calibration and validation rating is thus not dependent on whether the station was used during calibration. However, at the “Quevedo en Quevedo” station, which was not used during calibration,
the performance is worse during validation than during calibration. With respect to the “Zapotal en Lechugal” station, located in region 3 for which the parameters from region 1 were extrapolated, the bias during calibration indicates a low performance but the performance during validation is very good. A second observation is that the stations performing very good during the calibration period (“Daule en La Capilla” and “Quevedo en Quevedo”) are different from the stations with a very good rating during the validation period (“Vinces en Vinces” and “Zapotal en Lechugal”). An explanation is that the model performance at “Daule en La Capilla” and “Quevedo en Quevedo” is better during high flow periods (Appendix E) and high flow is more pronounced during the calibration period.

Taking into account the good ratings for the station with the largest discharge (“Daule en La Capilla”), the fact that the statistics are not close to the thresholds that define unacceptable model performance (NSE < 0 and PBIAS > 30 %) and the calculation of the statistics at multiple stations, it can be concluded that the model performs well on a monthly basis. An important shortcoming, however, is the lack of data at the watershed outlet. This impedes to estimate the model performance at locations more downstream than the streamflow stations. In addition, at some stations the baseflow is underestimated, peak flow volumes do not agree with the measurements or the slope of the recession curve is too low. With respect to the objective to simulate pesticides, the peak flows are the most important to be improved. This is because runoff is the main simulated transport route of pesticides to the rivers and the simulated pesticide concentrations are, in general, maximal during the rainy season (e.g. Figure 20). In this respect, the sensitivity of NSE towards high flows is advantageous.

6.1.2 Transport route and application timing
In literature, two important factors controlling the pesticide simulations are reported, being runoff and the application timing (Bannwarth et al., 2014). The importance of runoff was confirmed by the simulations, demonstrating a clear correlation between simulated runoff and pesticide dynamics. This observation underlines that it is necessary to accurately estimate the distribution of the water among the runoff and baseflow components. The use of a baseflow filter might help in this respect (section 6.2.3). The potential overestimation of the rainfall because of the use of a correction factor (section 6.2.1) might imply an overestimation of the pesticide transport. On the contrary, mainly positive PBIAS values for high flow periods (Appendix E) indicate an underestimation of the runoff, and thus an underestimation of the pesticide transport.

The importance of the second main controlling factor reported in the literature, the application timing, was not observed. This is probably because the application is distributed among seven days. A second reason might be the low detail of the model structure, having large subbasins with large times of concentration. This is the time required for water to flow from the remotest point in the subbasin to the subbasin outlet (Neitsch et al., 2011). As such, the pesticide transfer from the field to the outlet of the basin is smoothened out over multiple days. Thirdly, the monthly time step masks the pesticide peak occurring immediately after an application event. Besides, it is striking that the applied pesticides can cause a peak several months later or can be accumulated during several months. This is unlikely to occur in reality, as pesticides will be removed earlier because of irrigation, small rainfall events, uptake by plants, degradation or harvesting. To improve this in the model, the degradation half-lives or the threshold for wash-off might be set lower. Because pesticide accumulation during several months is improbable, the December peak observed for simulation 4 might not be realistic, underlying that simulated trends should be confirmed by field measurements.
6.2 Methodology
The application of SWAT for the Guayas River basin was performed in four steps: data gathering and selection, model development, streamflow calibration and pesticide simulations. Choices made during each of these steps will be discussed and suggestions for improvement will be given.

6.2.1 Data availability and selection
A challenge encountered when using SWAT in developing countries is the lack of (detailed) data (Estrada et al., 2009; Gassman et al., 2007). First of all, the development of a physically based, semi-distributed model imposes high data requirements with respect to data quantity, variety, accuracy and precision (Pandey et al., 2016). In addition, SWAT is developed primarily with regard to application in the United States (US), implying that climate and soil databases need to be extended when used elsewhere (Winchell et al., 2013). Data limitations encountered during the case study include the presence of data gaps, the limited spatial coverage and the absence of metadata. Therefore, methods to deal with these limitations were explored. Besides, increased insight into the data availability for the basin could be obtained. In this section it will be outlined on which aspects future data collection should focus in order to improve the model performance.

An improvement for the development of the hydrological model would be the collection of soil data. The available HWSD soil map is possibly outdated and has a coarse spatial resolution (Figure 9). In addition, for some of the required soil parameters no measurements were available (Table 11). As most of the hydrological processes during the land phase, e.g. evaporation and runoff, are influenced by soil parameters, an improvement in soil data is expected to increase the model performance (Wahren et al., 2016). In a first step, this improvement could be realised for the five most abundant HWSD soil classes (Anu, Lvf, Anh, Cmeb, Cme, representing 75% of the watershed area). Parameters recommended to measure are the texture, the saturated hydraulic conductivity and the profile depth, preferably at multiple locations throughout the basin (Wahren et al., 2016). An alternative is to sample for each of the most abundant land use and soil combinations. As such, the obtained parameters could be used for all the Hydrologic Response Units (HRUs) representing these combinations, revealing an interesting feature of the semi-distributed structure of the model. Such a sampling campaign is described by Matamoros (2004).

The meteorological data on which should be focused with priority is precipitation. This is because, on the one hand, precipitation is the driving input for hydrological models. On the other hand, some major limitations were encountered with respect to the available point precipitation data (Table 6). Therefore, it was chosen to use the WFDEI reanalysis dataset, having the best agreement with the stations dataset (Appendix C.1). This choice seems legitimate, demonstrated by the good streamflow statistics. However, as both rainfall and streamflow stations are absent in the south-eastern part of the basin (Figures 10 and 13), no information is available about the accuracy of the WFDEI dataset in this part. In addition, as the measured precipitation is only representative for one point (the location of the rain gauge), the measured value is expected to be more extreme than precipitation averaged over a whole grid (i.e. the WFDEI precipitation). Therefore, the application of the correction factor of 1.32 might lead to an overestimation of the rainfall. Considering the importance of precipitation data for hydrological modelling and the limitations of both datasets, it would be interesting to compare the current model performance with the one obtained when using the stations dataset. In addition, the precipitation data could potentially be improved by including elevation bands and accounting for orographic effects, using the methodology outlined by Strauch et al. (2016).
With respect to the reservoir data, more recent outflow (from 2010 onwards) measurements for the Daule Peripa Dam should be gathered if it is desired to run recent simulations. Moreover, as recently (after 2009) two new dams were constructed (Baba Dam and DauVin Project), data for these dams (outflow measurements or monthly target volumes) are required in order to implement them into the model (Arias-Hidalgo, 2012).

Concerning pesticide application data, detailed data for one specific pesticide product were difficult to obtain as also experienced by other studies (section 4.3). Because pesticide application is driven by a variety of factors a strict timing scheme does often not exist (Bannwarth et al., 2014). In addition, farmers not always keep track of the amounts they apply or do not want to share that information (personal communication). It was chosen to focus on the main crops, on two pesticides and to do one interview per crop. As such, the collected information was associated with a high uncertainty. First, this approach impeded to have spatially distributed information. For sugar cane, the spatial variation can be assumed to be limited as the cultivation area is concentrated in two regions and the farmer that was interviewed possesses one third of the total sugar cane cultivation area within the basin. Corn and banana, on the contrary, are cultivated throughout the basin and their spatial variation with respect to application practices can be more pronounced. Secondly, as the interviews were conducted at big farms, no information was gathered about the practices at small farms. Because of the uncertainty associated with the application data, it is not possible to make detailed predictions about the surface water pesticide concentrations. However, the pesticide simulations can be used for a system analysis. Even for a system analysis, it would be interesting to gather more information on the pesticide practices. This can be done by conducting interviews or collecting market data. The information that should be gathered is the AR \([\text{L product ha}^{-1}]\), the type of product (in order to recalculate the AR to kg active ingredient ha\(^{-1}\)) and the application timing.

With respect to the calibration data, an important limitation for this study was the lack of sediment and pesticide concentration data. Available sediment yield measurements, first, are scarce and outdated. This is because the spatial distribution of the gauging stations is too low to obtain reliable results and it was decided to stop monitoring suspended solids in 1980 (Castro and Andres, 2009). Promising for the future, however, is the announcement of a national monitoring network and a better sharing of information (Nolivos et al., 2015). Related to pesticide data, secondly, it is currently not realistic to obtain pesticide calibration data. This is because the required temporal and spatial resolution of these data is high due to their dynamic nature and pesticide analysis is expensive (Boithias et al., 2011; Holvoet, 2006). Nevertheless, the monitoring of pesticides at a lower temporal and spatial resolution can be interesting to confirm simulated trends. Important in this respect is to sample at locations corresponding with the simulations, thus at the outlets of the model's subbasins. While doing so, the simulations could be used to determine relevant locations (risk areas) and periods (e.g. wet season). As runoff forms an important contribution to pesticide transport and pesticide concentrations are highly dynamic, the sampling timing should ideally be after rainfall events. Alternatively, passive samplers might be used (Holvoet, 2006).

### 6.2.2 Choices related to the model development

In this section will be focused on the threshold drainage area (TDA) and the scheduling of management operations. The choice of 3 % for the TDA, first, was based on the objective to develop a first rather coarse model for the basin. In view of model refinement it would be interesting to investigate the effect of a smaller TDA on the model simulations. A smaller TDA will result in a more
detailed channel network, a larger amount of subbasins and more spatial variability in the input data (section 5.4.1), which might improve the accuracy of the predictions (Chiang and Yuan, 2015). In addition, the high TDA might be the reason for unrealistic calibrated parameter values (see below). However, it should be noted that in other studies the effect on the streamflow simulations was found to be small (Aouissi et al., 2013; Jha et al., 2004; Tripathi et al., 2006; Vilaysane et al., 2015). In addition, the lowest TDA does not necessarily yield the most accurate model (Gong et al., 2010). With respect to water quality, the influence could be more pronounced. Jha et al. (2004), for example, found the sediment yield predictions to be sensitive towards the watershed subdivision. This has several reasons. First, the peak runoff rate, used in the MUSLE equation to calculate the sediment yield, is dependent on the subbasin area. In addition, topographic parameters (overland slope and slope length) of this equation vary as a function of the watershed delineation. Lastly, the channel length influences the sediment routing, e.g. the amount of deposition (Jha et al., 2004; Neitsch et al., 2011). Likewise, pesticide dynamic simulations can be expected to be dependent on the chosen TDA, both directly due to varying subbasin and channel topographic parameters and indirectly due to varying sediment yield predictions. It is thus recommended to investigate the effect of different TDAs on the model performance and find an optimal value. As an alternative, the desired stream order could be formulated first and based on this, the TDA could be determined iteratively (Omran et al., 2016).

A second aspect is related to the heat units method to schedule management operations (section 5.5.3.2). As explained above, management operations (e.g. harvesting, pesticide application) could be scheduled by using either heat units or dates. Advantageous of the default heat unit method is that the temporal and spatial meteorological variation within the basin is taken into account, which makes management timing more realistic. However, it was opted to use the date scheduling method for the implementation of the pesticide practices because the application timing was expressed by dates. Alternatively, these dates could have been recalculated to accumulated heat units in order to keep using the default method. However, in that case, it would have been more difficult to estimate the effect of application timing on simulated pesticide dynamics, as the application timing would not have been the same throughout the basin. As the recalculation of the monthly NSE and PBIAS demonstrated, the streamflow simulations slightly change when adjusting the scheduling method. Adjusting the method for all HRUs – not only the HRUs where pesticide practices were implemented – is expected to have a larger impact on the streamflow simulations. A suggestion for model refinement is therefore to find the optimal scheduling method and associated parameters. Associated with these scheduling methods is SWAT’s plant growth model, used to estimate plant development, water uptake and evapotranspiration. Problems related to the use of this model in the tropics and possible solutions are discussed by Strauch and Volk (2013).

6.2.3  Calibration approach and parameter values

The case study watershed is a large and complex area, having a branched network of multiple important rivers instead of consisting of one main river. In addition, the available (spatially distributed) information about the catchment is limited and no streamflow station is present at the outlet. For these reasons, the calibration of the hydrological model might be challenging. In this section, the calibration approach used in this study will be commented and suggestions for improvement will be formulated. Thereafter, the calibrated parameter values will be examined.
A first decision that had to be made during calibration is how to make use of the model's semi-distributed structure. When using SWAT, the aim is to include spatial variability into the model as was done during model development e.g. land use and Manning's n. During the calibration, however, this aim is limited by the low density of the streamflow stations network. As it was not possible to calibrate for each of the 29 subbasins separately, the subbasins needed to be grouped into larger regions that were calibrated together. A question here is how to handle the large areas without streamflow station (e.g. Chimbo River, downstream part of the Babahoyo River, Figure 17). It was decided to calibrate for only two regions, considering these areas without station, the limited data impeding to physically determine certain parameters (e.g. all the groundwater parameters) and the fact that the calibration does not have the potential to bring a lot of spatial variation into the model. This is related to a second decision, being the amount and selection of the stations used for calibration. The amount of stations used for calibration in this study was intentionally limited, in contrast to the approach of Neitsch et al. (2002). This was with the philosophy that, certainly in the presence of large areas without stations, it would be useful to have an indication of the model performance at locations that were not used during calibration. If all stations were used during calibration, potentially good statistics for these stations could give a misleading idea of the model performance at other locations. This is also argued by Meixner et al. (2003), Mroczkowski et al. (1997) and Refsgaard (1997) and the multi-site approach is said to be a more powerful validation strategy than the split sample in time methodology. In addition, one station was not used for calibration because of its upstream location. Lastly, this approach was more time-efficient compared to calibrating for each station separately. Nevertheless, it should be noted that good statistics obtained for the stations that were reserved for validation not necessarily guarantee good model performance in regions where no station is located.

As there are several calibration approaches possible, it would be interesting to investigate the effect of a different calibration method on the model performance, for example, the subdivision of the subbasins into different regions (Figure 17). It can be argued that is more logical to group subbasins going from upstream to downstream than lumping the parameters along one river. As such, parameters of regions that are expected to have similar properties, according to the river continuum concept, are jointly calibrated (Vannote et al., 1980). This is similar to the approach suggested by Neitsch et al. (2002), however, a difference is the presence of multiple main rivers in this basin. In addition, given the location of the subbasins and the streamflow stations (rather upstream) this subdivision might not be evident. To end, the upstream subbasins located in the Andes might have different characteristics than the subbasins located in the proximity of the Daule Peripa Dam. A second aspect which could be considered for further improvement is the amount of stations used for calibration. The use of more streamflow stations can refine the spatial variability of the model, ideally in combination with the collection of more data (section 6.2.1) and the refinement of the delineated network (section 6.2.2). Meanwhile, the arguments for not using all the stations during calibration remain valid. Lastly, the calibration could focus on a smaller time step, in order to improve the simulation of specific runoff events being mainly responsible for the pesticide transport.

The physical meaning of the calibration parameters was described in section 5.5.1.2. If extreme values for these parameters were obtained during calibration (Appendix D), this can indicate the compensation for certain model structural shortcomings. The calibrated value for the baseflow alpha factor (ALPHA_BF), first, is rather low, indicating a slow response of the baseflow on a changing water table. The coarse delineated network might be the reason for this low value, as due to this
coarse network the streamflow is only simulated for large, slow responding rivers. However, equally low values were reported by other studies (Nair et al., 2011; Twigg et al., 2009; Van Liew et al., 2005). The use of a baseflow filter, for example the one developed by Arnold et al. (1995), can be used to estimate ALFA_BF based on measured streamflow data and to gain insight into the importance of groundwater contribution to the streamflow (Arnold et al., 2012a; Moriasi et al., 2007). The groundwater delay time, secondly, indicates a fast transfer from the subsurface to the aquifer. This value seems low compared to other studies, maybe because of compensation for the low ALPHA_BF (Holvoet, 2006; Shen et al., 2012b). The channel hydraulic conductivity (CH_K2), thirdly, should be equal to zero for perennial streams, which is the case here. However, in that case the streamflow simulations fluctuated strongly and it was not possible to solve this by changing other parameters. Consequently, a value greater than zero was used. The reason that this was necessary might be the coarse delineated network, where in reality tributary channels buffer the streamflow in the large rivers. Thus, a solution might be to use a lower TDA (section 6.2.2). It can be concluded that there were indeed some parameters that needed to compensate for model shortcomings and might not be physically realistic. A second reason for not guaranteeing that the calibrated parameter values reflect real world conditions is the occurrence of parameter equifinality\(^\text{10}\) (David, 2014).

### 6.2.4 Pesticide simulations methodology

With respect to the pesticide simulations, a first difficulty that was encountered was the uncertainty associated with the application data (section 6.2.1). A solution suggested in the literature to deal with this is to vary the application date throughout the basin, as SWAT models are found to be sensitive to application timing (section 4.3). However, the implementation of this suggestion would make the analysis of the effect of application on the simulated pesticide dynamics more difficult. In addition, SWAT was experienced to be inflexible with respect to the implementation of pesticide applications. For these reasons, it was decided to use a fixed application date throughout the basin (although spread out over one week). The use of heat units to schedule pesticide application, however, would be a convenient way to bring variation in application timing into the model (section 6.2.2). Nevertheless, the fact that the effect of the application timing on the pesticide simulations was not observed (section 6.1.2) suggests that it was not necessary for this study to vary the application timing throughout the basin. As an alternative to the collection of application data, lastly, one could assume application practices for a synthetic pesticide to obtain system insight.

A second aspect that should be noted is that recent application data and a recent land use map (2014) were used while the simulations were run for the year 2009. As already mentioned, if it is desired to run more recent simulations, more recent data (precipitation and reservoir outflow data) should be gathered and the two recently constructed dams should be implemented. In addition, only diffuse source pesticide pollution was taken into account, while point sources may have a large contribution to the occurrence of pesticides in the rivers (section 2.2). To end, as no pesticide calibration data were available, the model could not be calibrated for pesticide simulations.

\(^{10}\) The phenomenon of different parameter combinations yielding the same model results (Beven and Binley, 1992).
6.3 Evaluation of SWAT and further perspectives

In this last section, SWAT will be evaluated based on the experiences acquired during the case study. First, it will be questioned whether and why the use of SWAT to simulate pesticide dynamics in a data scarce context is justified. Secondly, case-specific limitations of the tool will be commented. To end, possible future applications of the developed model, on the one hand, and limits to its use, on the other hand, will be formulated.

6.3.1 Strengths of SWAT

A mechanistic model seems suitable to fulfil the objectives of this study (section 3.2). As such, spatially variable, dynamic outputs could be generated while taking into account the system characteristics. As pointed out in Table 1, one advantage of mechanistic models is that insights about dominant processes occurring in the watershed can be obtained. In addition, the model was able to generate detailed predictions, however, the accuracy of the pesticide simulations could not be verified because of data limitations. A last advantage listed in Table 1, being the potential to extrapolate the model to other scenarios, was not investigated.

By literature research, four potential tools were identified as corresponding to the requirements of the case study (Table 2). The main difference of SWAT compared to the other tools is its semi-distributed model structure. Although having limitations as reported in the literature (section 4.2), this balance between model complexity, spatial variation, data requirements and computational efficiency was experienced as very useful for this case study. On the one hand, it enables to differentiate between different land use and slope classes, which were required to implement the application practices and to observe the effect of slope on pesticide dynamics. On the other hand, the model was experienced as computationally efficient, opposed to distributed models (AnnAGNPS, MIKE SHE). Moreover, these tools would require more data which was already a limitation for SWAT. Compared to a lumped model (HSPF) that is limited to the generation of outputs at the outlet of a watershed, the semi-distributed model allows to investigate the pesticide dynamics within a watershed and to identify risk areas. Even more, as there is no streamflow station located at the outlet of the study area, no streamflow calibration and validation would have been possible using a lumped model. To end, this structure offers flexibility with respect to spatial detail (number of subbasins) and the use of HRUs facilitates the use of field measurements (section 6.2.1).

A second strength of SWAT that was experienced during the case study is the availability of an extensive online documentation and user support. In addition, many new tools are constantly developed, however, only the ArcGIS interface tool was tested during this study. This interface was found to be convenient for manipulating the input data layers. However, the tool was not always experienced as user-friendly (because of the unavailability of the source code and time-consuming generation of the input files). A third strength is SWAT’s broad range of potential applications being, however, constraint by case-specific limitations as will be discussed below. To end, the tool enables the implementation of a reservoir into the model. These strengths and the disadvantages of the other tools (Table 2), confirm that SWAT is the most suitable tool for this case study. However, it could be questioned if the study objectives are realistic considering the case-specific limitations.
6.3.2 Limitations of SWAT

The main limitation encountered during the case study is the high data requirement of SWAT, especially with respect to the simulation of pesticide dynamics. Main data limitations were discussed in section 6.2.1. Nevertheless, the good model performance for monthly streamflow simulations justifies this use. In addition, the pesticide simulations provided useful insights into the system functioning. A second disadvantage of mechanistic models in general (Table 1), and SWAT more specifically, is the time intensive model development. A third disadvantage mentioned in Table 1 comprises the challenging streamflow calibration (section 6.2.3). The limitations of SWAT with respect to pesticide limitations as reported in the literature (section 4.2) were less important for this case study because the simulations were used for system analysis. Nevertheless, other, case-specific limitations were encountered. First, the model development was found to be inflexible with respect to the delineation of the watershed and the river network, which could not be adjusted apart from choosing another TDA. This limitation is in contrast with the flexibility towards to the amount of subbasins mentioned above. A second limitation of the application of SWAT for the Guayas River basin is the fact that the tool is mainly intended for use in the US. It is frequently applied elsewhere but this involves some limitations with respect to the available databases and the plant growth model (section 6.2.1 and 6.2.2). Despite the importance of these limitations, especially the first one, SWAT enabled to obtain preliminary insights into the system functioning.

6.3.3 Future perspectives

Considering the good model performance with respect to monthly streamflow simulations, the hydrological model could be used as a valuable basis for future research. A useful application might be the use of the model for nutrient simulations, provided that nutrient data are available. In addition, research might focus on the effect of irrigation practices, reservoir management or climate change. Multiple examples of such applications are given by Gassman et al. (2014) and Krysanova and White (2015). Meanwhile, it should be noted that there is room for many model improvements, by collecting and using more data (section 6.2.1), refining the model (section 6.2.2) and calibrating more extensively (section 6.2.3). In addition, care should be taken when interpreting streamflow simulations at locations other than the locations used for model validation. Streamflow simulations at the outlet of the basin, for example, could not be validated. To end, conclusions based on model simulations should be verified by field measurements before influencing management decisions. The hydrological model can currently not be used for accurately predicting daily streamflow or groundwater parameters and processes. The previously mentioned improvements might, however, help to overcome these current limitations.

As demonstrated by the case study, the simulation of pesticide dynamics can provide useful insights into the system functioning. Future research could enlarge these insights by doing simulations for more pesticides and more years, investigating the influence of land using (by using the land use update operation option of SWAT) or by relatively comparing the effect of best management practices (BMPs) as was done by Holvoet (2006). Meanwhile, simulated trends should be confirmed by field observations (section 6.1.2) and the important limitations associated with the pesticide simulations (section 6.2.4) should be considered. Provided that data availability would improve in the future and the suggestions for model refinement would be followed, the simulation of pesticide dynamics might be a valuable tool to be used in a decision framework, e.g. the one presented by Arias-Hidalgo (2012). The objective to accurately predict pesticide concentrations, however, will require an enormous effort with respect to the collection of application and calibration data.
6.4 Implications for the Guayas River basin

A risk area that was identified based on multiple simulations comprises the drainage area of the Vinces River. Especially at the “Vinces en Vinces” station high concentrations were simulated due to the location of this station downstream of the main corn cultivation area (Figure 21). It was observed that the pesticide application at banana farms, located more upstream, also affect this catchment. In addition, the recent construction of the Baba Dam is expected to exert pressures on this river (Arias-Hidalgo, 2012). Unfortunately, during the sampling campaign of 2016 only five samples were taken for this river, impeding to confirm the identification of the catchment as a risk area. Therefore, it is recommended for future sampling campaigns to increase the sampling density along the Vinces River, especially in the vicinity of banana and corn fields. In addition, these samples should preferably be taken in February or March, associated with the occurrence of peak concentrations. Moreover, it would be interesting to sample at the downstream region of the Babahoyo river, to confirm or disprove the low simulated contribution of pesticide application at rice farms to river pesticide concentrations.

Additional insights provided by the simulations are the occurrence of peak concentrations during the wet season (February, March), while concentrations were low to zero during the dry season. Moreover, the slope of the cultivation areas had a major influence on the simulated concentrations (rice versus sugar cane). To end, the land use degradation rate of the pesticides was an important factor influencing the simulated pesticide concentrations.

Assuming these insights to be correct, it is recommended for decision makers to prioritise the Vinces catchment regarding the mitigation of pesticide pollution. A suggestion for river management is the implementation of runoff control measurements, runoff being identified as main pesticide transport route. Moreover, these measurements should, in the first place, be implemented at fields with a high slope (e.g. sugar cane farms). An example of a runoff control measurement is the implementation of plant rows parallel to the receiving water ways (Figure 2). Additionally, as reported by Arias-Hidalgo et al. (2013), pesticide practices within the basin should be made more sustainable, for example, by prohibiting the use of toxic pesticides. Another pesticide selection criteria for policy makers might be the land phase degradation rate of the pesticides, as this rate was observed to be an important factor influencing the surface water pesticide concentrations. Lastly, as peak concentrations occur during February and March, especially during these months measurements related to pesticide practices are required.
7 Conclusion

Agricultural intensification and the associated use of pesticides imposes a major stress on freshwater ecosystems. Especially in developing countries, where legislation is weak and data are scarce, it is urgent to gain more insight into this problem. To reduce the gaps of knowledge and to conserve or restore ecosystem health, the use of simulation models has a large added value. Applied to investigate the impact of pesticide use, mechanistic hydrological models extended for pesticide simulations are assessed as appropriate tools. The current study aimed at evaluating the use of the Soil and Water Assessment Tool (SWAT) to simulate pesticide dynamics within the Guayas River basin considering the boundary condition of limited data availability. This large and complex watershed is characterised by intensive agriculture and the presence of a hydropower dam. SWAT is a widely used tool to develop hydrological watershed models based on land use, soil and slope information. To our best knowledge, it is the first time that SWAT is applied at the extent of this watershed. In addition, the pesticide applications of SWAT in developing countries are rare.

The case-study application of SWAT was performed in different steps. First, the data required to develop the model (land use, soil, DEM, river network, reservoir data), to calibrate it (streamflow data) and to run the simulations (meteorological data, pesticide application data) were gathered. During this step, the main data limitations could be pinpointed and solutions for these limitations where sought for. Specific attention was given to the precipitation data, since precipitation is the driving input for water dynamics in a system. Because of data limitations associated with the records of the precipitation stations, it was chosen to use the global WFDEI reanalysis precipitation dataset after application of a correction factor. Pesticide application data for the most important crops were gathered by conducting interviews at big farms. The second step comprised the development of a hydrological model for the basin. This model was manually calibrated for streamflow on a monthly basis and using multiple stations throughout the basin. Model evaluation ratings for the streamflow station having the largest discharge, located on the Daule River, were very good and good on a monthly basis for the calibration and validation period respectively. Satisfactory to very good model performance was acquired at most of the stations, however, at some other stations high PBIAS values were obtained. The potentially low accuracy of the streamflow data might at least partly explain these high PBIAS values. Altogether, the hydrological model was evaluated as performing well on a monthly basis. In a last step, application practices for two pesticides were implemented, simulations were run and simulated trends were analysed. The simulations suggested the importance of system characteristics (precipitation, slope) and pesticide properties. In addition, risk areas (e.g. the Vinces catchment) could be identified and a strong seasonal variation was observed, which enabled to formulate recommendations for future sampling campaigns. However, these findings could not be verified by field measurements, presenting the main limitation associated with these simulations.

The application of SWAT for the Guayas River basin made it possible to identify case-specific strengths and shortcomings of the tool. A first main strength comprises the semi-distributed structure of the developed model, enabling to balance model complexity and efficiency according to the available data and study objectives. This model structure is characteristic of SWAT and differs from the structure (lumped or distributed) of other tools that are used to develop hydrological model extended for simulating pesticide dynamics. Additional strengths of SWAT include the extensive user support, the constant improvements and the possibility to implement hydropower dams into the
model. A main limitation that is often encountered during SWAT applications, especially in
developing countries, is the high data requirement of the tool. This is especially true when the
objective is to simulate pesticide dynamics, which requires detailed application data. Moreover, the
model development was experienced as inflexible and the model calibration as challenging. Despite
these limitations, the case study demonstrated the potential of SWAT to develop a hydrological
model for a complex watershed that performs well with respect to monthly streamflow simulations.
In addition, it was shown that useful insights into pesticide dynamics can be obtained. Based on
these results and SWAT’s strengths listed above, SWAT was identified as being the tool having the
best potential to simulate pesticide transport and fate within the Guayas River basin. As this
conclusion is partly based on case-specific characteristics (e.g. the absence of a station at the outlet
of the basin), its extrapolation to other data scarce study areas should be done with care.

Future opportunities related to the case study include the use of the calibrated hydrological model as
basis for further research and applications related to the simulation of pesticide dynamics. A
potential research field of the hydrological model, first, is the simulation of non-point nutrient
pollution. There is, however, still potential for improvement of this model. Model performance is
expected to increase by collecting and using more data (e.g. soil data), exploring different threshold
drainage areas (which affects the detail of the river network and the amount of subbasins) and
.calibrating more extensively (e.g. by using more stations). The model can currently not be used for
accurately predicting daily streamflow or groundwater parameters and processes. In addition, it
should be noted that the model performance at the outlet of the basin could not be evaluated due to
the absence of an outlet streamflow station. Potential research related to the simulation of pesticide
dynamics, secondly, is to investigate the influence of land use change and to relatively compare best
management practices. The main limitation associated with these simulations is the lack of surface
water pesticide concentration data required to verify simulation results. Nevertheless, in this respect
the pesticide simulations might already provide useful information about relevant locations and
periods to collect concentration data, potentially decreasing costs associated with this collection. A
remaining challenge will be the uncertainty associated with the pesticide application data. Interviews
at multiple, small and big farms and the collection of market data can reduce this uncertainty. The
use of the simulations to accurately predict pesticide concentrations is not expected to be possible in
the near future due to the lack of sediment and pesticide calibration data.

SWAT has proven to be a suitable tool to develop a hydrological model and obtain insight into
pesticide dynamics within the Guayas River basin. Although a number of improvements should be
made, this model can serve as a basis for pesticide simulations and other valuable applications, i.e.
modelling the fate of nutrients. The present research can help to identify focus points for further
development. Besides the obtained insight into the system’s dynamics of the river basin, a further
improved model can aid to define priorities in river management regarding pesticide use. With this,
the basis for a tool is available to help protect and restore the natural value of the freshwater
ecosystem of the Guayas River basin.
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Appendix A: Evapotranspiration implementation methods

A.1 Penman method

\[ \text{ET}_0 = \frac{1}{\lambda} \left[ \frac{\Delta}{\Delta + \gamma} \left( H_{\text{net}} - G \right) + \frac{\gamma}{\Delta + \gamma} \cdot E_a \right] \]  

(A.1.1)

Where:

\( \text{ET}_0 \) the reference evapotranspiration, with grass as reference crop [mm day\(^{-1}\)]

\( \lambda \) the latent heat of vaporization [MJ kg\(^{-1}\)]

\( \Delta \) the slope of the water vapor saturation curve [kPa °C\(^{-1}\)]

\( \gamma \) the psychrometric constant [kPa °C\(^{-1}\)]

\( H_{\text{net}} \) the net radiation [MJ m\(^{-2}\) day\(^{-1}\)]

\( G \) the soil heat flux [MJ m\(^{-2}\) day\(^{-1}\)]

\( E_a = f(u) \cdot (e_s - e) \) an expression for the ‘drying power’ of the air [m kPa day\(^{-1}\)], which increases with an increasing driving force (the difference between saturated and actual vapor pressure) and increasing wind speed

\( f(u) \) the wind function [m day\(^{-1}\)]

\( e_s \) the saturation vapor pressure [kPa]

\( e \) the actual vapor pressure [kPa].

This equation combines two parts, an energy balance or radiation term and a ventilation or aerodynamic term (\( E_a \)), each multiplied by a dimensionless weighting factor which is only temperature and pressure dependent (Stigter, 1978). The energy term is explained by the energy balance:

\[ H_{\text{net}} - G - H - \lambda \cdot \text{ET}_0 = 0 \]  

(A.1.2)

Where:

\( H \) the sensible heat

\( \lambda \cdot \text{ET}_0 \) the latent heat flux (Allen 1998).

The sensible heat \( H \) is difficult to determine and is not included in the Penman equation.

A lot of variations on this equation exists, particularly with respect to the empirical wind function. The original Penman wind function is:

\[ f(u) = 6.43 \cdot (1 + 0.53 \cdot u_2) \]  

(A.1.3)

Where:

\( u_2 \) the wind speed at a height of 2 m [m day\(^{-1}\)].
A.2 Penman-Monteith method

\[ ET_{\text{opt}} = \frac{1}{\lambda} \left[ \frac{\Delta}{\Delta + \gamma^* (1 + \frac{r_c}{r_a})} \ast (H_{\text{net}} - G) + \frac{\rho_a \cdot c_p}{\Delta + \gamma^* (1 + \frac{r_c}{r_a})} \ast (e_s - e) \right] \]  \hspace{1cm} (A.2.1)

Where:

- \( ET_{\text{opt}} \) the evapotranspiration under optimal conditions [mm day\(^{-1}\)]
- \( \lambda \) the latent heat of vaporization [MJ kg\(^{-1}\)]
- \( \Delta \) the slope of the water vapor saturation curve [kPa °C\(^{-1}\)]
- \( \gamma \) the psychrometric constant [kPa °C\(^{-1}\)]
- \( r_c \) the surface resistance [s m\(^{-1}\)]
- \( r_a \) the aerodynamic resistance [s m\(^{-1}\)]
- \( H_{\text{net}} \) the net radiation [MJ m\(^{-2}\) day\(^{-1}\)]
- \( G \) the soil heat flux [MJ m\(^{-2}\) day\(^{-1}\)]
- \( \rho_a \) the air density [kg m\(^{-3}\)]
- \( c_p \) the specific heat at constant pressure [MJ kg\(^{-1}\) °C\(^{-1}\)]
- \( e_s \) the saturation vapor pressure [kPa]
- \( e \) the actual vapor pressure [kPa]

As explained in Allen et al. (1998), the original Penman-Monteith equation together with the equations for the aerodynamic and surface resistances, for standard conditions and adjusted to the reference crop, lead to the following version of the Penman-Monteith equation:

\[ ET_0 = 0.408 \ast \frac{\Delta}{\Delta + \gamma^* (1 + 0.34 + u_2)} \ast (H_{\text{net}} - G) + \frac{\gamma}{\Delta + \gamma^* (1 + 0.34 + u_2)} \ast \frac{900 + u_2^2}{T + 273} \ast (e_s - e) \]  \hspace{1cm} (A.2.2)

Where:

- \( ET_0 \) the reference evapotranspiration [mm day\(^{-1}\)]
- \( \Delta \) the slope of the water vapor saturation curve [kPa °C\(^{-1}\)]
- \( \gamma \) the psychrometric constant [kPa °C\(^{-1}\)]
- \( u_2 \) the wind speed at a height of 2 m [m s\(^{-1}\)]
- \( H_{\text{net}} \) the net radiation [MJ m\(^{-2}\) day\(^{-1}\)]
- \( G \) the soil heat flux [MJ m\(^{-2}\) day\(^{-1}\)]
- \( T \) the main daily air temperature at 2 m height [°C]
$e_s$ the saturation vapor pressure [kPa]

e the actual vapor pressure [kPa] (Allen et al., 1998).
A.3 Priestley-Taylor method

This method uses a simplification of the combined equation, by stating that in many cases the ventilation term in the Penman equation can be neglected, leading to following equation (Fleischer et al., 2015):

\[ E_T_0 = \frac{\alpha}{\lambda} \Delta \lambda^{\frac{\Delta}{\Delta + \gamma}} (H_{\text{net}} - G) \]  \hspace{1cm} (A.3.1)

Where:

- \( E_T_0 \) the reference evapotranspiration [mm day\(^{-1}\)]
- \( \alpha \) an empirical coefficient to account for climate conditions (Fleischer et al., 2015), set to 1.28 in SWAT (Fleischer et al. (2015) proposes 1.26)
- \( \lambda \) the latent heat of vaporization [MJ kg\(^{-1}\)]
- \( \Delta \) the slope of the water vapor saturation curve [kPa °C\(^{-1}\)]
- \( \gamma \) the psychrometric constant [kPa °C\(^{-1}\)]
- \( H_{\text{net}} \) the net radiation [MJ m\(^{-2}\) day\(^{-1}\)]
- \( G \) the soil heat flux [MJ m\(^{-2}\) day\(^{-1}\)]
A.4 Hargreaves method

\[
ET_0 = \frac{1}{\lambda} \left[ 0.0023 \times H_0 \times \sqrt{(T_{\text{max}} - T_{\text{min}})} \times (T_{\text{av}} + 17.8) \right]
\]  \hspace{1cm} (A.4.1)

Where:

- \(ET_0\) the reference evapotranspiration [\(\text{mm} \text{d}\)]
- \(\lambda\) the latent heat of vaporization [\(\text{MJ} \text{kg}\)]
- \(H_0\) the extraterrestrial radiation [\(\text{MJ} \text{m}^2 \text{d}\)]
- \(T_{\text{max}}\) the maximum air temperature for a given day [\(^{\circ}\text{C}\)]
- \(T_{\text{min}}\) the minimum air temperature for a given day [\(^{\circ}\text{C}\)]
- \(T_{\text{av}}\) the average air temperature for a given day [\(^{\circ}\text{C}\)]
Appendix B: A brief description of the four reanalysis precipitation datasets

The ERA-Interim reanalysis dataset, first, is a product of the European Centre for Medium-Wave Forecasts (ECMWF) and covers the period from 1979 till nearly present. The dataset is established by using a forecast model and comparing these results once every 12 hours with observations. The majority of these observations consist of satellite data but also in situ wind, air temperature and specific humidity measurements are taken into account. The resulting gridded dataset include various 3-hourly surface parameters as well as 6-hourly upper-air parameters. As is the case with every reanalysis product, this dataset is not only consistent with the observations but is also physically coherent (Dee et al., 2011). The precipitation data was downloaded at http://apps.ecmwf.int/datasets/. An extensive description of the forecast model, data assimilation method and input datasets used to produce the dataset is given by Dee et al. (2011). An example of a study that investigates the use of ERA-interim precipitation data as input for a SWAT model, is the study of Nkiaka et al. (2017).

The WFDEI dataset, secondly, is the result of a post-processing technique (the WATCH Forcing Data methodology) applied to the ERA-Interim (WFDEI) dataset. Adaptations include interpolation to a 0.5° resolution, elevation correction and monthly bias correction. The resulting dataset includes eight, 3-hourly meteorological variables. Precipitation and temperature data were downloaded at https://dataguru.lu.se/app. Details on the WFDEI dataset can be found in Weedon et al. (2014). An example of a SWAT study that uses the WFDEI precipitation dataset is provided by Monteiro et al. (2015).

The Climate Forecast System Reanalysis (CFSR) dataset, thirdly, is a product of the National Centers for Environmental Prediction (NCEP). The forecast model consists of four coupled modules, being atmosphere, ocean, land surface and sea ice. This model is reinitialised every 6 hours, using in-situ and satellite observations. Climate and hydrological parameters are generated at an hourly time scale (Saha et al., 2010). The precipitation dataset was downloaded at https://globalweather.tamu.edu/. Extensive information on the dataset is given by Saha et al. (2010). An example of a SWAT study using this dataset is the study of Jajarmizadeh et al. (2016).

The Climate Hazards group Infrared Precipitation with Stations (CHIRPS) dataset, lastly, is one of the most recent reanalysis products. It provides precipitation data at a high spatial resolution. This dataset is established by integrating multiple datasets. Data from various satellites (e.g. infrared data) is bias corrected using data from rain gauge stations (Funk et al., 2015). The dataset was downloaded at ftp://ftp.chg.ucsb.edu/pub/org/chg/products/CHIRPS-2.0 The CHIRPS algorithm is described by Funk et al. (2015). A study that estimates the use of the CHIRPS dataset as input for a SWAT model is the study of Tuo et al. (2016).
Appendix C: Comparison station and reanalysis datasets

C.1 Reanalysis precipitation datasets


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<td></td>
<td>La Capilla</td>
<td>2.5</td>
<td>-0.5</td>
<td>0.80</td>
<td>0.88</td>
</tr>
<tr>
<td></td>
<td>Olmedo Manabi</td>
<td>3.3</td>
<td>1.7</td>
<td>0.68</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td>Pichilingue</td>
<td>2.6</td>
<td>0.1</td>
<td>0.87</td>
<td>0.93</td>
</tr>
<tr>
<td></td>
<td>Pilalo</td>
<td>3.9</td>
<td>1.0</td>
<td>0.22</td>
<td>0.79</td>
</tr>
<tr>
<td></td>
<td>Puebloviejo</td>
<td>3.3</td>
<td>1.2</td>
<td>0.78</td>
<td>0.91</td>
</tr>
<tr>
<td></td>
<td>Puerto Ila</td>
<td>3.5</td>
<td>-0.2</td>
<td>0.80</td>
<td>0.91</td>
</tr>
<tr>
<td></td>
<td>San Juan La Mana</td>
<td>6.0</td>
<td>2.1</td>
<td>0.59</td>
<td>0.92</td>
</tr>
<tr>
<td></td>
<td>Vincies</td>
<td>4.3</td>
<td>1.6</td>
<td>0.75</td>
<td>0.93</td>
</tr>
<tr>
<td></td>
<td>Zapotal Los Rios</td>
<td>2.9</td>
<td>0.1</td>
<td>0.77</td>
<td>0.90</td>
</tr>
<tr>
<td></td>
<td>Mocache</td>
<td>5.1</td>
<td>0.3</td>
<td>0.55</td>
<td>0.88</td>
</tr>
<tr>
<td></td>
<td><strong>Average</strong></td>
<td><strong>3.8</strong></td>
<td><strong>0.9</strong></td>
<td><strong>0.66</strong></td>
<td><strong>0.89</strong></td>
</tr>
</tbody>
</table>
### C.2 Original and corrected WFDEI dataset

Table C.2: Statistics for the monthly average of daily precipitation for 14 ground stations and the WFDEI dataset for the period 1990 – 2013, before and after application of the correction factor. RMSE: Root Mean Squared Error, B: bias, $R^2$: coefficient of determination, $\rho_s$: spearman correlation coefficient.

<table>
<thead>
<tr>
<th>Reanalysis Product</th>
<th>Station</th>
<th>RMSE [-]</th>
<th>B [mm]</th>
<th>$R^2$ [-]</th>
<th>$\rho_s$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>WFDEI original</td>
<td>Babahoyo</td>
<td>3.3</td>
<td>1.6</td>
<td>0.84</td>
<td>0.93</td>
</tr>
<tr>
<td></td>
<td>Camposano</td>
<td>1.5</td>
<td>0.7</td>
<td>0.91</td>
<td>0.92</td>
</tr>
<tr>
<td></td>
<td>Chiriboga</td>
<td>7.9</td>
<td>5.4</td>
<td>-0.17</td>
<td>0.65</td>
</tr>
<tr>
<td></td>
<td>El Corazon</td>
<td>3.7</td>
<td>0.4</td>
<td>0.69</td>
<td>0.91</td>
</tr>
<tr>
<td></td>
<td>La Capilla</td>
<td>2.5</td>
<td>-0.4</td>
<td>0.81</td>
<td>0.87</td>
</tr>
<tr>
<td></td>
<td>Olmedo Manabi</td>
<td>3.7</td>
<td>2.1</td>
<td>0.66</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td>Pichilingue</td>
<td>2.4</td>
<td>0.4</td>
<td>0.90</td>
<td>0.95</td>
</tr>
<tr>
<td></td>
<td>Pilalo</td>
<td>2.3</td>
<td>0.5</td>
<td>0.50</td>
<td>0.85</td>
</tr>
<tr>
<td></td>
<td>Puebloviejo</td>
<td>3.5</td>
<td>1.3</td>
<td>0.77</td>
<td>0.92</td>
</tr>
<tr>
<td></td>
<td>Puerto Ila</td>
<td>2.9</td>
<td>0.0</td>
<td>0.87</td>
<td>0.94</td>
</tr>
<tr>
<td></td>
<td>San Juan La Mana</td>
<td>5.9</td>
<td>1.9</td>
<td>0.62</td>
<td>0.91</td>
</tr>
<tr>
<td></td>
<td>Vinces</td>
<td>3.5</td>
<td>0.6</td>
<td>0.77</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td>Zapotal Los Rios</td>
<td>5.6</td>
<td>1.5</td>
<td>0.58</td>
<td>0.85</td>
</tr>
<tr>
<td></td>
<td>Mocache</td>
<td>2.3</td>
<td>1.0</td>
<td>0.90</td>
<td>0.93</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td></td>
<td><strong>3.7</strong></td>
<td><strong>1.2</strong></td>
<td><strong>0.69</strong></td>
<td><strong>0.89</strong></td>
</tr>
<tr>
<td>WFDEI corrected</td>
<td>Babahoyo</td>
<td>3.0</td>
<td>1.0</td>
<td>0.87</td>
<td>0.93</td>
</tr>
<tr>
<td></td>
<td>Camposano</td>
<td>1.5</td>
<td>-0.1</td>
<td>0.92</td>
<td>0.92</td>
</tr>
<tr>
<td></td>
<td>Chiriboga</td>
<td>5.8</td>
<td>0.0</td>
<td>0.37</td>
<td>0.64</td>
</tr>
<tr>
<td></td>
<td>El Corazon</td>
<td>3.9</td>
<td>0.0</td>
<td>0.66</td>
<td>0.92</td>
</tr>
<tr>
<td></td>
<td>La Capilla</td>
<td>3.0</td>
<td>-1.1</td>
<td>0.72</td>
<td>0.87</td>
</tr>
<tr>
<td></td>
<td>Olmedo Manabi</td>
<td>2.3</td>
<td>0.0</td>
<td>0.86</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td>Pichilingue</td>
<td>2.2</td>
<td>0.0</td>
<td>0.92</td>
<td>0.95</td>
</tr>
<tr>
<td></td>
<td>Pilalo</td>
<td>1.9</td>
<td>0.0</td>
<td>0.67</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td>Puebloviejo</td>
<td>3.4</td>
<td>0.7</td>
<td>0.78</td>
<td>0.92</td>
</tr>
<tr>
<td></td>
<td>Puerto Ila</td>
<td>2.8</td>
<td>0.0</td>
<td>0.88</td>
<td>0.94</td>
</tr>
<tr>
<td></td>
<td>San Juan La Mana</td>
<td>5.0</td>
<td>0.3</td>
<td>0.73</td>
<td>0.91</td>
</tr>
<tr>
<td></td>
<td>Vinces</td>
<td>3.4</td>
<td>-0.1</td>
<td>0.78</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td>Zapotal Los Rios</td>
<td>5.4</td>
<td>0.6</td>
<td>0.61</td>
<td>0.85</td>
</tr>
<tr>
<td></td>
<td>Mocache</td>
<td>2.0</td>
<td>0.0</td>
<td>0.93</td>
<td>0.93</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td></td>
<td><strong>3.2</strong></td>
<td><strong>0.1</strong></td>
<td><strong>0.76</strong></td>
<td><strong>0.89</strong></td>
</tr>
</tbody>
</table>
### C.3 WFDEI temperature dataset

Table C.3: Statistics for the monthly average of the daily minimum and maximum temperature for nine ground stations and the WFDEI dataset for the period 1990 – 2013. RMSE: Root Mean Squared Error, B: bias, $R^2$: coefficient of determination, $\rho_s$: spearman correlation coefficient.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Station</th>
<th>RMSE [-]</th>
<th>B [°C]</th>
<th>$R^2$ [-]</th>
<th>$\rho_s$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Minimum temperature</strong></td>
<td>Babahoyo</td>
<td>1.0</td>
<td>-0.2</td>
<td>0.43</td>
<td>0.69</td>
</tr>
<tr>
<td></td>
<td>ElCorazon</td>
<td>2.3</td>
<td>-2.1</td>
<td>-8.11</td>
<td>0.52</td>
</tr>
<tr>
<td></td>
<td>Pichilingue</td>
<td>4.3</td>
<td>4.3</td>
<td>-16.06</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td>Pilalo</td>
<td>4.1</td>
<td>4.0</td>
<td>-17.39</td>
<td>0.44</td>
</tr>
<tr>
<td></td>
<td>Puebloviejo</td>
<td>1.3</td>
<td>-0.5</td>
<td>0.16</td>
<td>0.61</td>
</tr>
<tr>
<td></td>
<td>Puerto Ila</td>
<td>1.7</td>
<td>1.5</td>
<td>-2.09</td>
<td>0.67</td>
</tr>
<tr>
<td></td>
<td>San Juan La Mana</td>
<td>2.7</td>
<td>2.4</td>
<td>-3.07</td>
<td>0.51</td>
</tr>
<tr>
<td></td>
<td>Vinces</td>
<td>2.8</td>
<td>-2.2</td>
<td>-1.17</td>
<td>0.45</td>
</tr>
<tr>
<td></td>
<td>Caluma</td>
<td>3.0</td>
<td>-2.7</td>
<td>-3.64</td>
<td>0.53</td>
</tr>
<tr>
<td></td>
<td><strong>Average</strong></td>
<td><strong>2.6</strong></td>
<td><strong>0.5</strong></td>
<td><strong>-5.66</strong></td>
<td><strong>0.58</strong></td>
</tr>
<tr>
<td><strong>Maximum temperature</strong></td>
<td>Babahoyo</td>
<td>4.6</td>
<td>-4.4</td>
<td>-11.86</td>
<td>0.53</td>
</tr>
<tr>
<td></td>
<td>ElCorazon</td>
<td>8.5</td>
<td>-8.4</td>
<td>-67.76</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>Pichilingue</td>
<td>1.2</td>
<td>-0.6</td>
<td>0.02</td>
<td>0.50</td>
</tr>
<tr>
<td></td>
<td>Pilalo</td>
<td>2.6</td>
<td>-2.4</td>
<td>-11.23</td>
<td>0.26</td>
</tr>
<tr>
<td></td>
<td>Puebloviejo</td>
<td>4.3</td>
<td>-4.2</td>
<td>-22.21</td>
<td>0.50</td>
</tr>
<tr>
<td></td>
<td>Puerto Ila</td>
<td>2.7</td>
<td>-2.5</td>
<td>-4.16</td>
<td>0.51</td>
</tr>
<tr>
<td></td>
<td>San Juan La Mana</td>
<td>2.0</td>
<td>-1.7</td>
<td>-2.03</td>
<td>0.42</td>
</tr>
<tr>
<td></td>
<td>Vinces</td>
<td>4.3</td>
<td>-4.2</td>
<td>-14.14</td>
<td>0.63</td>
</tr>
<tr>
<td></td>
<td>Caluma</td>
<td>7.0</td>
<td>-6.9</td>
<td>-39.97</td>
<td>0.44</td>
</tr>
<tr>
<td></td>
<td><strong>Average</strong></td>
<td><strong>4.1</strong></td>
<td><strong>-3.9</strong></td>
<td><strong>-19.26</strong></td>
<td><strong>0.44</strong></td>
</tr>
</tbody>
</table>
## Appendix D: Calibrated parameter values

Table D.1: Values for the calibration parameters determined during manual calibration. Range: range of possible parameter values as implemented in SWAT, R1: region 1, R2: region 2, R3: region 3.

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Range</th>
<th>Calibrated value R1 and R3</th>
<th>Calibrated value R2</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>AWC(n)</td>
<td>Available water capacity of soil layer n</td>
<td>0 - 1</td>
<td>Initial value (b)</td>
<td>Initial value (b)</td>
<td>mm H2O mm soil /</td>
</tr>
<tr>
<td>ALPHA_BF</td>
<td>Baseflow alpha factor</td>
<td>0 - 1</td>
<td>0.01</td>
<td>0.02</td>
<td>days ^ -1</td>
</tr>
<tr>
<td>CH_K2</td>
<td>Effective hydraulic conductivity in main channel alluvium</td>
<td>0 - 300</td>
<td>10</td>
<td>10</td>
<td>mm h / 2</td>
</tr>
<tr>
<td>CN2</td>
<td>SCS runoff curve number for moisture condition II</td>
<td>35 - 98</td>
<td>Initial value (c) * 1.5</td>
<td>Initial value (c) * 1.2</td>
<td>-</td>
</tr>
<tr>
<td>GW_DELAY</td>
<td>Groundwater delay time</td>
<td>0 - 500</td>
<td>1</td>
<td>1</td>
<td>days</td>
</tr>
<tr>
<td>GW_REVAP</td>
<td>Groundwater &quot;revap&quot; coefficient</td>
<td>0.02 - 0.2</td>
<td>0.115</td>
<td>0.2</td>
<td>-</td>
</tr>
<tr>
<td>GWQMN</td>
<td>Threshold depth of water in the shallow aquifer required for return flow to occur</td>
<td>0 - 5000</td>
<td>1000</td>
<td>3000</td>
<td>mm H2O</td>
</tr>
<tr>
<td>Temperature elevation bands</td>
<td>Five elevation bands per subbasin in order to adjust the temperature records to variation in elevation</td>
<td>-</td>
<td>Not included</td>
<td>Not included</td>
<td>-</td>
</tr>
</tbody>
</table>

(a) Value that was estimated for the different soil types using a pedotransfer function (Table 12).
(b) Determined in function of land cover and soil type according to Cronshey (1986).
## Appendix E: Evaluation statistics for low and high flow periods

Table E.1: Evaluation criteria for low and high flows for the calibration period (1993 – 2000) and average flows (Qav, Dry: dry season, Rainy: rainy season) registered during the same period. The stations for which manual calibration was done are indicated in grey. NSE: Nash-Sutcliffe efficiency (equation 5.7), PBIAS: percent bias (equation 5.8). L: calculated for low flows (simulated and registered flow < Qav), H: calculated for high flows (simulated and registered flow > Qav).

<table>
<thead>
<tr>
<th>Station</th>
<th>NSE monthly L (%)</th>
<th>PBIAS monthly L [%]</th>
<th>NSE monthly H (%)</th>
<th>PBIAS monthly H [%]</th>
<th>Qav [m³ s⁻¹]</th>
<th>Qav dry [m³ s⁻¹]</th>
<th>Qav rainy [m³ s⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baba dam</td>
<td>-0.04</td>
<td>56</td>
<td>0.24</td>
<td>-2</td>
<td>126</td>
<td>57</td>
<td>195</td>
</tr>
<tr>
<td>Daule en La Capilla</td>
<td>0.06</td>
<td>10</td>
<td>0.63</td>
<td>-3</td>
<td>412</td>
<td>256</td>
<td>561</td>
</tr>
<tr>
<td>Quevedo en Quevedo</td>
<td>0.55</td>
<td>23</td>
<td>0.04</td>
<td>-2</td>
<td>260</td>
<td>93</td>
<td>431</td>
</tr>
<tr>
<td>Vinces en Vinces</td>
<td>0.81</td>
<td>-9</td>
<td>-2.02</td>
<td>-13</td>
<td>267</td>
<td>120</td>
<td>412</td>
</tr>
<tr>
<td>Zapotal en Lechugal</td>
<td>0.70</td>
<td>12</td>
<td>-0.74</td>
<td>15</td>
<td>235</td>
<td>91</td>
<td>379</td>
</tr>
</tbody>
</table>

Table E.2: Evaluation criteria for low and high flows for the validation period (2001 – 2009) and average flows (Qav, Dry: dry season, Rainy: rainy season) registered during the same period. The stations for which manual calibration was done are indicated in grey. NSE: Nash-Sutcliffe efficiency (equation 5.7), PBIAS: percent bias (equation 5.8). L: calculated for low flows (simulated and registered flow < Qav), H: calculated for high flows (simulated and registered flow > Qav).

<table>
<thead>
<tr>
<th>Station</th>
<th>NSE monthly L (%)</th>
<th>PBIAS monthly L [%]</th>
<th>NSE monthly H (%)</th>
<th>PBIAS monthly H [%]</th>
<th>Qav [m³ s⁻¹]</th>
<th>Qav dry [m³ s⁻¹]</th>
<th>Qav rainy [m³ s⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baba dam</td>
<td>-1.33</td>
<td>58</td>
<td>0.34</td>
<td>7</td>
<td>91</td>
<td>27</td>
<td>155</td>
</tr>
<tr>
<td>Daule en La Capilla</td>
<td>-6.19</td>
<td>25</td>
<td>0.46</td>
<td>-2</td>
<td>220</td>
<td>113</td>
<td>328</td>
</tr>
<tr>
<td>Quevedo en Quevedo</td>
<td>0.27</td>
<td>17</td>
<td>-0.10</td>
<td>23</td>
<td>199</td>
<td>46</td>
<td>357</td>
</tr>
<tr>
<td>Vinces en Vinces</td>
<td>-0.25</td>
<td>-47</td>
<td>0.49</td>
<td>13</td>
<td>185</td>
<td>51</td>
<td>312</td>
</tr>
<tr>
<td>Zapotal en Lechugal</td>
<td>-0.31</td>
<td>-46</td>
<td>0.41</td>
<td>8</td>
<td>128</td>
<td>26</td>
<td>230</td>
</tr>
</tbody>
</table>
Appendix F: Streamflow time series


![Daily time series for the "Baba dam" station during the calibration period (1993 – 2000).](image1)

![Daily time series for the "Daule en la Capilla" station during the calibration period (1993 – 2000).](image2)
Figure F.1.3: Daily time series for the “Quevedo en Quevedo” station during the calibration period (1993 – 2000).

Figure F.1.4: Daily time series for the “Vinces en Vinces” station during the calibration period (1993 – 2000).

Figure F.1.5: Daily time series for the “Zapotal en Lechugal” station during the calibration period (1993 – 2000).
F.2: Daily time series of observed and simulated streamflow for the validation period (2001 – 2009)

Figure F.2.1: Daily time series for the “Baba dam” station during the validation period (2001 – 2009).

Figure F.2.2: Daily time series for the “Daule en la Capilla” station during the validation period (2001 – 2009).
Figure F.2.3: Daily time series for the “Quevedo en Quevedo” station during the validation period (2001 – 2009).

Figure F.2.4: Daily time series for the “Vinces en Vinces” station during the validation period (2001 – 2009).

Figure F.2.5: Daily time series for the “Zapotal en Lechugal” station during the validation period (2001 – 2009).
F.3: Monthly time series of observed and simulated streamflow for the calibration period (1993 – 2000)

Figure F.3.1: Monthly time series for the “Baba dam” station during the calibration period (1993 – 2000).

Figure F.3.2: Monthly time series for the “Daule en la Capilla” station during the calibration period (1993 – 2000).
Figure F.3.3: Monthly time series for the “Quevedo en Quevedo” station during the calibration period (1993 – 2000).

Figure F.3.4: Monthly time series for the “Vinces en Vinces” station during the calibration period (1993 – 2000).

Figure F.3.5: Monthly time series for the “Zapotal en Lechugal” station during the calibration period (1993 – 2000).
F.4: Monthly time series of observed and simulated streamflow for the validation period (2001 – 2009)

Figure F.4.1: Monthly time series for the “Baba dam” station during the validation period (2001 – 2009).

Figure F.4.2: Monthly time series for the “Daule en la Capilla” station during the validation period (2001 – 2009).
Figure F.4.3: Monthly time series for the “Quevedo en Quevedo” station during the validation period (2001 – 2009).

Figure F.4.4: Monthly time series for the “Vinces en Vinces” station during the validation period (2001 – 2009).

Figure F.4.5: Monthly time series for the “Zapotal en Lechugal” station during the validation period (2001 – 2009).
Appendix G: Streamflow scatter plots

G.1: Scatter plots to compare observed and simulated daily average streamflow for the calibration period (1993 – 2000)

Figure G.1.1: Scatter pots of daily average streamflow at the “Baba dam” station for the calibration period (1993 – 2000).

Figure G.1.2: Scatter pots of daily average streamflow at the “Daule en la Capilla” station for the calibration period (1993 – 2000).
Figure G.1.3: Scatter pots of daily average streamflow at the “Quevedo en Quevedo” station for the calibration period (1993 – 2000).

Figure G.1.4: Scatter pots of daily average streamflow at the “Vinces en Vinces” station for the calibration period (1993 – 2000).
Figure G.1.5: Scatter pots of daily average streamflow at the “Zapotal en Lechugal” station for the calibration period (1993 – 2000).
G.2: Scatter plots to compare observed and simulated daily average streamflow for the validation period (2001 – 2009)

![Scatter plot for Baba dam station](image1)

Figure G.2.1: Scatter plots of daily average streamflow at the “Baba dam” station for the validation period (2001 – 2009).

![Scatter plot for Daule en la Capilla station](image2)

Figure G.2.2: Scatter plots of daily average streamflow at the “Daule en la Capilla” station for the validation period (2001 – 2009).
Figure G.2.3: Scatter pots of daily average streamflow at the “Quevedo en Quevedo” station for the validation period (2001 – 2009).

Figure G.2.4: Scatter pots of daily average streamflow at the “Vinces en Vinces” station for the validation period (2001 – 2009).
Figure G.2.5: Scatter plots of daily average streamflow at the “Zapotal en Lechugal” station for the validation period (2001–2009).
G.3: Scatter plots to compare observed and simulated monthly average streamflow for the calibration period (1993 – 2000)

Figure G.3.1: Scatter plots of monthly average streamflow at the “Baba dam” station for the calibration period (1993 – 2000).

Figure G.3.2: Scatter plots of monthly average streamflow at the “Daule en la Capilla” station for the calibration period (1993 – 2000).
Figure G.3.3: Scatter plots of monthly average streamflow at the “Quevedo en Quevedo” station for the calibration period (1993 – 2000).

Figure G.3.4: Scatter plots of monthly average streamflow at the “Vinces en Vinces” station for the calibration period (1993 – 2000).
Figure G.3.5: Scatter plots of monthly average streamflow at the “Zapotal en Lechugal” station for the calibration period (1993 – 2000).
G.4: Scatter plots to compare observed and simulated monthly average streamflow for the validation period (2001 – 2009)

Figure G.4.1: Scatter plots of monthly average streamflow at the “Baba dam” station for the validation period (2001 – 2009).

Figure G.4.2: Scatter plots of monthly average streamflow at the “Daule en la Capilla” station for the validation period (2001 – 2009).
Figure G.4.3: Scatter plots of monthly average streamflow at the “Quevedo en Quevedo” station for the validation period (2001 – 2009).

Figure G.4.4: Scatter plots of monthly average streamflow at the “Vinces en Vinces” station for the validation period (2001 – 2009).
Figure G.4.5: Scatter pots of monthly average streamflow at the “Zapotal en Lechugal” station for the validation period (2001 – 2009).