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Original software publication

# SURFATM: A model for the exchanges of energy, ammonia, ozone, and pesticides between soil, vegetation, and atmosphere at the field scale

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## ABSTRACT

Surfatm is a two-layer resistance model to compute the exchanges of heat, water vapour, ammonia, ozone, and pesticides between the atmosphere, the vegetation, and the soil in several ecosystems at the field scale. After briefly describing its functioning and functionalities, some application studies using the model are presented. Surfatm is a tool suitable for research, decision-making, and lecturing activities in environmental sciences, specifically on heat, water, and pollutant exchanges between the atmosphere and the biosphere.

## Code metadata

Current code version  
Permanent link to code/repository used for this code version  
Permanent link to reproducible capsule  
Legal code license  
Code versioning system used  
Software code languages, tools and services used  
Compilation requirements, operating environments and dependencies  
If available, link to developer documentation/manual  
Support email for questions

V4.2  
<https://github.com/SoftwareImpacts/SIMPAC-2023-329>  
<https://codeocean.com/capsule/6769779/tree/v1>  
GPL, V3  
github  
C  
gcc,  
[support.surfatm@agroparistech.fr](mailto:support.surfatm@agroparistech.fr)

## 1. Introduction

Since the pre-industrial era, the concentrations of numerous atmospheric pollutants have sharply increased due to emissions related to human activities. The pollutants impact climate, ecosystems, materials, and human health [1]. Terrestrial ecosystems, either natural or under strong human influence and management (such as agricultural lands), are both part of the problem and the solution. On the one hand, they can be significant contributors to the total emissions, and on the other hand, they act as strong sinks helping to mitigate and reduce atmospheric concentrations of some compounds. The deposition of these air pollutants can induce adverse effects on the environment such as biodiversity decline, soil acidification, and loss of plant productivity [2].

In this context, agricultural lands are critical ecosystems [3] since: (i) they are the main contributor to pesticide emissions which have deleterious impacts on plants, animals [4], and human health [5,6], and ammonia emissions which is the major atmospheric acid-neutralizing agent that plays an important role in the formation of aerosols [7] leading to a series of impacts on human health [8], and the environment, labelled collectively as the Nitrogen Cascade [9]; (ii) they contribute to CO<sub>2</sub> and numerous pollutants removal from the atmosphere (e.g., 10–12). Nevertheless, the central role of agricultural land remains food supply production. Pollutant deposition can have substantial adverse effects on plant productivity and, therefore, on crop yield. It is mainly the case concerning ozone which induces crop yield losses between 2 to 15% according to the crop considered, and that could reach up to 20%

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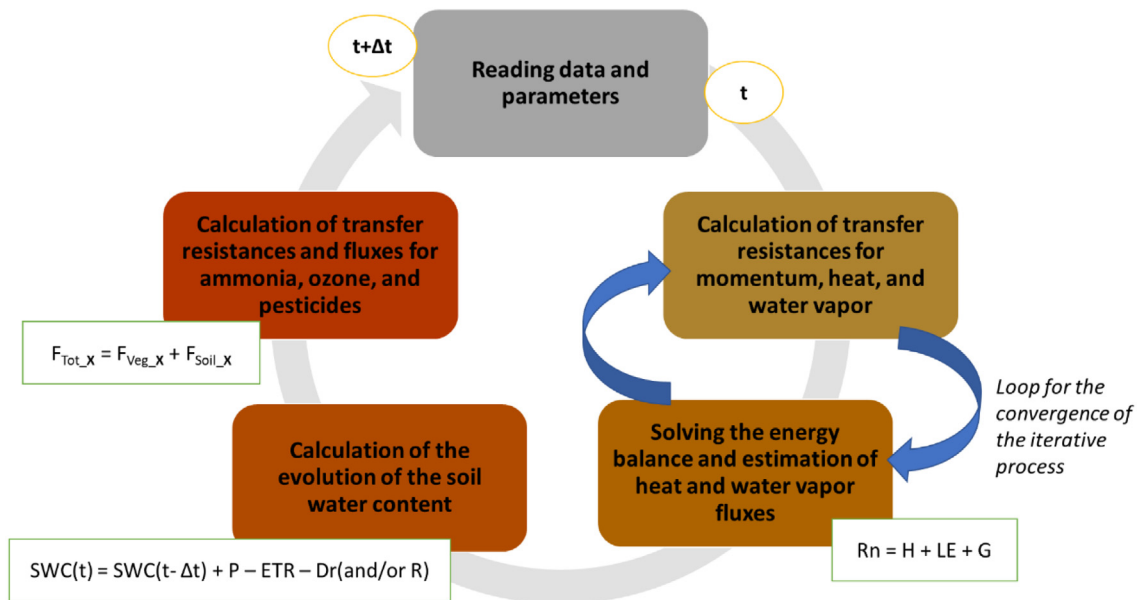


Fig. 1. Flowchart of the Surfam model for the five solver modules at each time step  $\Delta t$ , including the key equations of each solver.  $R_n$ ,  $H$ ,  $LE$ , and  $G$  are respectively the net radiation, heat, water, and ground energy fluxes between the surface (soil and vegetation) and atmosphere;  $SWC$ ,  $P$ ,  $ETR$ , and  $Dr$  (and/or  $R$ ) are the soil water content, precipitation, evapotranspiration and drainage and/or run-off occurring during the time step  $\Delta t$ ;  $F_{Tot\_X}$ ,  $F_{Veg\_X}$ ,  $F_{Soil\_X}$  are respectively the total, the vegetation, and the soil pollutant "X" ( $NH_3$ ,  $O_3$ , Pesticides) fluxes.

in the coming years [13,14], inducing consequently significant economic losses [15]. Yet, with the increase in temperature and heat wave frequency and the decrease in rainfall and available water for crop irrigation, estimating the water losses from these crops is particularly important for carbon balance and pollutant exchanges.

The Surfam model has been developed to quantify the exchanges at the field scale of water and energy together with ammonia, ozone, and pesticides, between the atmosphere, the vegetation, and the soil, with a strong emphasis on agroecosystems. It can quantify the role of terrestrial ecosystems in the emission and deposition of these pollutants and contribute to the estimation of crop yield losses due to ozone. It also helps farmers to assess the water, pesticides, and fertilizer needs and losses.

## 2. Description and functionalities

The Surfam model has been extensively described and validated for heat, ammonia, ozone, and pesticide exchanges [16–22] in several ecosystems, and distinguishing soil and plant surface exchanges. It uses resistive schemes for heat, water vapour, and pollutant exchanges to estimate the bidirectional surface–atmosphere fluxes. It accounts for air layer and surface resistances (soil, stomata, and cuticles) and includes the soil water budget with a reservoir-based approach and its links with the stomatal regulation, and the pesticide behaviour on the leaf surface (penetration, photodegradation). The model computes surface temperatures and concentrations at each time step, assuming these are in equilibrium (stationarity assumption).

To estimate the surface–atmosphere fluxes, the Surfam model follows the steps illustrated by the flowchart in Fig. 1. The input data and parameters are read in the first module to create the complete data set. The transfer resistances for momentum, heat, and water vapour are then calculated in the second solver module [16], allowing a first resolution of the energy balance and its components (sensible heat flux, latent heat flux, and soil conductive heat flux) in the third solver module [16] under neutral conditions. An iterative process is then initiated to account for the interdependency between the transfer resistances and the heat fluxes through the boundary layer thermal stratification expressed with the Monin-Obukhov Length. The model

usually converges within a few iterations to provide the equilibrium temperatures at the leaf and soil surfaces. The soil water budget is then updated to account for the evaporation, transpiration, runoff, and rainfall in the fourth solver module [16,17,20]. The last step consists in calculating the surface resistances of pollutants, using the previously estimated temperatures and humidity at the soil and leaf surfaces. Each pollutant has its parameterization for the surface concentrations and resistances. The pollutants fluxes are then computed in the last solver module [16,17,20]. These steps are performed for each input time step, typically set to 30 min.

Surfam requires standard meteorological conditions (solar or net radiations, rainfall, air temperature, humidity, and velocity at a reference height), structural ecosystem characteristics (canopy height, leaf area index, displacement height, and soil roughness length), and the atmospheric pollutant concentrations at a reference height. Parameters for the calculation of the transfer and surface resistances are also required. Some simulation options are available: the possibility to calculate the net radiation if not available as an input; the choice to use soil water content or soil water potential to compute the stomatal water stress function; the choice to save or not all input files at the end of the simulation. All the input files are provided in a tabulated-separated text file. The results of Surfam, stored in a comma-separated text file (CSV format), are the components of the energy balance and their partitioning in soil and vegetation components, the temperature and humidity at the soil and leaf surfaces, the evolution of the soil water budget, the transfer and surface resistances, and the pollutant fluxes and their partitioning into the soil, cuticular, and stomatal components.

## 3. Impact overview

The Surfam model has been initially developed to quantify the ammonia fluxes for grassland [16]. It has been used to evaluate the nitrogen losses after fertilization in the fields [16] and to identify the origin of the soil emissions and the determinants of the reduction of this soil emission (drying of the soil or accumulation of fallen leaves) [23]. It was similarly used to investigate the surface resistances for ammonia exchange using measured fluxes in a triticale crop [24]. In addition, it was tested on forest ecosystems by identifying the importance of

senescence and the role of emission or deposition on cuticles [25] and also used to assess daily  $\text{NH}_3$  fluxes in a semi-arid grazed ecosystem in Senegal [26]. Surf atm was also implemented in the landscape nitrogen flow model NitroScape as the surface exchange scheme for that model [27–29]. Furthermore, a new parameterization of the urease inhibitor effect on  $\text{NH}_3$  emissions from urea-based fertilizers was developed to investigate the impact of urease inhibitor on the dynamics and order of magnitude of  $\text{NH}_3$  fluxes. This parameterization was combined with an operational description of soil and stomatal emission potentials, implemented in the model, and then evaluated with field measurements of  $\text{NH}_3$  fluxes above fertilized corn field in central Illinois, USA [22].

The model has also been developed and used to quantify the total deposition fluxes of ozone to understand the different contributions of deposition pathways (i.e., soil, cuticular, and stomatal) and to assess their role as ozone sink [17,18]. Its capability to estimate the amount of ozone entering the plant through stomata, which is responsible for a decrease in the photosynthetic capacity, allowed to estimate the crop yield losses [18]. Surf atm has also been adapted for pesticides to estimate the volatilization fluxes of pesticides after their application on crops [20]. It allows the quantification of the relative contribution of processes competing with volatilization at the leaf scale such as pesticide leaf penetration and photodegradation. The model was evaluated using a French dataset including two pesticides applied on wheat crop and a Dutch dataset involving two pesticides applied on potato crop [21].

More recently, the Surf atm model has been coupled with the Town Energy Balance model [30] to retrieve the impact of urban greening on energy fluxes in urban areas and, therefore, the role of urban vegetation in mitigating the urban heat island effect [31].

Last but not least, the Surf atm model is also used in the practical lecturing activities at the AgroParisTech/Paris-Saclay University to illustrate and provide knowledge on the determinants controlling the exchanges of energy and pollutants between the atmosphere and the ecosystems.

Therefore, the Surf atm model is a suitable tool for research, decision-making, and lecturing activities in the field of environmental sciences with an emphasis on heat, water, and pollutant exchanges between the atmosphere and the biosphere. For instance, coupled with climate and atmospheric chemistry models, it can help to assess air quality predictions at the local and regional scale. Another potential application is to help crop management for water, assessments of the practices changes (fertilization, pesticides application) in terms of ammonia and pesticide emissions, optimize their usage and reduce the adverse impacts of cropping systems on the environment. It requires only a few easily accessible input data (meteorological data, plant and soil parameters such as leaf area, plant height and initial soil water content), and the output file format is simple, easing analysis and sharing.

#### 4. Further developments

The Surf atm model has been initially developed to estimate the pollutant exchanges between the soil, the vegetation, and the atmosphere. Further developments will concern the implementation of additional pollutant compounds whose current atmospheric concentrations are problematic, e.g., particulate matter and nitrogen oxides. The model will then be expanded to simulate fluxes of additional forms of atmospheric pollutants. The enhancement of Surf atm model by adapting it to other ecosystems is also needed. In fact, it will allow new studies concerning the impact of urban greening on both urban microclimate and air quality owing to its coupling with an urban microclimate model such as Town Energy Balance [30]. Indeed, as highlighted by Ernst et al. [32] using a bibliometric analysis, current scientific studies deal with the impact of urban vegetation on urban microclimate and air quality separately while they are effectively linked together. Hence, there is a need for studies coupling microclimate and air pollution modelling in urban areas. The Surf atm model would be a key tool since it has proved its ability to estimate heat and pollutant exchanges.

It may also be adapted for open and sparse canopies like vineyards and to coastal ecosystems such as salt marshes. Indeed, understanding the drivers of pesticide emissions from the vineyard is necessary to control pesticide losses into the atmosphere through volatilization after pesticide application as pesticide usage is high in vineyard and generates resident and environmental exposure. The adaptation of Surf atm to open and sparse canopies will also address the exchanges over vegetable gardening and annual crops in their development phase.

#### Authorship contribution statement

**Erwan Personne:** The general structure of the model and the couplings of the energy-pollutant interactions were developed based first on ammonia exchanges, Realized the adaptations to ozone, Carried out those for pesticides, Under P. Stella's impulse, the model in its current multipollutant version has been reconfigured and updated. **Carole Bedos:** Carried out the adaptations for pesticides. **Nebila Lichiheb:** Carried out the adaptations for pesticides. **Benjamin Loubet:** Realized the adaptations to ozone, Incorporated Surf atm in the NitroScape landscape model. **Patrick Stella:** Realized the adaptations to ozone, Under P. Stella's impulse, the model in its current multipollutant version has been reconfigured and updated.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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