Urban Europe and NSFC

Europe – China joint call on Sustainable Urbanization in the Context of Economic Transformation and Climate Change: Sustainable and Liveable Cities and Urban Areas

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UNCNET

Urban nitrogen cycles: new economy thinking to master the challenges of climate change

D2/2: Final concept of urban nitrogen flows including uncertainty considerations – Version 2

Due date of deliverable: **01/04/2020** Actual submission date of Version 2: **15/10/2021**

Start Date of Project: **01/04/2019** Duration: **35 + 6 months**
Organization name of co-chairs for this deliverable: **IIASA, CAS**

Authors: Katrin Kaltenegger, Samuel Guéret, Wilfried Winiwarter, Zhaohai Bai

1. Executive Summary

Building on results from WP on ammonia emissions, WP4 on N inputs and irrigation, WP5 on urban agriculture and WP6 on waste, with the draft concept for urban N flows, that has previously been developed in WP2, a final concept for urban N flows was developed as well as a concept for data exchange between the different models involved in UNCNET. The backbone structure that was set up using the STAN software (developed by Vienna University of Technology) was extended accordingly. This development was supplemented with a detailed analysis of the type of data needed for each model and the data transferred between the models. Eventually, a concept for uncertainty consideration describing the STAN-related requirements and treatment of uncertainty when implementing the collected data in the software was presented.

2. Objectives:

The UNCNET project has been established to meet several challenges associated with urban nitrogen flows. Some of these challenges are explicit (linking different environmental spheres and problem areas via a common denominator, which in this case is reactive nitrogen; optimizing flows via circular economy approaches), others are more implicit (identifying appropriate system boundaries and comparable data sources; representing trade across such boundaries; developing strategies to represent changes that are more prevalent in dynamic urban situations than for a whole country). The central model structure will need to be organized to meet these challenges. Hence, this report describes the final version of a structure to be tested on the challenges. The structure is supplemented with a concept on the linkages between existing models and data sets, sufficiently rigid to force datasets from different cities (in different world regions) into comparability, while still being flexible enough to learn from experience and allow improvements. As collected data is commonly accompanied by uncertainty, a concept for handling data uncertainty in a way that can be implemented in the central modelling structure of STAN is needed and provided in this report.

3. Activities:

Interaction with STAN developers (Oliver Cencic, Vienna University of Technology)

Expansion of the STAN model to include subsystems for urban agriculture

Development of a concept for data requirements and data transfer between the models

Uncertainty consideration

4. Results:

A complete flow model has been established in its final version – see attachment

A concept for data transfer has been developed – see attachment

A concept for uncertainty consideration has been established – see attachment

5. Milestones achieved:

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6. Deviations and reasons:

Delay due to the Corona crisis.
Revised version of the deliverable (first version submitted in 04/08/2020) with changes exclusively performed on the uncertainty concept section.

7. Publications:

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8. Meetings:

Kick-off meeting at PKU
CAS – IIASA bilateral meeting at CAS

Teleconferences

9. List of Documents/Annexes:

Annex:

A final nitrogen flow model to describe urban situations

A concept for data transfer

A concept for uncertainty considerations

REFERENCES

ANNEX

Final Nitrogen Flow Model to describe urban situations

Building on prior results from WP2 and results from WP5, a final concept for urban nitrogen flows was developed and implemented in STAN, the stock and flow model developed at the Technical University Vienna (Figure 1). This concept includes a detailed consideration of N flows within urban agriculture as well as into and from urban agriculture, characterized by its two main pools, urban animals and urban plants (Figure 2 and Figure 3). A detailed description of the stocks and flows included in urban agriculture can be found in D5.1.

The implementation of the subsystems of urban agriculture into STAN, enables the extraction of Excel Tables containing a detailed list of flows and stocks to which data needs to be collected. These Excel tables are not only essential for data collection but are a central piece of the development of the concept for data exchange between the different models involved.

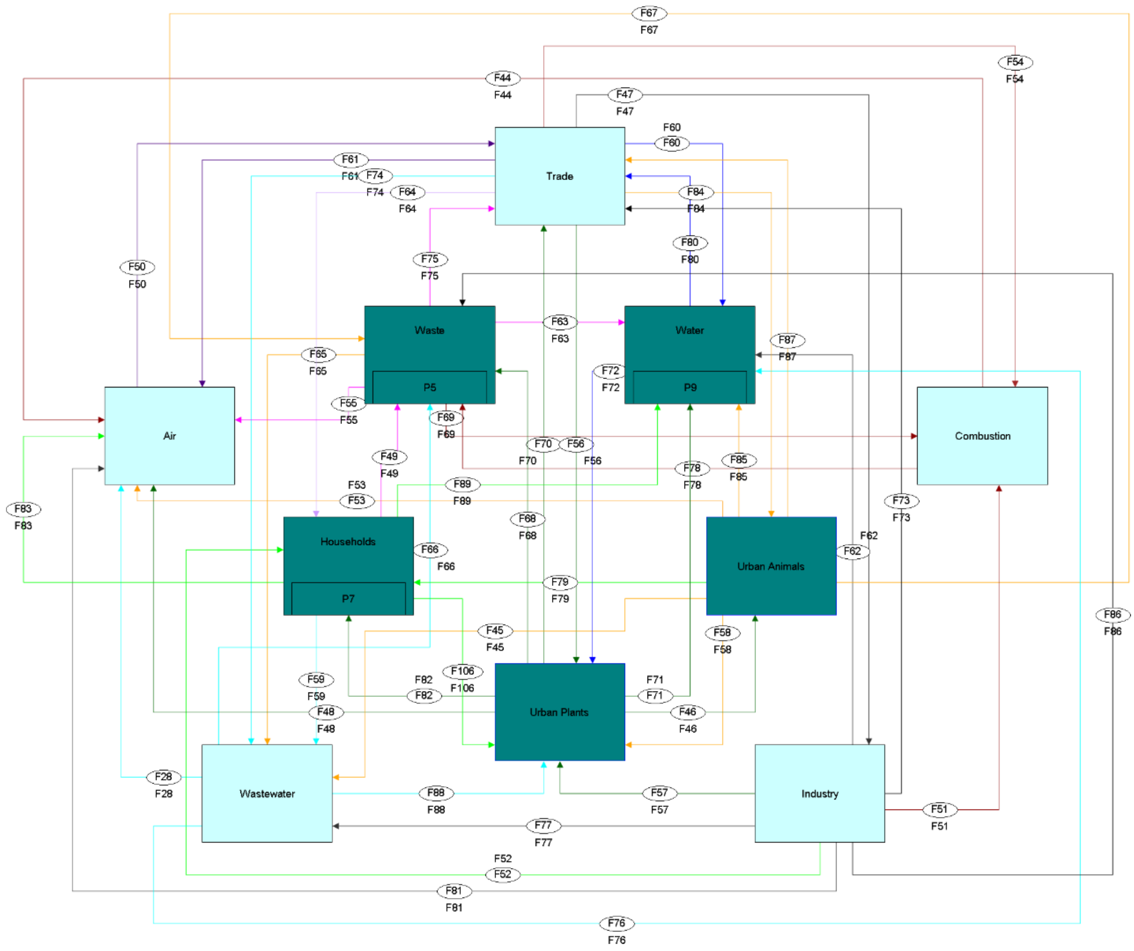

Figure 1 Final Concept of Urban Nitrogen Flows as implemented in STAN

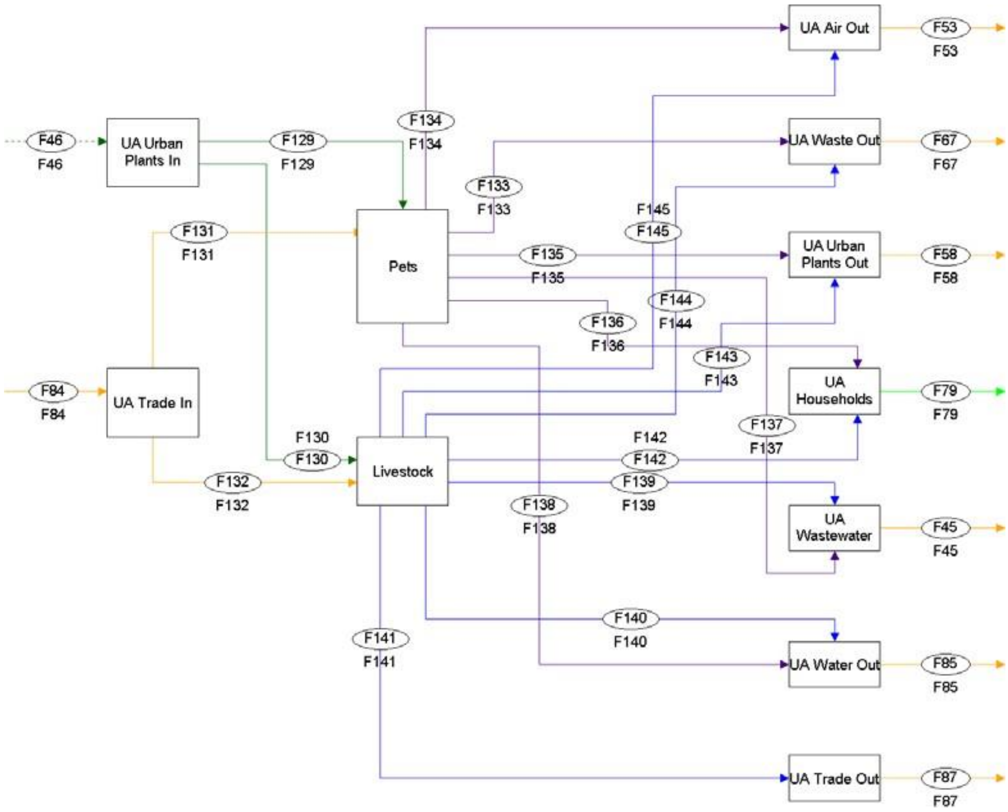

Figure 2 Stock and Flows considered in the subsystem 'Urban Animals'

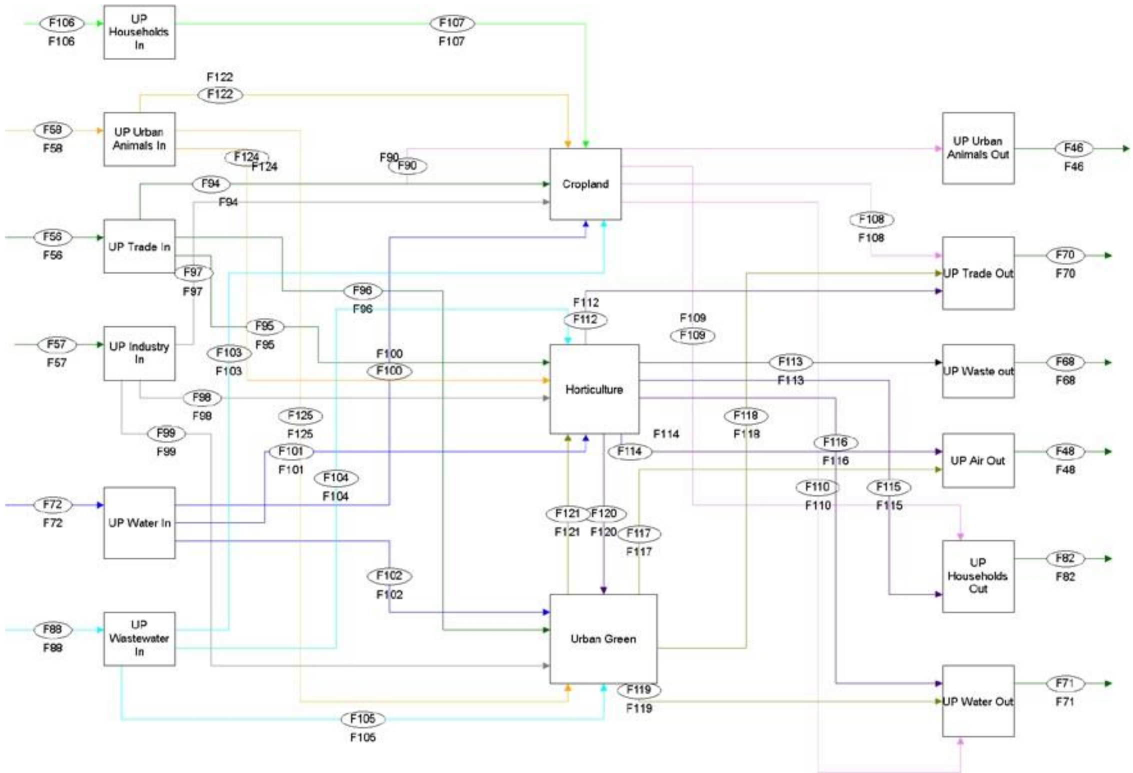

Figure 3 Stock and Flows considered in the subsystem 'Urban Plants'

Concept for Data Exchange

Several models will be involved in the calculation of urban N budgets. Therefore, a concept for data exchange between these models is needed. As STAN will be used for the final N budget calculation, it is the center piece of the data exchange. Depending on the other models' requirements data will be transported to or from STAN. Figure 4 gives an overview of the models involved and the type of data transferred between them.

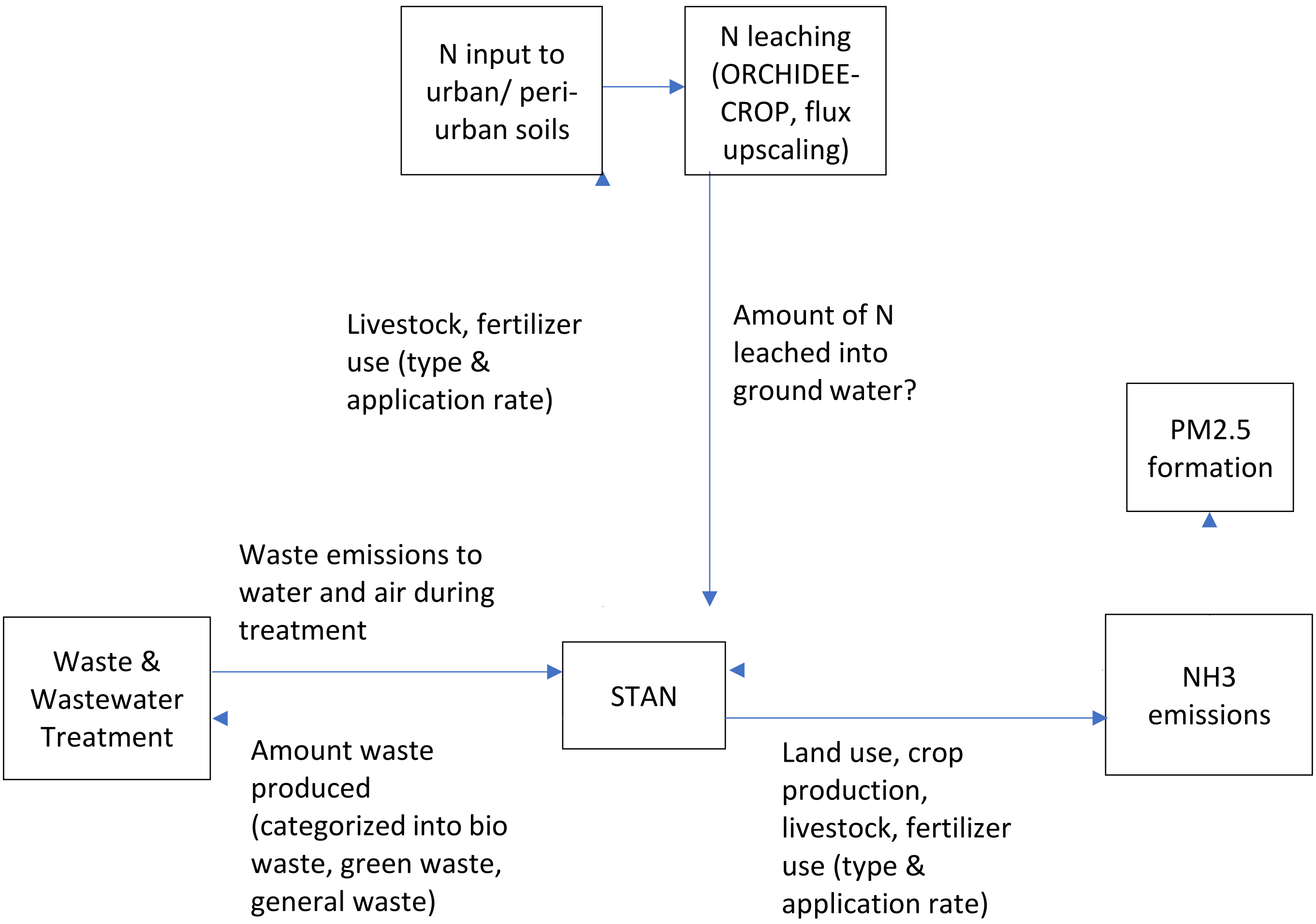

Figure 4 Data transfer between different models

Table 1-4 show details on the data used by each model. The first column indicates which data is needed by each model to arrive at the final results. The second column states the source that has been used so far. This source can also be another model. Data for which this column remains empty needs to be collected. Column three states the extent of the data which can be either global or limited to a city or region. In the latter case, global data or city specific data needs to be collected additionally. The fourth column states the years covered by each model while the fifth column indicates the resolution in which the data is available or required. Data available in higher resolution and greater extent can be aggregated to fit each city's extent using shape files which have previously been provided by each research team from the respective city. The seventh column gives information on other models to which data, either required for or calculated by each model, can be exported.

These tables will be central to the data collection as well as the data exchange. When all data noted down in these tables is available, it will be imported into STAN and urban N budgets for Beijing, Vienna, Zielona Góra and Shijiazhuang will be calculated.

Table 1 Data used in the NH3 model

	data available for all cities					
NH3 atmospheric model - Lin Zhang						
item	**source**	**extent**	**years covered**	**resolution**	**extra info**	**exported to**
Land use	MODIS	global	2005-2012	500 m		STAN
crops	Earthstat	global	2000	5'	18 crop types used (M3)	STAN
fertilizer type	IFA	global		countries/regions		STAN
fertilizer use	NBSC	China	2005-2016	province		STAN
pH						
CEC						
temperature	GEOS-FP	global		0.25deg x 0.3125deg		
wind	GEOS-FP	global		0.25deg x 0.3125deg		
livestock	GLW	global	2010	5'		STAN
livestock calibration	NBSC	China	2005-2016	province		
NH3 emission from non-agricultural activities	Kang et al. (2016)	China	2005-2012	1000m		

	data available for all cities					
NH3 atmospheric model - Lin Zhang						
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Land use	MODIS	global	2005-2012	500 m		STAN
crops	Earthstat	global	2000	5'	18 crop types used (M3)	STAN
fertilizer type	IFA	global		countries/regions		STAN
fertilizer use	NBSC	China	2005-2016	province		STAN
pH						
CEC						
temperature	GEOS-FP	global		0.25deg x 0.3125deg		
wind	GEOS-FP	global		0.25deg x 0.3125deg		
livestock	GLW	global	2010	5'		STAN
livestock calibration	NBSC	China	2005-2016	province		
NH3 emission from non-agricultural activities	Kang et al. (2016)	China	2005-2012	1000m		

Table 2 Data used in the N input and irrigation model

N inputs & irrigation model / leaching - Feng Zhou						
item	**source**	**extent**	**years covered**	**resolution**	**extra info**	**exported to**
water use	2nd National Water Reso	China	1965-2000	prefectures		STAN
water use	Water Ressources Bulleti	China	2001-2013	31 provinces		STAN
irrigated area per crop	statistical year book	China		31 provinces		STAN
irrigated areas	HYDE	global	-2017	5'		STAN
fertilizer use	several national surveys	China	county	~2900 counties	9 crop types	STAN
manure N applied to CL	Eubolism model	China	county			STAN
N deposition	LMDZ-OR-INCA	global		1.27deg x 2.5deg	validated only for chinese dat	STAN
agriculture management practice (e.g. tillage, cropping systems, application rate)		urban & suburban area	1995-2030 - base year 2015			
land use area (cropland horticulture etc)		urban & suburban area	1995-2030 - base year 2015			

Table 3 Data used for waste and wastewater calculations

Waste						
item	**source**	**extent**	**years covered**	**resolution**	**extra info**	**exported to**
Material Recovery Facility		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
Anaerobic digestion		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
landfilling		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
composting green waste						
check degree of utilisation & processes in city		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban	is composition assumed to be the same everywhere	
garden waste (mass & composition(&DOM, %DM, etc needed)	STAN (horticulture, urban	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban	all data on waste will be collected to fit STAN pools	
composting bio waste						
check degree of utilisation & processes in city		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
biowaste (mass & composition)	STAN (households)	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
composting sewage sludge						
check degree of utilisation & processes in city		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
sewage sludge (mass & composition)	wastewater component	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
mechanical-biological treatment biostabilization						
check degree of utilisation & processes in city		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban	mostly mixed municipal waste	
waste (mass & composition)	STAN (households)	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
mechanical-biological treatment biodrying						
check degree of utilisation & processes in city	mostly mixed municipal w	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
waste (mass & composition)	STAN	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
fermentation						
check degree of utilisation & processes in city		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban	mostly mixed municipal waste	
waste (mass & composition)	STAN	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
waste incineration						
check degree of utilisation & processes in city		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
waste (mass)	STAN	city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
combustion technology		city (urban vs peri-urban)	1995-2030 - base year 2015	divided into urban/peri-urban		
Wastewater						
population		city (urban vs peri-urban)	1995-2030 - base year 2015	gridded? 5'		STAN
country specific protein supply	Food Balance Sheets of F	city (urban vs peri-urban)	1995-2030 - base year 2015			STAN
check treatment systems & degree of utilisation		city (urban vs peri-urban)	1995-2030 - base year 2015		treatment systems: no treatment, primary (mechani	

Table 4 Data used in STAN

STAN							
item	**source / imported from**	**extent**	**years covered**	**resolution**	**extra info**	**exported to**	**STAN Flows**
urban animals							
urban livestock distribution							
spatial distribution, livestock systems	input/irrigation model?	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			
amount of manure N to cropland, horticulture and urban greens	input/irrigation model	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urba	trade between urban/peri-urb	input/ irrigation mod	F122, F124, F
urine flushed into wastewater in urban livestock system			1995-2030 - base year 2015		livestock system dependent (	waste model	F139, F45
manure N leached	leaching model		1995-2030 - base year 2015				F140, F85
export of urban livestock products (meat, milk, eggs etc)		city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urba	trade between urban/peri-urban area?		F141, F87
urban livestock products consumed in households		city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urba	trade between urban/peri-urban area? - probably p		F142, F79
disposed of manure, feed, carcasses etc in waste			1995-2030 - base year 2015		livestock system dependent (	waste model	F144, F67
N volatilization from livestock manure	NH3 model		1995-2030 - base year 2015		livestock system dependent (also resolution & exte		F145, F53
pets							
amount of pets and spatial distribution - urban, peri-urban		city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			
N volatilization from pet manure	NH3 model		1995-2030 - base year 2015				F134, F53
manure N excreted in urban greens (parks and gardens)	input/irrigation model?	city (urban vs peri-urban)	1995-2030 - base year 2015		pet specific N excretion rate?, spatial resolution de		F135, F58
pet manure N run-off to wastewater		city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			F137, F45
Amount of N from pets to households (manure)			1995-2030 - base year 2015				F136, F79
Amount of N from pets to water (manure leaching)	leaching model		1995-2030 - base year 2015				F138, F85
Amount of N from pets to waste (manure N from pets (collected manure N on walks disposed of in public waste bins)			1995-2030 - base year 2015			waste model	F133, F67
water							
amount and N content of water	leaching model?	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			
water useage shares for cropland, horticulture, urban greens	input/irrigation model	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			F100, F101, F
export of N in water e.g. from urban to suburban area		city (urban vs peri-urban)	1995-2030 - base year 2015				F80
waste water							
amount and N content of waste water	waste model?	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			
waste water useage shares for cropland, horticulture, urban greens	input/irrigation model	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban		input/irrigation mode	F103, F104, F
N emissions from wastewater	waste model	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			F28
sludge to waste (N content)	waste model		1995-2030 - base year 2015		waste model internal flow depends on waste and w		F66
share of treated wastewater to water	waste model		1995-2030 - base year 2015	divide between urban & peri-urba	dependent on distribution of wastewater treatment		F76
urban plants							
land use data (spatial distribution of horticulture, urban green, cropland) for disaggregation of data available as shape file	NH3 model	city (urban vs peri-urban)	1995-2030 - base year 2015	5' (peri-urban & urban)			
horticulture							
type and N content of flowers grown			1995-2030 - base year 2015		extent & resolution depends on land use data/ is derived from la		
amount of flowers exported (traded)			1995-2030 - base year 2015		trade between urban & peri-urban region, extent &		F112, F70
amount of flowers etc in horticulture to waste			1995-2030 - base year 2015		extent & resolution depends	waste model	F113, F68
amount of flowers etc to households (flowers indoors/on balcony - not in garden)			1995-2030 - base year 2015		trade between urban & peri-urban region, extent &		F115, F82
share of flowers etc to urban greens (flowers in parks, private gardens)			1995-2030 - base year 2015		trade between urban & peri-urban region, extent &		F120
N volatilization	NH3 model		1995-2030 - base year 2015		extent & resolution depends on land use data/ is d		F114, F48
N leaching	leaching model		1995-2030 - base year 2015		extent & resolution depends on land use data/ is d		F116, F71
cropland							
type and N content of crops			1995-2030 - base year 2015		extent & resolution depends on land use data/ is derived from la		
amount of crops exported			1995-2030 - base year 2015		extent & resolution depends on land use data/ is d		F108, F70
amount of crop N to urban livestock			1995-2030 - base year 2015		extent & resolution depends on land use data/ is d		F90, F130, F4
amount of crop N to pets							F90, F129, F4
N leaching	leaching model	city (urban vs peri-urban)	1995-2030 - base year 2015		extent & resolution depends on land use data/ is d		F110, F70
amount of crops to household as food			1995-2030 - base year 2015		trade between urban & peri-urban region		F109, F82
N volatilization	NH3 model	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urba	extent & resolution depends on land use data/ is derived from la		
urban greens							
type and N content of urban greens			1995-2030 - base year 2015		extent & resolution depends on land use data/ is derived from la		
N volatilization	NH3 model	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urba	extent & resolution depends on land use data/ is d		F117, F48
N leaching	leaching model	city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urba	extent & resolution depends on land use data/ is d		F119, F70
Amount of N from urban green to trade			1995-2030 - base year 2015				F118, F70
Amount of N from urban green to horticulture (green manure)			1995-2030 - base year 2015				F121
Amount of N from gardens etc to waste (garden waste)							
Industry							
type and location of industry in urban vs peri-urban areas		city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			
amount of industrial production to households, trade and urban plants (seeds, fertilizer, textiles etc - depending on industry)	fertilizer from input/irrigation model?		1995-2030 - base year 2015		trade between urban & peri-u	fertilizer data to inpu	F52, F73, F97
N emissions from industry			1995-2030 - base year 2015		extent & resolution depends on industry location da		F81
industrial waste (composition)			1995-2030 - base year 2015		extent & resolution depends	waste model	F86
Amount of N from industry to combustion (heating, etc)			1995-2030 - base year 2015				F51
Amount of N from industry to water (cooling water? Leaks?)			1995-2030 - base year 2015				F62
Amount of N from industry to wastewater	IPCC guidelines Table 6.11		1995-2030 - base year 2015				F77

trade statistics for cities - broken down from country statistics, per capita?			1995-2030 - base year 2015	divide between urban & peri-urban			
amount of traded goods going to industry, households, combustion, urban plants and urban animals (seeds, fertilizers, textiles, food, nitrogen enriched fuel, feed)		city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			F131, F132, F
Amount of N from trade to wastewater (e.g. waste water treated within boundaries coming from outside)		city (urban vs peri-urban)	1995-2030 - base year 2015			waste model	F74
Amount of N from trade to air (emissions from outside boundaries e.g. suburbs)			1995-2030 - base year 2015				F61
Amount of N from trade to water (N transported from outside to water inside boundaries)			1995-2030 - base year 2015				F60
Combustion							
location of combustion		city (urban vs peri-urban)		divide between urban & peri-urban			
N emissions from combustion to air (from industry trade and waste)		city (urban vs peri-urban)	1995-2030 - base year 2015	divide between urban & peri-urban			F44
Amount of N from combustion to waste (e.g Ash)			1995-2030 - base year 2015				F78
Air							
flow from air to urban plants - N deposition	NH3 model		1995-2030 - base year 2015		extent & resolution depends on land use data/ is derived from la		
Amount of N from air to trade (export of emissions)			1995-2030 - base year 2015				F50
Household							
spatial distribution of households - people per household?		city (urban vs peri-urban)		divide between urban & peri-urban			
any kind of waste - composition of waste (share of residual, organic, plastic, textiles??) needed			1995-2030 - base year 2015			waste model	F49
human excreta - population, country specific protein supply (IPCC/FAO Food Balance sheet)			1995-2030 - base year 2015		people per household needed	waste model	F59
N emissions (household-air) from heating/ cooking with gas or petroleum			1995-2030 - base year 2015				F83
Amount of N from households to urban plants (Fertilizer, compost)			1995-2030 - base year 2015				F106, F107
Waste							
location of & type of waste treatment plants		city (urban vs peri-urban)		divide between urban & peri-urban			
N emissions from waste	waste model		1995-2030 - base year 2015				F55
N leaching from waste	waste model		1995-2030 - base year 2015			leaching model?	F63
N (waste to wastewater) from dewatering in MBT eg	waste model		1995-2030 - base year 2015				F65
waste incineration	waste model		1995-2030 - base year 2015				F69
amount of waste traded (type of waste, N content)			1995-2030 - base year 2015				F75

Concept for Uncertainty Consideration

The integration of uncertainties is an important element of quality assurance as it helps to estimate the influence of imperfect information on the calculated quantities (EPNB 2011). This is also reflected in the STAN model used for the urban N budget calculations as for every quantity its standard error should be included.

According to its manual, the STAN model assumes uncertain quantities to be normally distributed and characterized by their mean value and standard deviation. Such an assumption would therefore allow STAN using methods like error propagation and data reconciliation which are based on the weighted least square approach (IWR, 2012).

In order to facilitate the understanding of the present uncertainty concept, the statistical notions of Standard Deviation (SD) and Standard Error (SE) are firstly briefly clarified hereunder.
While the SD acts as a descriptive statistic estimating the variability of the population from which a given sample is drawn; the SE (of the estimate of the mean) is defined as the SD of the sampling distribution of the mean and rather represents a measure of the precision of the sample mean. (Altman and Bland 2005)

If the SD appears on the one hand relatively independent of the sample size and the considered distribution; the SE is on the other hand inversely proportional with the sample size, hence falling as the extent of chance variation is decreased. The fact that the SE appears as a specific type of SD remains a large source of confusion in the literature and should therefore be carefully dealt with. (Olsen 2003)

The two parameters can be expressed as follows in Eqs. (1)-(2):

$$SD = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2}\ , \ where\ \mu = \frac{1}{N} \sum_{i=1}^{N} x_i \qquad (1)$$

$$SE = \frac{SD}{\sqrt{N}} \qquad (2)$$

Where:

- SD is the standard deviation
- SE is the standard error (standard uncertainty);
- N is the sample size;
- μ is the mean of the sample and;
- x_i are the collected samples' values (i=1, …, N).

In order to remain consistent with the above mentioned STAN assumptions, a normal distribution describing the collected data is therefore assumed in UNCNET. As seen in

Figure 5, more than 95% of the events following a normal distribution are encompassed within 2 SDs of the mean. The SD being a convincing estimate of the variability regardless of the distribution, it is worthwhile to note that about 95% of observations of any distribution would generally fall within 2 SDs of the mean. (Altman and Bland 2005)

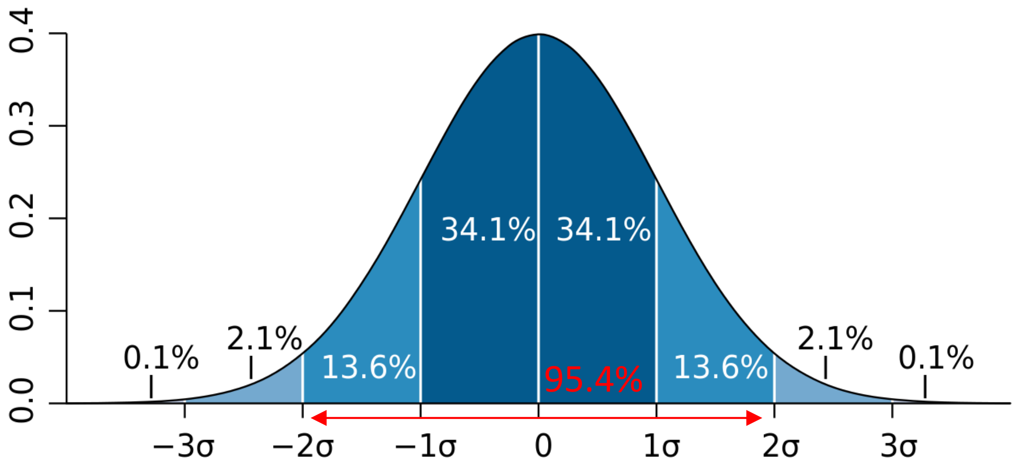

Figure 5 – Normal distribution of mean 0 and standard deviation 1σ. Adapted from (Wikipedia 2021).

Sample size

Depending on the sample size, different approaches to calculate the standard deviations of the various samples are taken. The present section describes the various procedures to be considered for the cases of sample sizes of N=1, N=2 and N>2.

- ***N = 1***

When only a single data point is available, Uncertainty Factors (UFs) derived from (Winiwarter and (EPNB) 2016) and associated to a given level of uncertainty are used, as seen in the following Table 5:

Table 5 – Levels of uncertainty and their corresponding field of application. Adapted from (Winiwarter and (EPNB) 2016)

Level	Uncertainty Factor (UF)	Relative Standard Deviation (RSD)	Application
1	1.1	0.048	current official statistics, measurement data, data from appropriate literature
2	1.33	0.145	expert estimates, outdated official statistics, unofficial statistics, presentations, industry reports
3	2.0	0.375	assumptions for which neither official statistics nor expert estimates were available often based on on-line data sources or publications without accurate literature reference
4	4.0	0.938	an estimate based on a calculation derived from assumptions only

The likely value of a given flow is both multiplied and divided by the corresponding UF to derive the range of the Uncertainty Interval (UI), as expressed by the following Equation (3):

$$r = (x * UF) - (x/UF) \tag{3}$$

Where:

- x is the likely value of the flow in [g. N. cap^{-1}];
- r is the range of the UI in [g. N. cap^{-1}] and;
- UF is the uncertainty factor (see Table 5).

Depending on the uncertainty level associated to the data, discrete values for the UF ranging from 1.1 to 4.0 are chosen.

On that basis, SDs and SEs of the various involved flows are then computed assuming a normal distribution of mean equal to the single collected data point x and of SD equal to a fourth of the UI's range r defined above. The latter specific assumption would in particular allow about 95% of the samples of such a distribution to fall between the UI (cf. Figure 5).

This is summarized through the following set of Eqs. (4) - (6):

$$UI = [x - \frac{r}{2}; x + \frac{r}{2}] \tag{4}$$

$$RSD = \frac{(UF - \frac{1}{UF})}{4} \tag{5}$$

$$SD = \frac{r}{4} = RSD * x \tag{6}$$

Where:

- UI is the uncertainty interval;
- RSD is the relative standard deviation (see Table 5) and;
- SD is the standard deviation of the considered normal distribution in [g. N. cap^{-1}].

- ***N = 2***

For the cases with more than a single collected data point, UFs are no longer used to derive the UI and the associated SD. The mean corresponds in the case of N=2 to the middle of the UI which is simply bounded by the two collected values, as expressed by the following Eqs. (7) - (9):

$$r = (x_2 - x_1) \tag{7}$$

$$UI = [x_1;\ x_2] \tag{8}$$

$$\mu = \frac{(x_2 - x_1)}{2} \tag{9}$$

Where x_1 and x_2 are the two collected values in [g. N. cap-1] and $x_1 < x_2$.
SDs and SEs remain computed following the Eqs. (2) and (6) with the updated values of r and N.

- ***N > 2***

For the rest of cases encompassing sample sizes strictly greater than two data points, the standard deviation and mean of the sample are straightforwardly computed according to their formula, that respectively correspond to Equ.(1). and the following Equ. (10):

$$\frac{1}{N}\sum_{i=1}^{N} x_i \tag{10}$$

Where:

- N is the sample size;
- x_i are the collected samples' values (i=1, …, N).

The following Table 6 summarizes the relevant parameter formulas for the different above mentioned cases:

Table 6 – Parameter computation summary in function of the sample size tier.

	N=1	N=2 (x_1, x_2), $x_2 > x_1$	N>2 $(x_1, x_2, \ldots, x_N)$
Mean	x	$(x_2 - x_1)/2$	$\frac{1}{N}\sum_{i=1}^{N} x_i$
Standard Deviation (SD)	RSD* x	$(x_2 - x_1)/4$	$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2}$
Standard Error (SE)	$\frac{SD}{\sqrt{N}}$		

Covariance and Correlation

Another requirement for the calculation of error propagation, supporting the data reconciliation tool in STAN, is the independence of input data. The combination of dependent data can lead to an underestimation of the overall uncertainty (Winiwarter & Rypdal, 2001; Winiwarter & Muik, 2010). To test the relation between separate flows going into one pool, Spearman's Rank Correlation Hypothesis Testing will be applied to check their correlation in case more datapoints are available for each flow. Spearman is chosen as it is a non-parametric measure for correlation using a monotonic function to assess relationships between input data rather than expecting a purely linear relationship (Dytham, 2011).

D … rank difference
n … number of data pairs

$$r_s = 1 - \frac{6\sum D^2}{n(n^2-1)} \quad (10)$$

Once the Spearman correlation coefficient has been calculated, hypothesis testing can be used to check whether the Nullhypothesis of no correlation ($r_s = 0$) is rejected using a predefined significance level (α). This check can be done either using Spearman's rho table to find the corresponding r_s for the significance level chosen or by calculating t according to (11) and comparing it to critical t of the chosen significance level taken from a table or calculated.

$$t = \frac{r_s}{\sqrt{\frac{1-{r_s}^2}{n-2}}} \quad (11)$$

Sensitivity Analysis

The Spearman coefficient can also be used to get information of each inflow's contribution to the total outflow using Monte Carlo simulation (Winiwarter & Rypdal, 2001).

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