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Global sensitivity analysis in wastewater applications: A comprehensive comparison of different methods

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ABSTRACT

Three global sensitivity analysis (GSA) methods are applied and compared to assess the most relevant processes occurring in wastewater treatment systems. In particular, the Standardised Regression Coefficients, Morris Screening and Extended-FAST methods are applied to a complex integrated membrane bioreactor (MBR) model considering 21 model outputs and 79 model factors. The three methods are applied with numerical settings as suggested in literature. The main objective considered is to classify important factors (factors prioritisation) as well as non-influential factors (factors fixing). The performance is assessed by comparing the most reliable method (Extended-FAST), by means of proposed criteria, with the two other methods. In particular, similarity to results obtained from Extended-FAST is assessed for sensitivity indices, for the ranking of sensitivity indices, for the classification into important/non-influential factors and for the method's ability to detect interaction among factors and to provide results in a reasonable time.

It was found that the computationally less expensive SRC method was applied outside its range of applicability $(R^2) = (0.3-0.6) < 0.7$. Still, the SRC produced a ranking of important factors similar to Extended-FAST. For some variables significant interactions among the factors were revealed by computing the total effect indices S_{Ti} using Extended-FAST. This means that to obtain reliable variance decomposition and to detect and quantify interactions among the factors, the use of the Extended-FAST is recommended. Regarding the comparison between Morris screening and Extended-FAST a poor agreement was found. In particular, the Morris screening overestimated the number of both important and non-influential factors compared to Extended-FAST for the analysed case study.

1. Introduction

In the field of mathematical modelling sensitivity analysis represents a very powerful tool as it provides information about how the variation in the outputs of the model can be apportioned to the variation of the model (input) factors (Saltelli, 2000). "Factors" is a term widely used in the sensitivity analysis literature and includes model parameters and model input variables. Saltelli (2000) singles out three main classes of sensitivity analysis methods: screening methods, local methods and global methods. Screening methods are economical and qualitative methods. Local methods provide a measure of how the model output is affected by infinitesimal factor changes at a specific location in factor space. Global sensitivity analysis (GSA) provides information on how the model outputs are influenced by factor variation over the whole space of possible input factor values (Homma and Saltelli, 1996; Saltelli et al., 2004).

In the environmental modelling field the majority of sensitivity analysis applications are local. Moreover, often a one-at-a-time approach is used that does not allow identifying interacting factors. In recent years, several GSA techniques have been developed. Among them the most widely used are: (i) global screening methods such as the Morris screening method (Morris, 1991; Campolongo et al., 2007); (ii) variance decomposition methods such as Fourier Amplitude Sensitivity Testing (FAST), Extended-FAST and the Sobol indices method (Cukier et al., 1973; Schaibly and Shuler, 1973; Saltelli et al. 1999; Sobol, 2001); and (iii) regression-based methods such as the standardised regression coefficient (SRC) method (Saltelli et al., 2008). GSA may help the

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List of symbols and abbreviations

MBR	Membrane BioReactor
FAST	Fourier Amplitude Sensitivity Test
SRC	Standardised Regression Coefficient
GSA	Global Sensitivity Analysis
ASM	Activated Sludge Models
UCT	University of Cape Town
SMP	Soluble Microbial Product
TSS	Total Suspended Solids
VSS	Volatile Suspended Solids
COD	Chemical Oxygen Demand
NH_4-N	Ammonia nitrogen
NO_2-N	Nitrite nitrogen
NO_3-N	Nitrate nitrogen
N_{TOT}	Total nitrogen
P_{TOT}	Total phosphorus
COD_{TOT}	Total COD model variable
S_{NH_4}	Ammonia nitrogen model variable
S_{NO_3}	Nitrate nitrogen model variable
S_{PO_4}	Soluble inorganic phosphorus model variable
MLSS	Mixed liquor suspended solid
COD_{SOL}	Soluble modelled COD
CTN	Total nitrogen model variable
y	Model output
x_i	ith model factor
b_i	Regression slopes
ε	Random error of the regression model
σ_{x_i}	ith factor standard deviation
σ_y	Model output standard deviation
β_i	ith factor sensitivity index
EE	Elementary Effect
p	Sampling level of Morris screening method
Δ	Factor perturbation
μ	Mean of the EEs function
σ	Standard deviation of the EEs function
IF	Interaction among factors
μ^*	Mean of the absolute EEs function
r	Sampling repetition for Morris screening method
n	Model factors number
Var(Y)	Total variance of the model output
S_i	First order effect index of the ith factor
S_{Ti}	Total effect index of the ith factor
N_{MC}	Number of Monte Carlo simulations
S_{Ni}	Normalised interaction index
ρ_s	Spearman's rank correlation index
r_P	Pearson correlation index
PF	Position Factor
Rel	Relevance
NS	Number of simulations
PAOs	Phosphorus Accumulating Organisms
$Rel_{IMPORTANT}$	Relevance of important factors
$Rel_{NON-INFLUENTIAL}$	Relevance of non-influential factors
k_H	Maximum specific hydrolysis rate
$\eta_{NO_3,HYD}$	Correction factor for hydrolysis under anoxic conditions
η_{FE}	Correction factor for hydrolysis under anaerobic conditions
K_O	Half saturation parameter for SO_2 for X_H
S_{O_2}	Dissolved oxygen
X_H	Ordinary heterotrophic organisms
X_S	Particulate biodegradable organics
X_H	Ordinary heterotrophic organisms
K_{NO_3}	Half saturation parameter for S_{NO_3} for X_H
K_x	Half saturation parameter for X_S/X_H
S_F	Fermentable organic matter
S_A	Fermentation product (considered to be acetate)
X_{PAO}	Phosphorus accumulating organisms model variable
X_{PP}	Stored polyphosphates in PAOs
X_{PHA}	Storage compound in PAOs
S_{ALK}	Alkalinity (HCO_3^-)
X_{AUT}	Autotrophic nitrifying organisms
S_{BAP}	Soluble biomass associated products
S_{UAP}	Soluble utilisation associated products
S_I	Soluble undegradable organics
X_I	Particulate undegradable organics
$K_{O,HYD}$	Half saturation/inhibition parameter for S_{O_2}
$K_{NO_3,HYD}$	Half saturation/inhibition parameter for S_{NO_3}
μ_H	Maximum growth rate of X_H
q_{FE}	Rate constant for fermentation/Maximum specific fermentation growth rate
$\eta_{NO_3,H}$	Reduction factor for anoxic growth of X_H
b_H	Decay rate for X_H
K_F	Half saturation parameter for S_F
K_{FE}	Half saturation parameter for fermentation of S_F
K_A	Half saturation parameter for S_A
$K_{NH,H}$	Half saturation parameter for S_{NH_4} for X_H
K_P	Half saturation parameter for S_{PO_4} for X_H
$K_{ALK,H}$	Half saturation parameter for S_{ALK} for X_H
q_{PHA}	Rate constant for S_A uptake rate
q_{PP}	Rate constant for storage of polyphosphates
μ_{PAO}	Maximum growth rate of X_{PAO}
$\eta_{NO_3,PAO}$	Reduction factor for anoxic growth of X_{PAO}
b_{PAO}	Endogenous respiration rate of X_{PAO}
b_{PP}	Rate constant for Lysis of polyphospates
b_{PHA}	Rate constant for respiration of X_{PHA}
K_{PS}	Half saturation parameter for S_{PO_4} uptake
K_{PP}	Maximum ratio of X_{PP}/X_{PAO}
K_{MAX}	Half saturation parameter for X_{PP}/X_{PAO}
K_{IPP}	Half inhibition parameter for X_{PP}/X_{PAO}
K_{PHA}	Saturation constant for X_{PHA}/X_{PAO}
$K_{O,PAO}$	Half saturation parameter for S_{O_2} for X_{PAO}
$K_{NO_3,PAO}$	Half saturation parameter for S_{NO_3} for X_{PAO}
$K_{A,PAO}$	Half saturation parameter for S_A for X_{PAO}
$K_{NH,PAO}$	Half saturation parameter for S_{NH_4} for X_{PAO}
$K_{P,PAO}$	Half saturation parameter for S_{PO_4} as nutrient (X_{PAO} growth)
$K_{ALK,PAO}$	Half saturation parameter for S_{ALK} for X_{PAO}
μ_{AUT}	Maximum growth rate of X_{AUT}
b_{AUT}	Decay rate for X_{AUT}
$K_{O,A}$	Half saturation parameter for S_{O_2} for X_{AUT}
$K_{NH,A}$	Half saturation parameter for S_{NH_4} for X_{AUT}
$K_{ALK,A}$	Half saturation parameter for S_{ALK} for X_{AUT}
$K_{P,A}$	Half saturation parameter for S_{PO_4} for X_{PAO}
$k_{H,BAP}$	Hydrolysis rate coefficient for S_{BAP}
$k_{H,UAP}$	Hydrolysis rate coefficient for S_{UAP}
$k_{LaT,3}$	Overall oxygen transfer coefficient aerobic tank
$k_{LaT,4}$	Overall oxygen transfer coefficient MBR tank
Y_H	Yield for X_H growth
f_{X_I}	Fraction of X_I generated in biomass decay
Y_{PAO}	Yield for X_{PAO} growth
Y_{PO_4}	Yield for X_{PP} requirement per X_{PHA} stored
Y_{PHA}	Yield for X_{PP} storage per X_{PHA} utilised
Y_A	Yield of X_{AUT} growth per S_{NO_3}
f_{BAP}	Fraction of S_{BAP} generated in biomass decay
f_{UAP}	Fraction of S_{UAP} generated in biomass decay