**Addressing the Ability of a Land Biosphere Model to Predict Key Biophysical Vegetation Characterisation Parameters with a GSA study**

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**ABSTRACT**

Sensitivity Analysis (SA) of the SimSphere Soil Vegetation Atmosphere Transfer (SVAT) model has been performed in our research using a cutting edge and robust Global Sensitivity Analysis (GSA) approach, based on the use of the Gaussian Emulation Machine for Sensitivity Analysis (GEM-SA) tool. The sensitivity of the following model outputs was evaluated: the ambient CO2 concentration and the rate of CO2 uptake by the plant, the ambient O3 concentration, the flux of O3 from the air to the plant/soil boundary and theflux of O3 taken up by the plant alone. The most sensitive model inputs for the majority of outputs were: The Leaf Area Index (LAI), Fractional Vegetation Cover (Fr), Cuticle Resistance (CR) and Vegetation Height (VH). The influence of the external CO2 on the leaf and O3 concentration in the air as input parameters was also significant. Our study provides a step forward in the global efforts towards SimSphere model verification which is important given the increasing interest in the use of SimSphere as an independent modelling or educational tool. Results of this study are also timely given the ongoing global efforts focused on deriving, at an operational level, the spatio-temporal estimates of energy fluxes and soil moisture content using SimSphere synergistically with Earth Observation data.

**Keywords**: *Sensitivity Analysis*, *CO2 flux, ambient CO2, O3 flux, SimSphere, Gaussian process emulators, BACCO GEM-SA.*

**1. INTRODUCTION**

 The complex interplay between the different facets of land-surface interactions play a fundamental role in the spatio-temporal variations of carbon dioxide (CO2) and ozone (O3)fluxes within the Earth system. Within the atmospheric boundary layer, the exchange of CO2 at the surface is primarily the result of complex vegetation processes (Boussetta et al, 2013). CO2 is assimilated in vegetation by photosynthesis (expressed as gross primary productivity) and is returned to the atmosphere by a variety of above-and below- ground metabolic processes (Bloemen et al., 2013). Stomatal behaviour provides the main short-term control of both transpiration and CO2 assimilation. Crops grown under CO2 enrichment usually exhibit increased mass, which is attributed to greater photosynthetic capacity and enhanced water use efficiency (Olvera et al., 2013). Carbon assimilation and water dynamics are inherently linked to crop yield and so an understanding of these relationships is fundamental to our ability to understand, or predict, plant productivity. The Intergovernmental Panel on Climate Change (IPCC) predicts concentrations of atmospheric CO2 to continue rising from their current concentrations of ~395ppmv to > 420ppmv by 2050 (IPCC, 2001). Therefore, understanding the interactions between plants and environment is a central requirement when forecasting the effects of future climate change and variability (Williams et al., 2012).

 Tropospheric ozone is a phytotoxic air pollutant responsible for crop and forest damage worldwide (Panek, 2004). The impact of O3 exposure usually manifests as necrotic lesions, decreased photosynthesis and accelerated senescence (Pell et al., 1997; Wiese and Pell, 1997). The exact mechanism by which O3 stress is imposed is unclear but probably occurs through the formation of reactive oxygen species such as superoxide and hydrogen peroxide (Pell et al., 1997). Furthermore, stomatal control may be reduced following exposure to O3 which causes greater susceptibility to drought stress (McLaughlin et al., 2007). This has major implications for tree and crop performance in the future climate as temperatures are predicted to increase (thus increasing transpiration) along with a greater areas affected by more frequent drought (IPCC, 2014). The effect of O3 stress on stomatal regulation and implications for drought susceptibility has been found to offset much of the projected benefit of rising CO2 for plant growth in some biogeochemical models (Ollinger et al., 2002). The direct reduction in forest productivity currently caused by O3 stress is estimated to be 1-10% for forests in Europe and North America (Broadmeadow, 1998). Thus O3 is clearly an important economic factor in biomass production and there is a need to understand its influence on plant processes (Ainsworth et al., 2012; Konovalov, et al., 2012). To this end, an improved quantification of the effect of atmosphere-land-surface interactions on the spatio-temporal distribution of CO2 and O3 fluxes will enable the development of coherent plans to manage ecosystems for future climate mitigation and agricultural production (Pitman et al., 2012; Williams et al., 2012).

 In this context, a representative description of land surface-atmosphere interaction requires mathematical models able to accurately describe interdependent physical and biological processes in vegetation and soil, as well as physical processes within the atmospheric boundary layer (Marras et al., 2011). Several modelling approaches have been developed to represent the terrestrial carbon cycle depending on the main goals of the modelling effort. Aggregated ‘big leaf’ models for instance, act to simulate selected mass, water and energy transfers from a representative leaf surface which is scaled up to the whole canopy, either based on simple linear scaling or on a non‐linear scaling by partitioning between sunlight and shaded leaves (Ganzeveld et al., 2012). Generally, these models are widely regarded as the simplest group of models, but behold vast application value such as data gap filling and tracing gas fluxes (Baldocchi, 2010). SVAT models are more complex ‘distributed multilayer models’ which differ in their approach to estimate surface exchanges. These embedded modelling efforts are numerical representations of the multifarious interactions of energy and mass transfers through the soil/vegetation/atmospheric 1-dimensional vertical column (Marras et al., 2011). They require an application context constrained by input variables (atmospheric forcing and vegetation variables) and input parameters (soil and vegetation properties, initialisation) to simulate the water and energy budget at the surface. The number of parameters is generally related to the complexity of the model and their calibration requires the development of optimisation methodologies (Coudert and Ottle, 2007).

 A variation on the SVAT model architecture, termed SimSphere, was originally developed by Carlson and Boland (1978) within the Department of Meteorology of Pennsylvania State University, USA, and has continued to be developing over a period of more than two decades. Notably, during this period the model has undergone significant modifications by a number of contributors, most recently by Petropoulos et al. (2013a). Briefly, it is a one-dimensional boundary layer model with a plant component implicitly referring to a horizontal area of undefined size that can be composed of a mixture of bare soil and vegetation. In addition to its use as a stand-alone modelling tool, it is also integrated synergistically with Earth Observation (EO) data, via a method termed the “triangle” method (Carlson, 2007; Petropoulos & Carlson, 2011). This method interprets the relationship between a Vegetation Index (VI) and surface radiative temperature (Ts) derived from a satellite-derived scatter plot, linked with a SVAT model to deduce evaporative fraction (EF) over large areas (Long and Singh, 2013). Variants of this method are at present being considered for the development of operational products from EO data, some anticipated to be delivered on a global scale (Chauhan et al., 2003; ESA STSE, 2012). However, being a mathematical representation of natural processes, such modelling approaches require a considerable number of assumptions on model structure, model parameter values and model input variables. These input parameters can lead to output uncertainty and inaccuracy (Cosenza et al., 2014; Vanuytrecht et al., 2014). Thus, Sensitivity Analysis (SA) is an essential and well-established tool that has been used in evaluating robustness of model based results (Feyissa et al., 2012; Ratto et al., 2012). In particular, SA quantifies the influence of each uncertain factor (parameter or driving variable) on the model’s output variability (Gan et al., 2014). It can help to determine the relationship between independent and dependent variables to get a better understanding of the model performance. Reasons for performing SA are diverse; it allows for Factor Fixing (FF), where factors that are non-influential can be set to a fixed value anywhere in their uncertainty range and it would not affect model output variance. Factor Prioritisation (FP) on the other hand, is where the modeller focuses on the parameters that have the potential to maximally reduce model output variance if determined. For the case of FP, SA allows for better estimation of the actual factor value and distribution (Nossent et al., 2011; Gamerith et al., 2013).

 SA methods are generally classified as either Local Sensitivity Analysis (LSA) or Global Sensitivity Analysis (GSA). In LSA methods each factor is perturbed in turn from randomly generated reference parameter sets, whilst holding all others to their central value and computing the difference in the outputs (Wainwright et al., 2013; Baroni and Tarantola, 2014). Although a computationally frugal method, LSA can be criticised for being inadequate for analysing complex biophysical process models which may have many parameters, and may be high-dimensional and/or non-linear (Song et al., 2012; Wainwright et al., 2013). Compared with LSA, GSA provides quantitative importance measures that relate the variance of the output with each input dependent variable on different sources of variation over the entire parameter space (Wei et al., 2013). Furthermore, GSA approaches are not limited by model complexity and provide robust sensitivity measures in the presence of non-linearity and interactions amongst parameters. However, the model complexity and high number of parameters can be computationally intensive and inefficient (Gatelli et al., 2009; Wainwright et al., 2013; Gan et al., 2014). Given the intricacy of the physical interconnections involved in modelling land surface-atmosphere interactions, GSA has become popular in the environmental modelling field in recent years. The complexity of such models and their ability to incorporate parameter interactions can be a significant advantage when deriving simulation outputs that are fully analogous of the real world system in terms of accuracy, generality and realism (Anderson et al., 2008). A number of studies have thus performed advanced GSA on SimSphere based on a Gaussian process emulator (Petropoulos et al. 2009b, 2010, 2013b–d). These allowed, for the first time, an insight into the model architecture and the mapping of the sensitivity between the model inputs and outputs. However, SA studies on SimSphere have been limited to only a small number of output parameters, and the effect of different simulation times on model sensitivity has yet to be explored.

 In this context, the objective of this study is two-fold: i) To perform a GSA to explore the sensitivity of target quantities simulated by SimSphere for the model inputs/outputs, which have not been previously investigated. These parameters are namely; the ambient CO2 concentration [ppmv], the rate of uptake of CO2 by the plant [*µmol m-2 s-1*], the ambient O3 concentration [*ppmv x 10-3*], the flux of O3 from the air to the plant/soil boundary [*mg m-2 s-1*], the flux of O3 taken up by the plant alone [*mg m-2 s-1*].

ii) To extend the GSA on SimSphere and to explore the sensitivity of the same target quantities at different simulation times (9:30/11:30/13:30), which coincide closely to the satellite overpass times of different satellite sensors. These objectives will allow us to foster our understanding of the model structure and further establish its coherence.

**2. SimSphere SA Studies**

SimSphere is a one-dimensional boundary layer model with a plant component implicitly referring to a horizontal area of undefined size that can be composed of a mixture of bare soil and vegetation. An overview of the model use was recently provided by Petropoulos et al. (2009a). An excellent systematic overview of the SimSphere model architecture and its initialisation process is available in Gillies (1993); The model is able to simulate the various physical processes and interactions that take place in a column that extends from the root zone below the soil surface up to the surface mixing layer over a 24-h cycle at a chosen time step (typically 3 minutes), starting from a set of initial conditions given in the early morning (at 06.00 h local time). The model simulates a number outputs including the surface energy (H, LE and soil heat) fluxes at the soil surface and in, around and above the vegetation canopy, the transfer of water in the soil and in the plants, the flux of CO2 between the atmosphere and the plants (the carbon assimilation rate), the surface O3 flux, a number of other parameters. SimSphere is globally distributed and maintained from Aberystwyth University, UK (http://www.aber.ac.uk/simsphere).

A number of studies based essentially on relatively basic empirical or LSA methods have been performed on the SimSphere model (Lynn and Carlson, 1990; Olioso et al., 1996). However, Petropoulos et al (2009b) demonstrated for the first time, the use of a GSA method using the Bayesian Analysis of Computer Code Outputs (BACCO) method for performing SA on SimSphere to identify the most responsive model inputs to the simulation of key model outputs. GSA methods, despite their often high computational demands, have become popular in environmental modelling due to their ability to incorporate parameter interactions and their relatively straightforward interpretation (Makler-Pick et al., 2011). Results by these investigators showed that the method was able to detect interactions between model parameters and derive absolute sensitivity measures concerning the model structure. Furthermore, in this initial study, the dominant input parameters were found to consistently control the predictions of the considered outputs by the model, namely, the topography parameters (slope, aspect), as well as the Fractional Vegetation Cover (Fr) and surface moisture. Petropoulos et al. (2010) expanded on this work by performing a comparative study of various emulator types including BACCO GEM, investigating the effect of sampling method and size on the sensitivity of key target quantities simulated by SimSphere. Their results showed that the sampling size and method did affect the SA results in terms of absolute values, but had no bearing in identifying the most sensitive model inputs and their interactions for model outputs on which SA was performed. Petropoulos et al., (2013c-d) also used the BACCO method in performing SA on SimSphere, aiming to further understand model structure and establish its coherence. Authors examined the effect of assuming uniform Probability Distribution Functions (PDFs) for the model inputs/outputs on the sensitivity of key quantities simulated by SimSphere. Furthermore, authors also explored the sensitivity of new, previously unexplored variables simulated by the model, namely of the Daily Evaporative, Non-Evaporative Fractions and Radiometric Temperature. Findings reinforced the conclusions of previous SA works on SimSphere that, regardless of the PDF assumption, only a small number of model input parameters exerted a significant influence on the model outputs, with the majority of parameters inconsequential. Petropoulos et al., (2013c) also examined the effect of assuming different PDFs for the model’s inputs/outputs on the sensitivity of key quantities simulated by SimSphere. Their results suggested that the assumption of different PDFs for the model inputs/outputs did not have significant bearing on mapping the most responsive model inputs and interactions, but only the absolute SA measures. However, they subsequently expanded the study to also examine the effect of changing the atmospheric sounding profile to the sensitivity of key variables predicted by the model. Notably, results did not show dramatic changes in the nature or ranking of influential model inputs using an atmospheric sounding derived from a different region to previous studies. Consequently, the previous work conducted on the BACCO method of SA on SimSphere represents a significant step forward in the global efforts on the model verification, especially given that its use is explored at present towards the development of global operational products from its synergy with EO data (Chauhan et al., 2003; Piles et al., 2011; ESA STSE, 2012). Our study anticipates to expand on these previous studies to enhance our knowledge of SimSphere model structure and establish further its coherence and correspondence to that of a natural system’s behaviour.

**3. GLOBAL SENSITIVITY ANALYSIS**

Herein we employed a sophisticated, cutting edge meta-modelling GSA method adopting a Bayesian analysis of computer code outputs (BACCO) SA on the model using the freely available software tool GEM SA (Kennedy, 2005). The theory related to the BACCO method of GSA is presented by Oakley and O’Hagan (2004), while the statistical theory and mathematical principles dominating the Gaussian Process (GP) emulation are documented by Kennedy and O’Hagan (2001) and Kennedy (2004).

Initially, BACCO SA implementation uses an efficient space-filling design of training input points and fits a Gaussian process model to the corresponding code runs to yield an emulator of the model (O’Hagan, 2006). The emulator is a mathematical function built from SimSphere to quantify the relationships between the model output and the model input, specifically the sensitivity of the former to the latter. Following this, the emulator itself is used to compute a number of statistical parameters to characterise the sensitivity of the targeted model output in respect to its inputs (Kennedy and O’Hagan, 2001).

For implementation of the BACCO SA, initially, a prior belief based on a Gaussian processes model about the actual model is inferred. The Bayes' theorem and a set of the model runs are considered together to refine the prior information to yield the posterior distribution of the output (Qin et al., 2013). On this basis, the emulator is used to calculate a mean function, which passes through the observed runs and the same time it quantifies the remaining uncertainty due to the emulator being an approximation to the true code (O’Hagan, 2006). Within BACCO, various measures of sensitivity, each of which requires integration of the model output with respect to probability distributions on the inputs, are generated. These include the *main effects* or *first order sensitivity indices (Si).* The main effect of a single input parameter component (*Xi*) measures the expected change in the output *f(X)* as *Xi* is varied, averaged with respect to the distribution of the remaining parameters (Parry et al., 2013). Thus, in other words this statistical measure quantifies the relative importance of an individual input variable *Xi,* in driving the total output uncertainty, indicating where to direct future efforts to reduce that uncertainty.

Similarly, using the same approach, higher order interactions (joint effect indices) of a group of input components (e.g. *Xi, Xj*) are generated to calculate the expected change in model output as a function of those inputs. Additionally, subsequent measures based on variations in the input parameters together induce a total variation in the output. These *total effects* can therefore be used as a measure of the combined influence of an input (Saltelli et al, 2000; Oakley and O’Hagan, 2004), where the sum of all inputs' *total effects* with respect to each model outcome will be greater than 100% (Parry et al., 2013; Qin et al., 2013). Use of the BACCO method has already been demonstrated in a large number of environmental modelling problems, providing useful insights in various disciplines and in various SA studies (Kennedy and O’Hagan, 2001; Kennedy et al., 2012; Parry et al., 2013; Petropoulos et al., 2009b).



 **Figure 1:** *Overview of the SA implementation in this study*

**4. SA EXPERIMENT IMPLEMENTATION**

The BACCO GEM-SA was implemented along the lines of GSA studies applied previously to SimSphere (Petropoulos et al., 2009b, 2010, 2013b–d). However, differently to previous studies, the sensitivity of several new, yet to be studied, model outputs were studied herein (Table 1). In addition, the sensitivity of the SA results to the time of the model simulation output was also explored, specifically here for the model output times 9:30/11:30/13:30. Again, effect of simulation times on model sensitivity is yet to be explored. These particular times were selected because they are close to the overpass times of most of the polar-orbiting satellites which provide data suitable for the “triangle” technique implementation on which SimSphere is also used. In particular, the sensitivity of the SimSphere outputs exhibited in Table 1 were examined primarily due to their importance in studies related to vegetation:

**Table 1:** *Summary and description of the SimSphere outputs examined in this study.*

|  |  |
| --- | --- |
| Parameter | Description |
| *CO2 Canopy ()* | the ambient CO2 concentration [ppmv] |
| *CO2 Flux ()* | the rate of uptake of CO2 by the plant [µmol m-2 s-1] |
| *O3 Canopy ()* | the ambient O3 concentration [ppmv x 10-3] |
| *Global O3 Flux ()* | the flux of O3 from the air to the plant/soil boundary [mg m-2 s-1] |
| *O3 Flux in Plant ()* | the flux of O3 taken up by the plant alone [mg m-2 s-1] |

To ensure consistency, comparability and a continuation of this study to previous SA experiments on SimSphere, the same implementation setting and dataset was used to that previously adopted (Petropoulos et al., 2009b; 2013b-d). In summary, a design space of 400 SimSphere simulations was developed using the LP-tau sampling method. All SimSphere inputs (Table 2) were allowed to vary across their full range of variation. An exemption to this was the geographical location (latitude/longitude) and atmospheric profile, for which a priori real observations for August 2002 were used from the Loobos CarboEurope site, located in The Netherlands (52° 10' 04.29" N, 05° 44' 38.25" E). Both cases of normal and uniform probability distribution functions for the inputs/outputs from the model were explored. For all variables, the theoretical ranges of values were defined from the entire possible theoretical range which they could take in SimSphere parameterisation and each of the model outputs were exported on three occasions relating to the different simulation output times. In addition, the emulator performance was evaluated based on the “leave final 20% out” method offered in GEM-SA, again in accordance to previous studies conducted to the model.

**Table 2:** *Summary of the SimSphere inputs considered in the GSA implementation using the BACCO GEM SA method. In parentheses are also provided the units of each of the model inputs.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Model input short name** | **Actual name of the model input** | **Process in which each parameter is involved** | **Min value** | **Max value** |
| **X1** | Slope *(degrees)* | time & location | 0 | 45 |
| **X2** | Aspect *(degrees)* | time & location | 0  | 360 |
| **X3** | Station Height *(meters)* | time & location | 0 | 4.92 |
| **X4** | Fractional Vegetation Cover *(%)* | vegetation | 0 | 100 |
| **X5** | LAI *( m2m-2)* | vegetation | 0 | 10 |
| **X6** | Foliage emissivity *(unitless)* | vegetation | 0.951 | 0.990 |
| **X7** | [Ca] (external [CO2] on the leaf) *(ppmv)*  | vegetation | 250 | 710 |
| **X8** | [Ci] (internal [CO2 ] of the leaf) *(ppmv)* | vegetation | 110 | 400 |
| **X9** | [03] (ozone concentration in the air) *(ppmv)* | vegetation | 0.0 | 0.25 |
| **X10** | Vegetation height *(meters)*  | vegetation | 0.021 | 20.0 |
| **X11** | Leaf width *(meters)*  | vegetation | 0.012 | 1.0 |
| **X12** | Minimum Stomatal Resistance *( sm-1)* | plant  | 10 | 500 |
| **X13** | Cuticle Resistance *( sm-1)* | plant | 200 | 2000 |
| **X14** | Critical leaf water potential *( bar)* | plant | -30 | -5 |
| **X15** | Critical solar parameter *(Wm-2)* | plant | 25 | 300 |
| **X16** | Stem resistance *( sm-1)* | plant | 0.011 | 0.150 |
| **X17** | Surface Moisture Availability *(vol/vol)* | hydrological | 0 | 1 |
| **X18** | Root Zone Moisture Availability *( vol/vol)* | hydrological | 0 | 1 |
| **X19** | Substrate Max. Volum. Water Content *(vol/vol)* | hydrological | 0.01 | 1 |
| **X20** | Substrate climatol. mean temperature *( oC )*  | surface | 20 | 30 |
| **X21** | Thermal inertia *( Wm-2K-1)* | surface | 3.5 | 30 |
| **X22** | Ground emissivity *(unitless)* | surface | 0.951 | 0.980 |
| **X23** | Atmospheric Precipitable water *(cm)* | meteorological | 0.05 | 5 |
| **X24** | Surface roughness *(meters)* | meteorological | 0.02 | 2.0 |
| **X25** | Obstacle height *(meters)* | meteorological | 0.02 | 2.0 |
| **X26** | Fractional Cloud Cover *(%)* | meteorological | 1 | 10 |
| **X27** | RKS (satur. thermal conduct.*(Cosby et al., 1984)* | soil | 0 | 10 |
| **X28** | Cosby B *(see Cosby et al., 1984)*  | soil | 2.0 | 12.0 |
| **X29** | THM (satur.vol. water cont.) *(Cosby et al., 1984)* | soil | 0.3 | 0.5 |
| **X30** | PSI (satur. water potential) *(Cosby et al., 1984)* | soil | 1 | 7 |

**5. RESULTS**

**5.1 Emulator Performance**

 Emulator performance was initially assessed using the self-test mechanism of the BACCO approach, based upon the quantitative evaluation of a series of statistical measures calculated by GEM-SA (Table 3). In addition, the roughness value of each input parameter, a unitless value, was computed internally by GEM-SA to specify the relationship that exist between model output and input (linearity or nonlinear) (Kennedy, 2004; Qin et al., 2013). A comprehensive description of the statistical measures computed by GEM SA is available in Kennedy and O’Hagan (2001) and O’Hagan (2006).

**Table 3:** *Emulator performance statistics for the SA tests conducted in this study under normal PDF assumptions for the model inputs/outputs at each different time scenario.*



 As can be observed from Table 3, sigma-squared values for the **and** parameters were low, ranging from 0.01 to 1.05, indicating only moderate deviations from linearity. However, sigma-squared values for the **, **and **parameterswere all relatively high. The majority of values ranged from 1.46 to 3.53, where only the **11:30 scenario displayed a value below 1 (0.86), suggesting a high degree of non-linearity.

 The cross- validation RMSD also displayed a variation in accuracy dependent on model output and simulation time. For the**,**, and ** model outputs the range of error was relatively low for all simulated time periods ranging from 3.10 (**– 11:30) to 8.16 *mg m-2 s-1* (**– 13:30). The error range for the *and *model outputs was on average slightly lower, ranging from 3.38 ppvm to 4.96 ppvm x 10-3. The cross-validation root mean squared standardised error values were all moderately close to 1 for all model outputs and simulation times, with the majority of values ranging from 0.15 (**– 11:30) to 1.97 (**– 9:30). Notably, a number of model outputs exhibited lesser accuracy at certain simulation times where values reached above 2, ranging from 2.01 (**– 11:30) to 2.37 (**– 11:30). The majority of values for the cross-validation root mean square relative error were below 5%, ranging from 1.22% to 4.84%. Three of the 15 scenarios exhibited values above 5% (ranging from 6.54% to 9.66%). However, these values are still relatively low, indicating a good overall emulator performance able to provide simulations of the target quantities examined with an accuracy ranging between 1.21% and 9.66%. The overall emulator accuracy results obtained herein were largely comparable to previous GSA studies on SimSphere (Petropoulos et al., 2009b, 2010, 2013b–d).

 For each of the model outputs, roughness value of 30 input parameters was calculated for the three different simulation times (9:30h/11:30h/13:30h). Any values of below 1 suggested a generally smooth response from the emulator to variations in its inputs, an important requirement for effective emulator build (Petropoulos et al., 2013c,d). Notably, roughness values for the majority of the model inputs were low, below 1, with few exceptions based on certain model outputs and time scenarios. For example, the 9:30 Leaf Width, Surface Moisture Availability, Substrate Max. Volume Water Content, Thermal Inertia, and Surface Roughness input parameters showed roughness values ranging from 0 to 0.05 for all model outputs, where 17 of the 25 roughness values for the 5 model outputs was 0. On the other hand, LAIfor the **model output exhibited roughness values exceeding 1. Variations were also visible within the individual input parameters dependent on simulation time. For example, the Critical Leaf Water Potential input parameter for the 09:30 and 11:30 scenarios exhibited roughness values of 0 for the **output, adverse to the 2.03 roughness value exhibited at the 13:30 time scenario, indicating that simulation time can have a major effect on model parameter relationships. In summary, roughness values above were relatively rare and indicated some degree of non-linearity between model inputs and outputs; however, apart from some exceptions, in the majority of cases these were not significant enough to suggest an extreme level of non-linear relationships. Overall, results indicate that the model output can be an approximate linearity function of the inputs.

**5.2 SA Results**

 The sensitivity of the model input parameters with respect to the decomposition of the examined model outputs for the cases of all the 3 different time scenarios (i.e. 9:30/11:30/13:30) has been summarised in Table 4. Figure 3 displays the input parameter sensitivity rankings with regards to each model output. Table 5 summarise the highly sensitive and moderately sensitive input parameters. Figure 2, exemplifies the main and total effects for each model output, for the case of the 3 different times at which SA was examined.

**Table 4***: Summarised results from the implementation of the BACCO GEM SA method on the different outputs simulated by SimSphere. Computed main (Main) and total effect (Total) indices by the GEM tool (expressed as %) for each of the model parameters are shown, whereas the last three lines summarise the percentages of the explained total output variance of the main effects alone (ME), the 1st order interactions only (1st) and the 2nd or higher order interactions only (2nd). Input parameters with a variance decomposition of greater than 1% are highlighted. The tables below show the summarised results for a) The 9:30 scenario b) The 11:30 scenario and c) the 13:30 scenario.*

 *(a) (b) (c)*



T**able 5:** *Summary of the most sensitive SimSphere inputs with respect to each of the model outputs of which their sensitivity was examined in our study.  is the ambient O3 concentration [ppmv x 10-3],  is the flux of O3 from the air to the plant/soil boundary [mg m-2 s-1], is the flux of O3 taken up by the plant alone [mg m-2 s-1], is the ambient CO2 concentration [ppmv], is the rate of uptake of CO2 by the plant [µmol m-2 s-1].*

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**5.2.1 Sensitivity for** **

 The SA results showed that the percentage variance contribution of each input parameter’s main and total effects for this parameter were significantly higher compared to all other model output results, ranging from 0% to 99.71% and 0% to 99.82% for the main and total effects respectively. Although these ranges are considerably greater than all other model outputs, there is only one significant input parameter contributing to the main effects for all time scenarios. The external CO2 on the leaf [Ca] parameter’s individual contributions dominate the total variance with ranges from 97.22% to 99.71%, followed by negligible contributions for all other input parameters (<1%). Main effects results also shows that first order interactions for the parameter range between 98.15% and 99.78%, being the only significant contribution to variance decomposition. This is also reinforced by the considerably low percentage influence of 2nd order (or higher) interactions which range from 0.13% to 0.83%. These trends are mirrored in the total effects where [Ca] ranges from 98.58% to 99.82%, with all other parameters again negligible (<1%). Furthermore, no significant (>1%) first order interaction were recorded (Table 4 and Figure 2d).

**5.2.2 Sensitivity for** 

 Percentage contributions from each input parameter to the total variance ranged from 0.01% to 26.10%, and 0.02% and 42.70% for the main and total effects respectively (Table 4 and Figure 2e). The summarised percentages of the main effects alone were relatively high, exhibiting comparable ranges for all three time scenarios, ranging between 68.91% and 71.91%. Highest individual contributions to first order main effects is given by Cuticle Resistance, followed by Fr and [Ca], which together contribute to ~50% of all first order main effects, suggesting that there are significant higher order interactions between these parameters. Second order interactions are less significant ranging from 5.78% to 7.86%. The same parameters were also important in terms of total effects, yet with increased percentage contributions. In addition many other factors also became important in the case of total effects, the most significant being internal CO2 of the leaf [Ci] and LAI. Six significant first order interactions (joint effects higher than 1%) were found for all three time scenarios. These included; Fr and Cuticle Resistance, Fr and [Ca], [Ca] and Cuticle Resistance, LAI and Cuticle Resistance, Fr and [Ci], and [Ci] and Cuticle Resistance. Although all three time scenarios shared the same six significant first order interactions, the percentage contribution and order of significance varied between different simulation times.

**5.2.3 Sensitivity for** 

 The input parameter’s main and total effect variance contribution to the simulation of the  output by SimSphere showed relatively wide variations in range dependent on computation time (Table 4, and Figure 2a). Main effects ranged from 0.03% to 32.58%, and total effects ranged from 0.63% to 68.48% respectively for all time scenarios. The model input with the lowest main effect of 0.03% (Leaf Width) was included within the 9:30 scenario, whereas the 11:30 scenario included the model input with the highest main effect of 32.58% ([03] in the Air). With regards to the total effects, the 9:30 and 11:30 scenarios again included the same model inputs with the lowest and highest total effect of 0.03% (Leaf Width) and 68.48% ([03] in the Air) respectively. The summarised percentages of the explained total output variance of the main effects alone, show that model output was mainly affected by the variance decomposition of input parameters during the 9:30 and 11:30 scenarios, which displayed main effects of 60.63% and 58.45% respectively. As Table 3 shows, the Cuticle Resistance, VH and [03] in the Air parameters had the largest percentage variance contributions for all time scenarios, suggesting significant first order interactions between these parameters. In terms of the total effects, Cuticle Resistance, VH and [03] in the Air were again the most important parameters for the simulation of  in all time scenarios, although there were a number of other significant contributors (e.g. LAI, Saturated Water Potential (PSI), Saturated Thermal Conductivity (RKS) and Surface Roughness) (Table 4). It should be noted that the 2nd order interactions are also significant here as they account for between 13.98% and 34.57% of variance.

 Significant first order interactions (higher than 1% joint effects) varied with simulation times; however, all time scenarios exhibited at least a minimum of 5 interactions. The most important interactions were i) 9:30 - VH and CR (5.95%) ii) 11:30 - [03] in the Air and VH (7.19%) iii) 13:30 – LAI and [03] in the Air (4.37%). Notably, VH, CR and [03] in the Air were incorporated in some part in the majority of interactions.

**5.2.4 Sensitivity for** 

 Main effects and total effects ranged from 0.01% to 32.79% and 0.02% to 79.95% respectively for all time scenarios (Table 4 and Figure 2b), where Main Effects (ME) results suggested all simulation times exhibited comparable ranges between 38.47% and 44.88%. The input parameters with the largest percentage variance contribution were similar to that of the, where [03] in the Air and CR were significant contributors. Higher than first order interactions for the parameter range between 16.85% and 26.37% dependent on time scenario, contributing to significant variance decomposition. In terms of the individual total effects, as well as mirroring the main effects, several other significant parameters exhibited high percentage variance (e.g. Thermal Inertia, LAI, VH) which were important contributors to total effects (>10%).

 Over thirty significant first order interactions were found for this output with the most important being i) 9:30 - LAI and Atmospheric Precipitable Water (3.58%) ii) 11:30 - LAI and CR (21.67%) iii) 13:30 – Fr and Thermal Inertia (2.13%) As was seen for the first order interactions of the, vegetative input parameters contributed significantly to the percentage variance, where interactions between Fr and LAI, [03] in the Air and Cuticle Resistance, LAI and VH, and LAI and [O3] in the Air also had significant contribution above 1%. Notably the first two time periods shared a number of significant first order interactions which were not deemed significant for the 13:30 scenario, suggesting that simulation time has a considerable effect on the performance of certain model inputs.

**5.2.5 Sensitivity for** 

 Values of percentage contributions from each parameter to the main and total variance again vary for the different simulation times. SA results showed ranges in main effects and total effects for all time scenarios ranged from 0.01% to 35.83% and 0.01% to 75.96% respectively (Table 4 and Figure 2c). The percentages of the explained total output variance of the main effects alone again showed comparable ranges with minimal variance, ranging from 47.68% to 53.43%. Parameters with the highest individual contributions were Cuticle Resistance, LAI and [03] in the Air which, with lesser contributions by VH, Thermal Inertia, and RKS amongst others (Table 4). Contributions by other parameters were negligible (<1%). Together the contributions from the three most significant parameters amount to over 60%, suggesting significant first order interactions between these model input parameters. This was also mirrored in the total effects results obtained, yet at higher percentage contributions (e.g. 11:30 – 35.83% increases to 75.96% for Cuticle Resistance), where a large number of additional parameters contributed > 1% to the total effects also (e.g. Station Height, Critical Solar Parameter, Surface Roughness) (Table 3).

 For the 29 significant first order interactions (>1%) the most important were i) 9:30 - VH and CR (7.58%) ii) 11:30 - CR and Substrate Climatological Mean Temperature (8.37%) iii) 13:30 – LAI and CR (3.63%). Similarly to the most significant first order interactions for both the and , the most important interactions included some contribution from vegetative input parameters, and the majority of the highest percentage contributions correlated between the three model outputs. Several other significant first order interactions were also recorded including [03] in the Air and CR, LAI and [03] in the Air, LAI and VH, and CR and Obstacle Height amongst others. Again the first two time scenarios shared a considerable number of first order interactions which were not deemed significant at the later simulation time. This again suggests the important effect of simulation time on model input contributions.

**Figure 2:** *Bar graphs displaying the results from the implementation of the BACCO GEM SA method on the different outputs simulated by SimSphere. The values on the x axis show the 30 input parameters examined in our study and the y axis displays the percentage contribution of each input parameter to the model output. Contributions of the input parameters to main effects and total effects variance decomposition, for each of the three time scenarios are displayed a) SA results for the O3 Canopy model output b) SA results for the Global O3 Flux model output c) SA results for the O3 Flux in Plant model output d) SA results for the CO2 canopy model output e) SA results for the CO2 flux model output.*



a)



b)

c)



c)

**Figure 3:** *Input parameter sensitivity rankings for the different model outputs for both main and total effects a) Input parameter sensitivity rankings for the 09:30 scenario main and total effects b) Input parameter sensitivity rankings for the 11:30 scenario main and total effects c) Input parameter sensitivity rankings for the 13:30 scenario main and total effects.*

**6. DISCUSSION**

In terms of the **simulation, it is clear that this parameter within SimSphere is dominated by the [Ca] and [Ci] input parameters (internal leaf CO2 and external, ambient, CO2). This is logical due to the fact that both components will be inherently linked in regards to the processes and feedbacks associated with photosynthesis. In essence, [Ca] represents the ambient concentration of CO2 in the atmosphere within, and above the canopy. Therefore [Ca], directly affects the carbon assimilation rates through the formation of concentration gradients that promote the diffusion of CO2 through the stomata and into the mesophyll. The significant influences of [Ca], as well as several vegetative parameters, are again apparent for the **model output. This is due to the integrated effect of carbon assimilation rates within the plant structures and CO2 uptake by plant canopies affecting the diffusive flux of CO2 (Fernández et al., 2013). The effect of vegetative parameters on the **model output can be explained by the process of CO2 diffusion by plants for use in photosynthetic carbon assimilation. Within a plant structure, stomatal behaviour directly affects assimilation by being able to regulate when to open if photosynthetic demand for CO2 is high or close if water supply becomes inadequate (Gordon and Olsen, 2013). In *Pinus ponderosa,* water potential alone explains 82% of the day-to-day variation in stomatal conductance (Panek, 2004). Fr and LAI were also identified as important determinants of ** . Fr is an input parameter to scale the vegetation cover on the ground, i.e. it determines the size of the vegetated portion of the land surface that will be communicating with the atmosphere. LAI is the total one‐sided area of leaf tissue per unit ground surface area characterising the canopy of an ecosystem, which is inherently linked to stomatal density and aperture (Bréda, 2003; Barlage and Zeng, 2004). Fr and LAI in essence determine the amount of biomass available for assimilation and transpiration, as well as being inherently linked to stomatal density and aperture (Bréda, 2003; Barlage and Zeng, 2004). Furthermore, the LAI, for example, determines canopy photosynthesis and plant productivity by providing the potential for light interception (Levis, 2010; Oikawa et al, 2013). Thus, given these plant physiological traits, these parameters determine the amount of CO2 uptake into a canopy for photosynthesis and transpiration (through the amounts and rates of CO2 diffusion through the stomata), as well as the amount of CO2 produced within a leaf structure through respiration (e.g. the higher the values of Fr and LAI, the greater the amount of CO2 uptake, diffusion and production), thus explaining the influence of these parameters on the **output.

CO2 diffusion through the cuticle can be up to 100 times less intensive than through the stomata (due to the cuticle on the epidermis being almost impermeable to CO2. However, this varies with leaf age and thickness, and is still an important influence on the dynamics of CO2 flux within the troposphere (Kvesitadze et al., 2006; Kirkham, 2011). The cuticle controls water loss from the leaf and the permeability of cuticles depends upon their evolutionary origin (Riederer and Schreiber, 2001). As properties of the cuticle are responsible for the loss of water, the effect of the leaf cuticle on **may be the influence of water dynamics affecting stomatal conductance which explains the significance of the CR parameter on the **model output. In addition, stomatal conductance has been shown to decline in taller trees due to hydraulic limitation, which may reduce intercellular CO2 concentrations within leaves and result in declines in assimilation, explaining the significance of VH on this output parameter (Sendall and Reich, 2013).

It is clear from the results obtained that vegetative parameters have a significant influence on several of the model outputs relating to O3 (CR, LAI, Fr, and VH). In terms of the modelled*,  and *simulation by the SimSphere model, the influence of these vegetative parameters can be explained by the fact that ozone has a sink at the ground surface as well as in the leaves, and since the cuticular resistance is typically many times that of the stomatal resistance, most of the ozone ingested by the leaf is through the stomates. However, an approximately equal flux is deposited at the ground surface in and around a plant canopy (Tuzet et al., 2011; Ganzeveld et al., 2012). In the case of full vegetation cover or dense canopies (large percentages of LAI, VH and Fr) this is mainly governed by stomatal aperture where O3 uptake is a function of both ambient O3 levels and stomatal conductance (Mauzerall and Wang, 2001). Quantified as stomatal resistance against the diffusion of O3 molecules into the sub‐stomatal cavities (Emberson et al., 2000), uptake increases with stomatal pore number or density (Eichert and Burkhardt, 2001). This is directly linked to the structural properties of a plant or plant canopy which is in turn represented by Fr and LAI. Essentially, the specific leaf area on a dry weight basis, or the area of assimilatory leaf material per dry weight unit thus becomes the main determining factor of amount of O3 uptake (WHO, 2006). This link between Fr, LAI and stomatal uptake of O3 explains the significant influence of the Fr and LAI input parameters on the**, *and *model outputs*.* Furthermore, vegetation height can play a role in the amount of available O3 for uptake due to possible vertical variations in mean O3 concentration within the canopy air space, with some experiments recording it to be as large as 10–30 ppb within forests and grasslands (Utiyama et al., 2004; Jäggi et al., 2006; Launiainen et al. 2013). Variations in canopy or plant height can thus affect the amount of O3 available for deposition which explains the influence of the VH parameter on these model outputs.

 The conventionally termed non-stomatal O3 removal pathways can also have some effect on O3 plant uptake, these include external plant parts (e.g. cuticles, bark, twigs etc.) the ground surface underlying the vegetative canopy (including soil, litter moss etc.) and the associated in-canopy aerodynamic resistance to O3 transfer to the ground surface. Non-stomatal O3 ﬂux has been attributed mainly to physical and chemical O3 depletion at the plant and soil surfaces through thermal decomposition (Cape et al., 2009), aqueous reactions in the liquid water accumulated at the surface (Altimir et al., 2004, 2006), light-stimulated reactions (Coe et al., 1995) and the gas-phase reactions of O3 with reactive Biogenic Volatile Organic Compounds (BVOC) and Nitrous Oxide (NO) (Wolfe and Thornton, 2011; Wolfe et al., 2011a,b). The extent of uptake depends on the time-integrated absorbed O3 flux (i.e. the dose), which is a function of non-stomatal conductance and ambient O3 concentration (Wohlfahrt et al., 2009). Concentration of ambient O3 in the troposphere (within the canopy, sub-canopy, canopy air space, ground surface) thus has some control on the rates of environmental O3 flux and plant deposition, explaining the influence of the [O3] in the Air parameter on the **, **and **model outputs. This would further explain the number of first order interactions which incorporated vegetative parameters with the [O3] in the Air input. However it should be noted that the relationship between ambient O3 concentration and uptake is non-linear, where highest rates of uptake are found during periods where stomatal conductance is highest and stomata are relatively unconstrained by stress factors, not when ambient O3 concentrations are at their maximum (Bytnerowicz et al, 2003).

In forest trees, the uptake of O3 also depends upon the daily diurnal rhythms that control the opening and closing of stomata. Diurnal fluctuations in the stem radius of large trees have been observed in a number of species and control the supply of water to the meristematic tissues (Zweifel et al., 2005; McLaughlin et al., 2007). Exposure of forest trees to increased levels of O3 was found to amplify these diurnal patterns indicating that the trees were experiencing reduced hydration. The annual reduction in growth rate ranged from -14 to -63% in a year in which O3 exposure was particularly high but was also dependent upon species, with a drought tolerant species (*Q. prinus*, chestnut oak) showing greatest resistance (McLaughlin et al., 2007). In a second tree species, *Pinus ponderosa*, growing under seasonal drought conditions in California, the uptake of O3 was highest in early summer when water availability was higher (Panek, 2004). However, as the summer progressed and water became limiting, O3 uptake was highest in the morning even though the concentration of was higher later in the day (Panek, 2004). The conclusion of both of these aforementioned studies was that the uptake of O3 does not depend upon concentration but the availability of water that drives the opening of the stomata and allows O3 to penetrate the leaf (Panek, 2004; McLaughlin et al., 2007). In the instance of external plant parts, deposition on the cuticles can be limited under dry conditions (Cape et al., 2009), but on wet canopies this process may represent a major sink for O3 (Altimir et al., 2006), particularly when O3 concentrations are low, explaining the significant influence of the CR parameter on these model outputs.

The general contention reported in the literature is that sensitivity analyses of models tend to be perfunctory. However, Shin et al. (2013) have identified a number of questions which need to be considered when performing SA of any model, highlighting two key issues related to uncertainty and identifiability. Questions of parameter range selection, data sampling size and SA method all need to be addressed to minimise uncertainty in SA. For example, reducing or expanding the variations in input parameter ranges can affect the sensitivity index, thus it is important that the ranges used yield parameter sets that are considered plausible, such that results are not biased by implausible model realisations. We tried to address this issue through refining a-priori values from real observations to allow for the determination of more plausible input parameter sets and to yield the posterior distribution of each model output considered. Questions related to the identifiability of models in SA are concerned with changing objective functions, parameter fixing, changing model structures or changing data periods amongst others. For example, as was the case in our study, there can be a change in the number of insensitive model parameters if different data periods are used, although some model parameters are insensitive for all data periods. While a modeller can easily use SA to help assess and improve their model in a particular case study, consideration of such issues must be taken when interpreting any results to avoid drawing generalisations or trying to apply generalisations to new situations.

Results obtained herein can be used practically to assist in future model parameterisation and implementation in diverse ecosystem conditions. Such findings provide further confidence to current ongoing efforts which focus on the development of operationally distributed products based on the synergy of the SimSphere model with EO data. The results of this study are not directly related to the development and future exploitation of such operational products but have significant implications for the development of the model as a useful and practical educational tool. Our results extend our understanding of the model structure and further establish its coherence to that of a natural system’s behaviour. This development represents a significant step towards the all-inclusive validation of the SimSphere model which is of high interest to the global user community.

**7. CONCLUSIONS**

 The SA study performed herein has attempted to analyse the performance of SimSphere for a number of yet unexplored parameters that are important contributors to a number of atmosphere-land surface interactions and feedbacks between the different components of the land surface. Results confirmed that model outputs are only significantly sensitive to a small group of model inputs based primarily on vegetative factors, CO2 and O3 fluxes (Table 4). Fr, LAI, CR and VH were the most important vegetative parameters which had most influence on all but one output. The influence of [Ca] and [O3] in the air were also significant parameters, especially in the case of the CO2 Canopy output. To our knowledge there have been few studies so far exploring the validation and verification of the SimSphere model. To this end, this study represents a significant step forward in contributing to current global efforts in that direction. All in all, our findings provided further evidence supporting the model coherence and correspondence to the behaviour of real world processes, natural feedbacks and interactions. Future research should aim to further explore our understanding of the SimSphere structure through performing direct comparisons of model outputs against reference data from actual *in-situ* observations and at different ecosystems worldwide. This would allow further confirming its potential role as an operational tool for climate research, land cover and land use change monitoring, environmental management, water resources and agricultural sustainability.

**Acknowledgments**

Dr. Petropoulos gratefully acknowledges the financial support provided by the Marie Curie Career Re-Integration Grant “TRANSFORM-EO” project supporting the implementation of this research work. Authors are also grateful to the anonymous reviewers for their constructive comments which results in improving the manuscript.

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