The New WIMOVAC

Windows Intuitive Model Of Vegetation response to Atmospheric & Climate change (WIMOVAC) has been used widely as a generic modular mechanistically-rich model of plant production. It can predict responses of leaf, canopy and growth level properties under different environmental conditions. Here we represent a JAVA version user-friendly WIMOVAC which can be easily used by plant biologists, crop breeders, ecologists and agronomists without reliance on any programming skill. In this article, we describe the structure, equations, user guide and the potential application of WIMOVAC.

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Using Java WIMOVAC -- A User-Friendly Means to Scale from the Biochemistry of Photosynthesis to Whole Crop Canopies and Production in Time and Space

Qing-Feng Song[1,2*], Dairui Chen[1,2*],Stephen P Long[3,4#], Xin-Guang Zhu[1,2,3#]

1. CAS Key laboratory of Computational Biology, CAS-MPG Institute of Computational Biology, Shanghai, China, 20003

2. State Key Laboratory of Hybrid Rice, CAS-MPG Institute of Computational Biology, Shanghai, China, 200031

3. Institute for Genomic Biology, University of Illinois at Urbana Champaign, Urbana IL, 61801

4. Department of Crop Sciences, University of Illinois at Urbana Champaign, Urbana IL, 61801

* Joint first author

[#]Correspondence Author:

Xinguang Zhu

CAS-MPG Partner Institute for Computational Biology

Chinese Academy of Sciences

Shanghai, China, 200031

Steve P Long

University of Illinois at Urbana Champaign

slong@uiuc.edu

Abstract: Windows Intuitive Model Of Vegetation response to Atmospheric & Climate change (WIMOVAC) has been used widely as a generic modular mechanistically-rich model of plant production. It can predict from biochemical and biophysical mechanisms the responses of leaf and canopy carbon balance, as well as production in different environmental conditions, in particular those relevant to global change. Here we introduce an updated JAVA user-friendly version of WIMOVAC. This makes the software platform independent, and it can be easily downloaded to a laptop and used without any prior programming skill. In this article, we describe the structure, equations, user guide and illustrate some potential applications of WIMOVAC.

Key words: crop yield, biomass, breeding, decision support system, climate change, photosynthesis

INTRODUCTION

In the IC (integrated circuits) design industry, computational modeling has been a critical factor in the rapid improvement and generation of new IC. Growth in capacity to mathematically model crop growth and developmental processes, incorporating various levels of mechanism have been developed, reviewed in (Hammer *et al.*, 2010, Jones *et al.*, 2003, Zhu *et al.*, 2011), has failed to have the same impact. One of the potential reasons is that, these models have been written for distinct research purposes, often to predict yields of specific crops or production of vegetation types within an ecosystems or landscape context. As a result these models may lack transparency and user-friendliness to non-specialist users, can require advanced programming skills and come with varying degrees of mechanism and documentation. As a result there is little involvement of the experimental community, who are seen as "data-gatherers" and not interacting partners. WIMOVAC is designed as a generic mechanistic model, with transparency and ease of access, fundamental to its development. With its strong basis in biochemical and biophysical mechanism for leaf and canopy photosynthesis and related processes, WIMOVAC can be used to study a wide range of environmental responses over seconds, days or years, scaling from biochemistry to production. By providing an interface to the parameter database, users can adapt the model to specific plants and genotypes without a need to change the underlying code. Though WIMOVAC has been used for more than two decades (Humphries & Long 1994), the original model and subsequent versions were coded in Visual Basic and so became difficult to transfer between platforms and unworkable under the most recent operating systems. We have therefore rebuilt WIMOVAC in a general-purpose object-oriented language that would be widely and freely available, providing a write-once, run-anywhere code (WORA). This made JAVA the obvious choice fitting all of these requirements and providing a General Public License (GNU) making it widely accessible. Here we describe the model equations, implementation, example applications and download instructions.

2. Basic features of the Java version WIMOVAC

WIMOVAC describes various processes related to photosynthetic CO_2 uptake, partitioning of assimilated carbon and interaction between plants with atmosphere and soil processes (Humphries & Long, 1995). This Java-version WIMOVAC retained many features of the original WIMOVAC. First, its equations are organized into different sections representing different physical and physiological processes, which interact with each other (Figure 1). For example, the light and temperature calculated from the macroclimate model are used by the canopy photosynthesis

model in WIMOVAC to calculate light and temperature profiles at different layers inside a canopy. The calculated microclimate inside a canopy is in turn used to calculate the leaf photosynthesis and transpiration, which further affects canopy microclimate and photosynthesis. Secondly, WIMOVAC is designed as a multi-scale simulation software. Simply, it can simulate processes from leaf biochemistry up to the ecosystem levels. It includes the basic biochemical models of C_3 and C_4 photosynthesis at the leaf level, the canopy photosynthesis and transpiration process, and the whole plant growth processes.   The detailed interdependence between the different processes and the scaling from leaf to stand processes is detailed in the supplemental section and has also been described in earlier publications (Miguez *et al.*, 2009). Thirdly, it is built to be user-friendly. To enable the model easily accessible by the research community, this Java version is easily transferable across different platforms and computers. The software can be used after the software package is copied directly onto any WINDOWS, Linux or Mac OS computer with Java runtime environment (JRE) installed. No other software installation is needed.

User Guide of WIMOVAC

We use the leaf level simulations as the example. In this example, WIMOVAC is here used to build a curve showing the responses of leaf CO_2 uptake rates of a leaf at different intercellular light levels (A/Q) by working through the following WIMOVAC screens. First click the "C3/C4 leaf assimilation" icon and the form for the "C3/C4 leaf assimilation module" appears (Figure 2B). Choose "Assimilation" as the dependent variables and "Light_0" as the independent variable which spans from 0 to 2000 μmol m^{-2} s^{-1} with an interval of 25 μmol m^{-2} s^{-1}. After this, enter the three CO_2 levels to be used in the simulation. Then enter O_2 concentration to be 210 mbar, temperature 25.0 $^{\circ}$C, and relative humidity 70%. C3 or C4 photosynthesis, can then be chosen via a toggle switch by clicking the button of "C3/C4 photosynthesis" at the left bottom corner of the form (Figure 2B). Simulation is invoked by clicking the "Start" button. Simulation results are directly displayed via a graphical user interface immediately after each simulation run is completed (Figure 2C). Users can obtain the numerical data in the Excel format from WIMOVAC_OutputFile_leaf which will appear in the same folder as the WIMOVAC software.

In addition to pre-population of climatic variable tables that the user can alter directly, such as CO_2 in the preceding example, WIMOVAC comes with the model parameters stored in a parameter files. Values used are derived from a series of sources, with an aim to providing best estimates for an "average plant". These can be viewed and modified by clicking "Parameter File" (Fig. 3A). Once in the Parameter file, users can change these according to their

simulation needs (Fig. 3B). For example, a user may have estimated leaf maximum rate of Rubisco limited

carboxylation ($V_{c,max}$) and whole chain electron transport supporting carbon metabolism (J_{max}) for a particular crop

and now wish to predict canopy assimilation. Within the parameter table they may add their values, store the

revised parameter table and then use this in their simulation by clicking "Save" (Fig. 3C) after the modification in

the "Customer Designed Parameter File" (Fig. 3B). Users can use the original default values by clicking "Load

Original Data". Users can gain more information about the sub-models and equations of WIMVOAC using the

Help menu (Fig. 3A).

Major Applications of WIMOVAC

Predicting the responses and adaptation of ecosystems under a future climate

WIMOVAC provides a means to explore, from underlying primary biochemical processes of net assimilation and

biophysical processes at the leaf and canopy level, how net assimilation over seconds to years would be affected by

rising temperature, altered humidity and rising CO_2. Equally, where acclimation at the leaf level has been defined

the user can explore impacts on canopy assimilation and productivity. Similarly, it allows adaptation to be explored.

Would a canopy under elevated CO_2 assimilate more carbon over the course of a day or growing season with more

or less leaf area? It also provides a means to quantitatively assign acclamatory changes in production to different

underlying processes. For example, Wittig et al (2005) used WIMOVAC to simulate the gross primary production

from recorded leaf photosynthetic properties, leaf area index, and meteorological conditions over a 3-year rotation

cycle of poplar forest ecosystem under both current and future elevated CO_2 conditions. The relative changes in the

simulated gross primary productivity (GPP) were consistent with the estimated GPP change based on biomass

increment and turnover. The modeling results provided new insight showing that the decline in stimulation of gross

primary production under elevated [CO_2] was due to earlier canopy closure, not photosynthetic acclimation (Wittig

et al., 2005). This is because the responses of photosynthesis to elevated CO_2 is most pronounced in saturating light

in contrast to limiting light conditions, as can be explained from the underlying biochemical/biophysical processes

(Long *et al.*, 2004).   Early observations of plant responses to rising [CO_2] noted a decline in N-content and Rubisco,

and suggested this was a negative response that could eliminate any production benefit from rising [CO_2], especially

under conditions of limiting N (Adam *et al.*, 2000). Rogers and Humphries (2000) used WIMVOAC to show that

the acclimation can be fully attributed to changes in the Rubisco activity (Drake *et al.*, 1997). From theory, in

elevated [CO_2] less Rubisco is needed. This can be easily shown in WIMOVAC by lowering $V_{c,max}$ and raising [CO_2] and then examining the effect on leaf CO_2 uptake rate (*A*) at elevated [CO_2]. Ainsworth & Long (2005) reviewing all FACE experiments, showed that the decline in N at elevated [CO_2] was attributable almost entirely to Rubisco, i.e. it was not a general decline in N. Since less Rubisco is needed at elevated [CO_2] it was possible by a combination of mechanistic modeling and FACE measurements, to show that this loss of N was acclamatory not detrimental, in the sense that it fits the plant better to its new environment. This usually occurs when photosynthesis exceeds the capacity for carbohydrate export and utilization, a response exacerbated by genetic limitations, such as determinate growth patterns, and environmental limitations, such as N deficiency or low temperature (Ainsworth *et al.*, 2004).

Teaching Tool   WIMOVAC was developed with the philosophy of easy access and easy application. Therefore, it can be used as a teaching tool. WIMOVAC includes multiple forms, with each form simulating a typical physiological process and can be used to explore the effects of different factors on these physiological processes. For example, users can load the form of "C3/C4 leaf assimilation" and simulate the effects of modifying light, temperature, CO_2, O_2 and humidity on photosynthetic CO_2 uptake rate. Users can modify the environmental parameters and the other key physiological parameters, e.g. the maximal rate of RuBisco limited photosynthesis, using a user friendly interface without having to know any programming language. The help system of WIMOVAC provides the detailed mechanistic basis which can help students to interpret the predicted changes of photosynthesis under perturbation. Right now, WIMOVAC is used by more than 20 countries in classroom teaching, in particular in the subject areas of photosynthesis and productivity.

Summary

This new Java version WIMOVAC is designed to provide a user friendly interface. Users can easily input parameters for each particular crop in different conditions to test specific hypothesis. We envisage this new platform can be used as a generic tool to support plant and environmental science research for another decade to come. The WIMOVAC software can be obtained from either http://www.picb.ac.cn/PSB/a/DOWNLOAD/ or Plant Cell and Environment article website http://onlinelibrary.wiley.com/journal/10.1111/%28ISSN%291365-3040 .

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Figure legends:

Figure 1 The mechanisms incorporated in WIMOVAC.   A shows the procedure used to calculate canopy photosynthesis. Canopy photosynthesis is calculated as the sum of photosynthetic CO_2 uptake rate contributed by sublit leaves (AC_{sunlit}) and canopy photosynthetic CO_2 uptake contributed by the shaded leaves (AC_{shaded}). The AC_{Sunlit} is calculated based on the leaf area index of the sunlit leaves (LAI_{sunlit}) and the photosynthetic rate (A) of the sunlit leaves. The A is further determined based on the leaf photosynthetic properties, stomatal conductance properties, and also leaf temperature, which are all influenced by ambient air temperature. The ambient air temperature can be either input or calculated based on the latitude and time of day. The air temperature will in turn determined by the latitude and time of day. B shows the overall structure of WIMOVAC. During the photosynthate partitioning and plant growth process, the growth stage is determined based on both the environment (e.g. temperature) and plant properties, i.e. thermal time needed to reach a particular developmental stage. The partitioning coefficients and relocation coefficient depend on the developmental stages. The relocated carbon as well as daily produced photosynthate together are partitioned to different organs to support organ growth. Organs can senescence and contribute to the carbon and nitrogen pool for partitioning. The detailed equations and parameters for WIMOVAC are available in Supplementary file xxxxx.
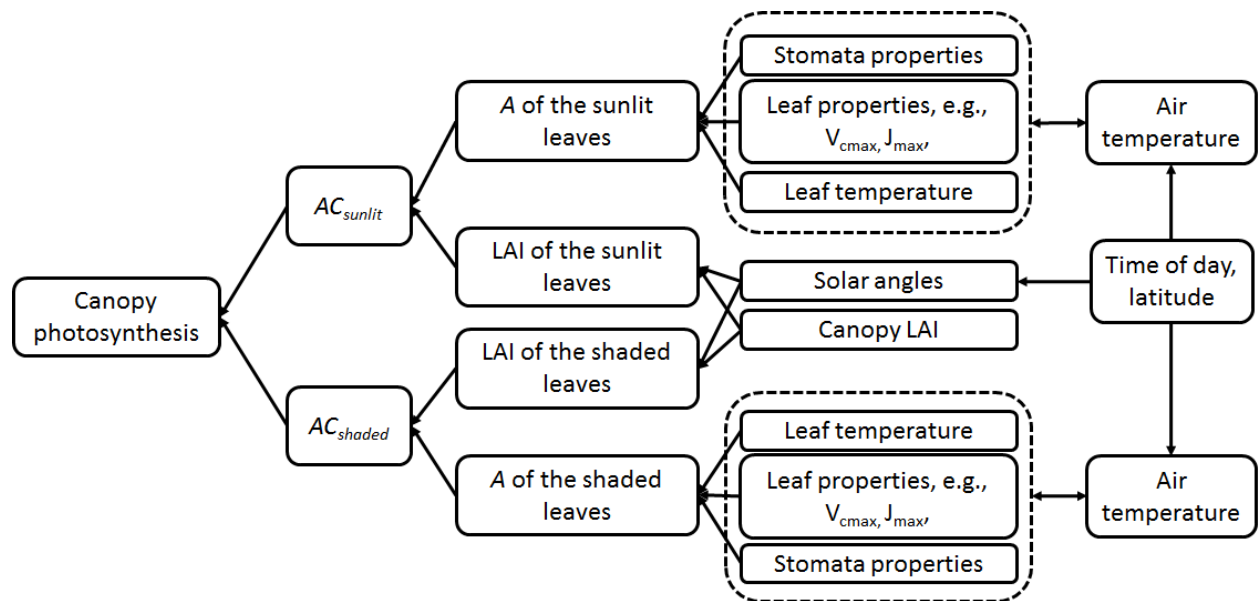
Figure 2. The graphic user interface (GUI) of WIMOVAC showing a procedure of using WIMOVAC to perform a simulation. A. the first WIMVOAC interface; as a default, the 'C3/C4 Leaf Assimilation Module" is selected. Users can also select the other three modules to perform different simulations. Once the "Start" button is clicked, the Form B is shown. On this form, different parameters can be selected to predict leaf photosynthetic rates under different conditions. Simulation can be invoked by clicking 'Start" button and the results are shown in graph format (C). D shows the module used to simulate a whole plant growth process. E shows the biomass changes of different organs during a growing season.

Figure 3. The procedure to access the parameter table of WIMOVAC. The parameter table can be accessed through clicking the "Parameter File" in either "C3/C4 Leaf Assimilation Module" or "Sunlit/Shaded Cnaopy MicroClimate Module" or 'Sunlit/Shaded Canopy Assimilation Module" or the 'Plant Growth Module'. By clicking the 'Parameter File" in each of these Modules, the users can access the parameters associated with this module (A). The parameter
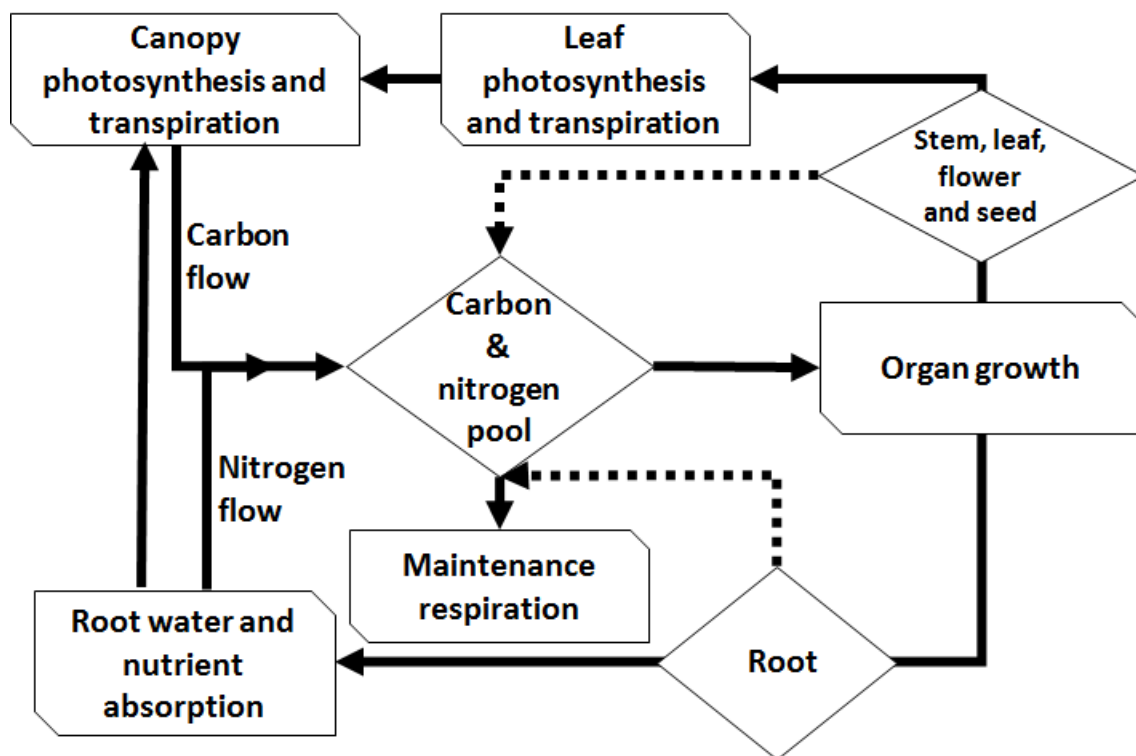
values can be modified and saved through the 'Customer Designed Parameter File' (B). By clicking the "Load

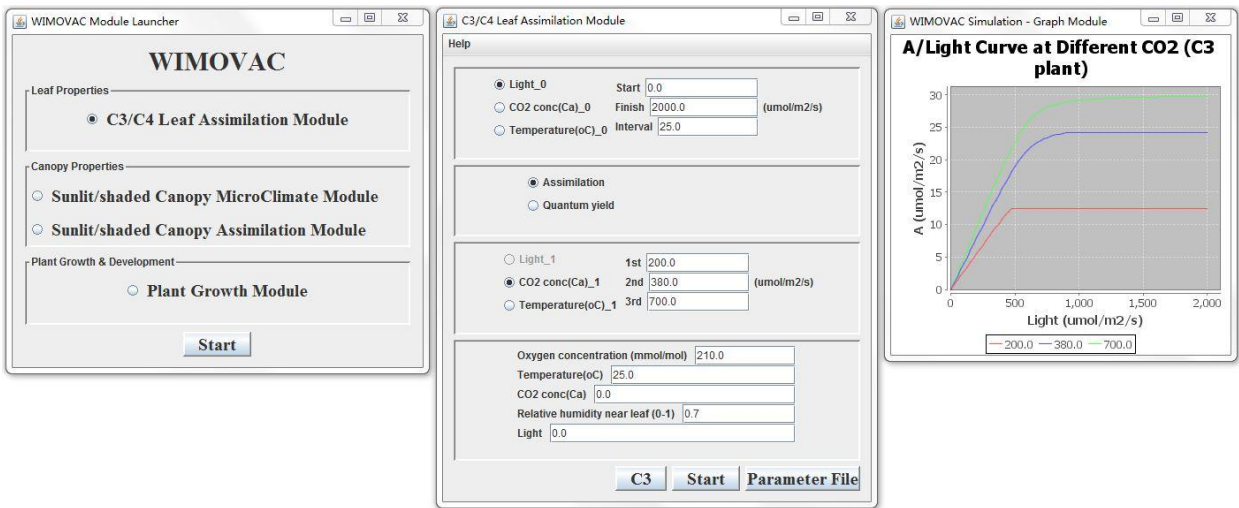Original Data", users can also load the default model parameters values.
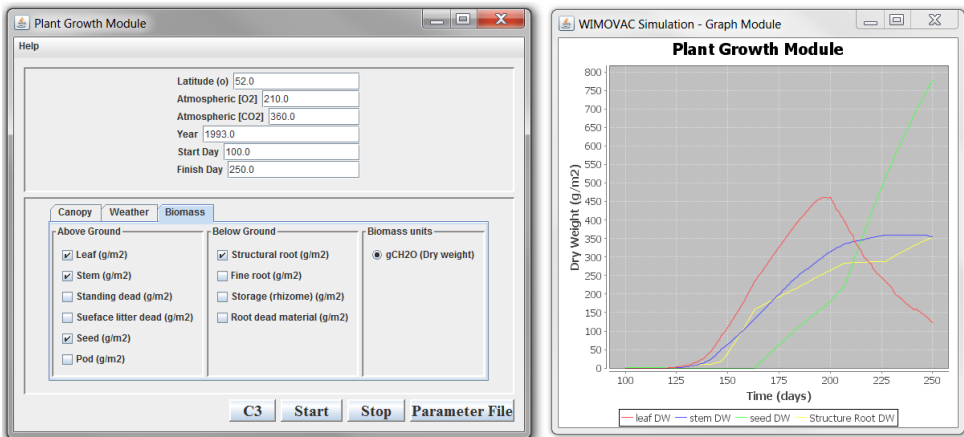
[Figure 1]

A

B.

[Figure 2]

A

B

C

D

E

[Figure 3]

C3/C4 Leaf Assimilation Module

Help

- ● Light_0
- ○ CO2 conc(Ca)_0
- ○ Temperature(oC)_0

Start 0.0
Finish 2000.0   (umol/m2/s)
Interval 25.0

- ● Assimilation
- ○ Quantum yield

- ○ Light_1
- ● CO2 conc(Ca)_1
- ○ Temperature(oC)_1

1st 200.0
2nd 380.0   (umol/m2/s)
3rd 700.0

Oxygen concentration (mmol/mol) 210.0
Temperature(oC) 25.0
CO2 conc(Ca) 0.0
Relative humidity near leaf (0-1) 0.7
Light 0.0

C3   Start   Parameter File

Customer Designed Parameter File

Customer Designed Parameter File

Leaf_Vcmaxo	90.0
Leaf_C4StomatalSlopeFactor	4.7824
Leaf_Reflectance	0.2
Leaf_Curvature_Factor	0.7
Leaf_Koo	278.0
Leaf_Stomatal_Coef_g1	9.8465
Leaf_Stomatal_Coef_g0	19.148
Leaf_Nitrogen_Vcmax_K4	12.4
Canopy_Q10TemperatureResponse	1.85
Leaf_Nitrogen_Vcmax_K3	35.7
Leaf_C4CO2ResponseSlope	0.22
Leaf_Stomatal_Coef_g1_650	11.35
Leaf_C4StomatalInterceptFactor	32.061
Leaf_TPUNitrogenHarleyK2	5.13
Leaf_TPUNitrogenHarleyK1	0.63
Leaf_C4CurvatureParam2	0.93
Leaf_C4CurvatureParam1	0.83
Leaf_JMaxo	170.0

Save   Load Saved Data   Load Original Data