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Calibration and validation of APSIM-Wheat Model in Mediterranean areas

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ABSTRACT

The Agricultural Production Systems sIMulator-Wheat (APSIM-Wheat) model is one of the most widely used agricultural models. It is a powerful simulator that has been successfully calibrated and tested for many locations in the world, especially in Western Australia (WA). However, there is a noticeable lack of a standard guide for realizing the calibration validation of APSIM-Wheat that could be applied in areas with a Mediterranean climate similar to that of WA. Therefore, this study aims to examine crop simulations reported in published articles and to provide a detailed description of input data and statistical assessment, which represent the two main components of the calibration-validation protocols. The PRISMA (PREFERRED Reporting Items for Systematic Reviews and Meta-Analyses) method was used to identify and select relevant papers for this review. Following the analysis of 31 calibration protocols extracted from selected eligible articles, it was found that regardless of the objective of using APSIM-Wheat, the same category of data is required for calibration. As far as meteorological data is concerned, the information essential to this study was daily maximum and minimum air temperatures, rainfall (mm), and solar radiation. In the case of soil data, information about the texture and hydraulic characteristics, especially PAWC, DUL and LL was required. Regarding agricultural management data, this pertains to cultivated crops, Nitrogen fertilization (rate and time of application) and sowing (date and density). For the statistical evaluation, it was observed that 90 percent of studies analyzed in this review revealed the use of RMSE.

KEYWORDS: APSIM-Wheat, Calibration, Data input, Statistical assessment, Crop simulation

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INTRODUCTION

The world population is expected to reach approximately 9.8 billion people in 2050 (Beltran-Peña *et al.*, 2020). As a result, agricultural production systems must evolve to satisfy the increasing demand for food in the future (Godfray *et al.*, 2010; Holt-Giménez *et al.*, 2012). Therefore, there is an important need for advanced agricultural models to identify suitable solutions (e.g., the most effective farming practices) for challenges facing the agriculture sector, such as, soil degradation, groundwater pollution, and the declining yields of crops (Chisanga *et al.*, 2017; Zaman & Maitra, 2018). In response to that need, substantial improvements have been made in agricultural models to promote a better understanding of the current and future effects of critical global issues (e.g., global warming, food security) (Ammar *et al.*, 2022; Tyczewska *et al.*, 2023).

One such model is the Agricultural Production Systems Simulator (APSIM). It has been recently recognized as an

effective system for simulating farming systems, especially when there is a need for more understanding of the ecological outcomes of agricultural practices (Boote *et al.*, 2010; Holworth *et al.*, 2014). It is a software that was developed by the Agricultural Production Systems Research Unit in Australia to satisfy the need for simulating agroecosystems with sufficient sensitivity (McCown *et al.*, 1996). Improvements to the simulator over the years have allowed modellers to produce a more accurate representation of the responses of soil to the different interactions between climate and farming practices by using its interconnected modules (Keating *et al.*, 2003; Brown *et al.*, 2018). Globally, there is an extensive literature on the description of these modules (Probert *et al.*, 1998; Hammer *et al.*, 2010). The broad range of topics to which they have been applied is well described in the literature, such as conservation agriculture (Yang *et al.*, 2018; Bahri *et al.*, 2019; Chaki *et al.*, 2022), genotype-environment interactions (Bustos-Korts *et al.*, 2019), agroecosystem services (Luo *et al.*, 2011) and climate change adaptation (Bai *et al.*, 2022; Li *et al.*, 2022).

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The considerable expansion of APSIM applications and features, resulting in reliable simulations, is the result of a robust calibration process implemented by users (Hao *et al.*, 2021). Calibration is the most important part of the procedure undertaken to test the performance of all process-based models, including agricultural models (Wimalasiri *et al.*, 2021). The process of calibration involves the adjustment of model parameters to minimize the difference between simulated and observed values for different variables under assessment (Wallach *et al.*, 2021). In other words, the calibration approach is based on two main steps: 1) integrating measured data collected from field experiments and other estimated data into the model and 2) assessing the fit of predicted values to experimental values by calculating performance indicators (e.g., Root Mean Square Error and Mean Bias Error) (Kersebaum *et al.*, 2015).

The APSIM Model has been widely calibrated and tested in diverse locations around the world, for instance, in Asia (Gaydon *et al.*, 2017), China (Zeng *et al.*, 2016), Africa (Carcedo *et al.*, 2023) and Spain (Kamali *et al.*, 2022). Also for various crops including wheat (Kouadio *et al.*, 2015; Asseng *et al.*, 2002; Kheir *et al.*, 2021), rice (Gaydon *et al.*, 2012), Maize (Lobell *et al.*, 2013; Peake *et al.*, 2013) and soybean (Archontoulis *et al.*, 2014). APSIM has also been extensively used in Australia, especially in the Mediterranean climate of Western Australia, for modelling the wheat crop (Chen *et al.*, 2020), with demonstrated robustness to simulate important agricultural indicators such as crop yield and crop phenology under climate change scenarios (Anwar *et al.*, 2015). However, there is no compilation of calibration protocols from past studies conducted in this region that can serve as suitable guidelines for APSIM-Wheat model validation. Indeed, there remains a lack of papers that provide a description of standard calibration approaches that can be applicable and replicated in areas around the world that are characterized by the same climate conditions as the Western Australia, such as some regions belonging to many countries in the world like Morocco, Tunisia, the United States, Spain, Portugal, and Italy.

Against this background, the main objective of this study is to review and critically examine the existing datasets and statistical assessment methods that were adopted by users in Western Australia to calibrate and validate the APSIM-Wheat model. To attain this goal, a comprehensive literature research of peer-reviewed publications related to the APSIM-Wheat simulations of experiments in Western Australia is conducted. This review provides a valuable reference that can help future users of this model in enhancing its reliability and accuracy.

MATERIAL AND METHODS

Literature Research

A literature search was conducted in May 2023 through two electronic databases: ScienceDirect and Scopus. In order to limit our search to APSIM-Wheat simulation studies conducted in Western Australia, the following combination of keywords: “APSIM-Wheat” NOT “APSIM” AND “Australia” OR “Western

Australia” AND “Mediterranean” AND “Wheat” was used. The initial search through the Scopus database yielded 21 articles, while 93 articles were extracted from the second database (ScienceDirect). After merging results from the two databases, eight book chapters and five duplicate articles were eliminated, giving a total of 101 articles. The first screening of these articles, by title, resulted in 36 articles being removed. The second screening, based on abstracts and keywords, resulted in 33 articles being removed (Figure 1 shows details of the screening steps), reducing the sample to 32 articles.

Selection Criteria

32 articles were read in full and selected if the following criteria were met:

- Only peer-reviewed articles that reported the description of the calibration process
- The comparison between simulated and observed values was well-described
- The statistical calibration metrics were reported

Papers were excluded if they:

- Provided an incomplete list of experimental data or measurements used for calibration
- Provided an incomplete list of estimated data used for calibration

After screening the full texts of the articles according to the above selection criteria, 18 articles were eliminated due to the lack of a detailed description of the calibration process. These 18 articles reported that the calibration process had been conducted previously and that this model was well-calibrated and tested in various locations across Western Australia (WA). However, the most cited author is Asseng, and the most cited reference is Asseng *et al.* (1998). Overall, 14 eligible articles were considered which yielded 31 datasets of APSIM-Wheat calibration processes.

RESULTS AND DISCUSSION

Overview of the APSIM-Wheat Model

The Agricultural Production Systems Simulator for Wheat (APSIM-Wheat) is one of the five key modules implemented within the APSIM Model (Meinke *et al.*, 1997; Chen *et al.*, 2023). It simulates the growth and development of wheat crops on a daily time step (Ludwig & Asseng, 2006). The modelling process is based on daily weather data (temperature and solar radiation), soil moisture and soil nutrients, as well as management practices (Tang *et al.*, 2003). According to Ahmed *et al.* (2016), APSIM-Wheat comprises 11 phases that describe the phenology development (sowing, germination, emergence, etc.). These phases (except from sowing to germination) are determined by the accumulation of thermal time and other factors such as photoperiod and vernalisation (Brown *et al.*, 2018). Apart from simulating wheat growth and phenology, APSIM-Wheat can also assist with, for example, leaf area expansion, soil water available to crop, nitrogen uptake and

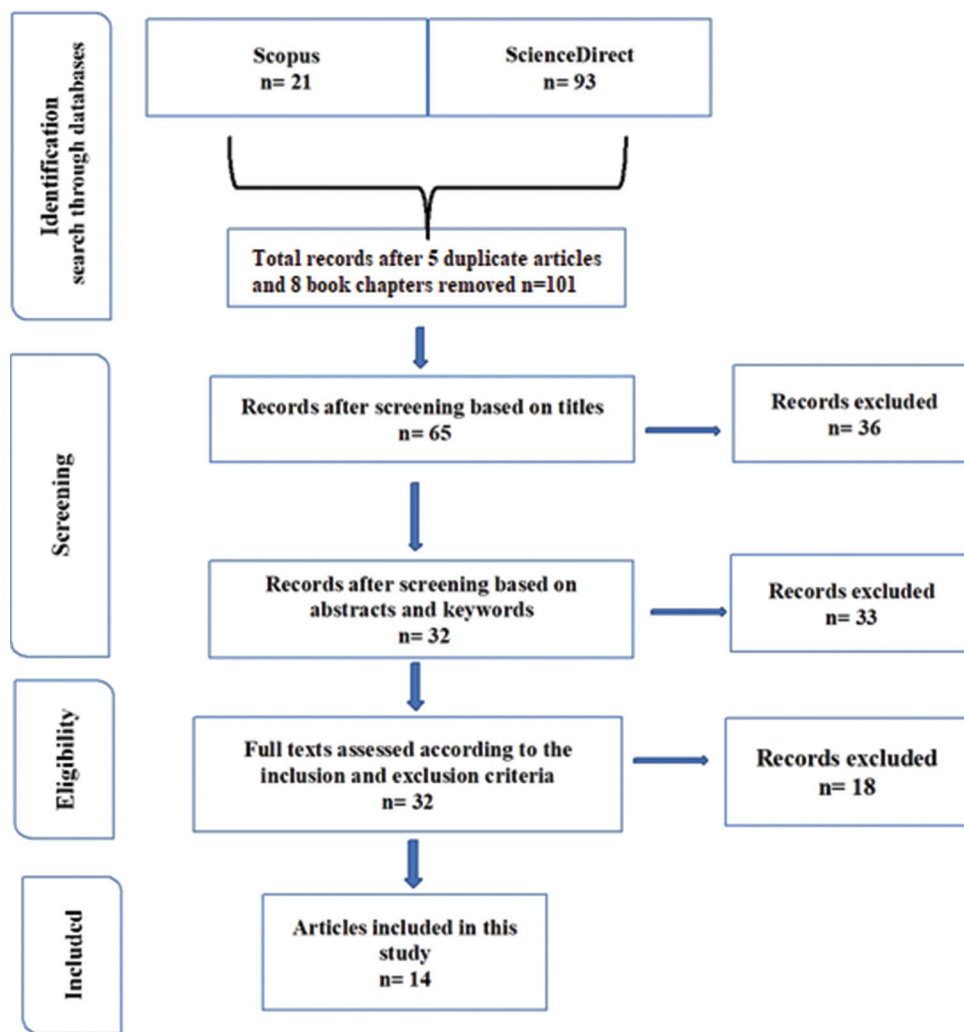


Figure 1: Flow Diagram of the paper selection process according to PRISMA Methodology

biomass partitioning in the four main parts of wheat: root, heat, leaf and stem (Holzworth *et al.*, 2018).

Overall Description of the General Results

Through an extensive examination of published studies, we sought to identify common approaches utilized by modelers in calibrating the APSIM-Wheat model, with a specific focus on the input data and statistical metrics employed. The final database included 14 articles, published between 1998 and 2015, yielding 31 calibration datasets collected from diverse locations around Western Australia (WA) (Table 1). Field experiments included in the present study occurred at 11 locations (Table 1), representing four regions across WA: Wheatbelt, South West, Goldfields and Midwest, as shown in Table 1. Wheatbelt is the most represented region with 23 datasets (Table 1). However, the most representative locations are Wongan Hills, Esperance, Moora and Buntine with seven, five, four and four calibration protocols respectively.

Building upon these observations, our examination of the calibration datasets further revealed the utilization of seven

distinct types of variables for testing the validation of the model calibration (Table 1). Yield is the most tested variable (68%), and other variables comprise Biomass, Phenology, grain protein, N uptake, soil water content and Plant Available Water Capacity (PAWC). A significant portion of the papers reviewed (42.8%) cover topics related to water use efficiency, 28.5 percent of those articles are dedicated to the evaluation of the performance of APSIM-Wheat, 14.3 percent deal with topics related to Nitrogen management and 14.3 percent are focused on ecosystem services (Table 1).

Input Data Description

The success of the applicability of a novel model in a new geographic region requires the identification and implementation of appropriate and reliable data (Aggarwal, 1995). As highlighted by Klepper and Rouse (1991), the quality of input data affects the model outcomes. The input interface of the APSIM Wheat model is composed of three main categories of data: daily weather records, soil properties and crop management information (Archontoulis *et al.*, 2014). In this review, we analyzed datasets from Western Australia to

Table 1: List of datasets extracted from selected papers used in this study

Dataset No.	Region	Location	Variable to test	APSIM Use	References
1	Wheatbelt	Moora	Yield	Water and nitrogen use efficiency	Asseng <i>et al.</i> , 2001
2	Wheatbelt	Wongan Hills	Yield	Water and nitrogen use efficiency	Asseng <i>et al.</i> , 2001
3	Wheatbelt	Merredin	Yield	Water and nitrogen use efficiency	Asseng <i>et al.</i> , 2001
4	Not Specified	WA	Yield	Sustainable intensification, ecosystem services, food security	Bryan <i>et al.</i> , 2014
5	Wheatbelt	Buntine	Biomass and yield	Sacrificing a wheat crop for grazing rather than harvesting it for grain	Bell <i>et al.</i> , 2009
6	Wheatbelt	Moora	Soil water content	Water use efficiency	Dolling <i>et al.</i> , 2006
7	Wheatbelt	Wongan Hills	Soil water content	Water use efficiency	Dolling <i>et al.</i> , 2006
8	South West	Katanning	Soil water content	Water use efficiency	Dolling <i>et al.</i> , 2006
9	Wheatbelt	Buntine	Yield	Water use efficiency	Lawes <i>et al.</i> , 2009
10	Wheatbelt	Buntine	Yield	Water use efficiency	Lawes <i>et al.</i> , 2009
11	Wheatbelt	Bodallin	Yield	Water use efficiency	Oliver & Robertson, 2013
12	Goldfields	Neridup	Soil water content	Water use efficiency	Robertson <i>et al.</i> , 2005
13	Goldfields	Mt Madden	Soil water content	Water use efficiency	Robertson <i>et al.</i> , 2005
14	Goldfields	Wittenoom Hills	Soil water content	Water use efficiency	Robertson <i>et al.</i> , 2005
15	Goldfields	Scaddan	Soil water content	Water use efficiency	Robertson <i>et al.</i> , 2005
16	Goldfields	Esperance Downs Research Station	Soil water content	Water use efficiency	Robertson <i>et al.</i> , 2005
17	Wheatbelt	Wongan Hills	Yield	Nitrogen Management	Monjardino <i>et al.</i> , 2015
18	Wheatbelt	Buntine	Yield, PAWC	Water use efficiency	Oliver <i>et al.</i> , 2006
19	Wheatbelt	Beverley	Biomass and yield	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 1998
20	Wheatbelt	Merredin	Biomass and yield	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 1998
21	Wheatbelt	Moora	Biomass and yield	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 1998
22	Wheatbelt	Wongan Hills	Biomass and yield	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 1998
23	Wheatbelt	Cunderdin	Grain protein	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 2002
24	Wheatbelt	Wongan Hills	Grain protein	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 2002
25	Wheatbelt	Cunderdin	Phenology, biomass and yield	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 2004
26	Wheatbelt	Wongan Hills	Phenology, biomass and yield	Evaluation of the performance of APSIM-Wheat	Asseng <i>et al.</i> , 2004
27	Wheatbelt	Beverley	Biomass, yield and N uptake	Evaluation of the performance of APSIM-Wheat	Wang <i>et al.</i> , 2003b
28	Wheatbelt	Merredin	Biomass, yield and N uptake	Evaluation of the performance of APSIM-Wheat	Wang <i>et al.</i> , 2003b
29	Wheatbelt	Moora	Biomass, yield and N uptake	Evaluation of the performance of APSIM-Wheat	Wang <i>et al.</i> , 2003b
30	Wheatbelt	Wongan Hills	Biomass, yield and N uptake	Evaluation of the performance of APSIM-Wheat	Wang <i>et al.</i> , 2003b
31	Mid West	Three Springs	Yield	Water use efficiency	Wong & Asseng, 2006

identify important information used by modelers as input data when the APSIM model is successfully calibrated and performed optimally, delivering reliable results.

Meteorological data

The first major group of model input data concerns the climate. These data represent an essential pillar for building model simulations and understanding the dynamics of agroecosystems (Hoffmann *et al.*, 2015). In this review, the evaluation of 31 datasets shows the use of the same weather data for model inputs (Table 2) relating to the daily maximum and minimum air temperature, rainfall (mm), and solar radiation. Usually, these data are recorded by weather stations close to the field

experiments. Additionally, in some very limited cases, the evapotranspiration parameter is given (Bryan *et al.*, 2014).

Soil data

The second major group of model parameters concerns the edaphic data. Soil characteristics are fundamental to initiate crucial functions in the model that rely on the information related to important properties such as soil texture, soil water retention and plant available water (Cichota *et al.*, 2021). Soil type is the parameter we find in all datasets. Depending on the model used, detailed information about soil type, such as color and texture is provided. The second main category of soil properties is the soil hydraulic characteristics, which include

Table 2: Description of input data used in calibration protocols extracted from selected papers

Number of dataset	Soil data	Climate data	Management data	References
3	Soil type/LL, DUL/PAWC	Historical daily weather data (T, rain and radiation)	Sowing date, sowing depth, plant density, cultivars, N fertilizer applications	Asseng <i>et al.</i> , 2001
1	Soil type/soil water holding capacity	Historical daily weather data (T, rain and radiation)	Fertilization and residue management	Bryan <i>et al.</i> , 2014
1	Soil type/PAWC	Historical daily weather data (T, rain and radiation)	Sowing date, sowing depth, plant density, row spacing, cultivars, N fertilizer applications, SOM	Bell <i>et al.</i> , 2009
3	Soil type/volumetric soil water fraction (θ_v)/LL/DUL	Historical daily weather data (T, rain and radiation)	Sowing date/N fertilization	Dolling <i>et al.</i> , 2006
2	Soil type/pH, EC, NO ₃ , NH ₄ , P, K and S, CLL, DUL/PAWC	Historical daily weather data (T, rain and radiation)	Sowing date/Applied N (Kg/ha)/crops cultivated	Lawes <i>et al.</i> , 2009
1	Soil type/ph, Nh ₄ , No ₃ , PAWC	historical daily weather data (T, rain and radiation)	Sowing date/Applied N (Kg/ha)/crops cultivated/cultivars	Oliver & Robertson, 2013
5	Soil type/DUL/PAWC/CLL/SAT	Historical daily weather data (T, rain and radiation)	Crop sequences/cultivars/sowing date/density/fertilizer applied (N: P: K)	Robertson <i>et al.</i> , 2005
1	Stype/soil water holding capacity	Historical daily weather data (T, rain and radiation)	Sowing date/sowing density/Applied N (Kg/ha)	Monjardino <i>et al.</i> , 2015
1	Soil type/PAWC/CLL/DUL	Historical daily weather data (T, rain and radiation)	Applied N (Kg/ha)	Oliver <i>et al.</i> , 2006
4	Soil type/LL, DUL/OC (organic matter)	Historical daily weather data (T, rain and radiation)	Applied N (Kg/ha)/sowing date/sowing density/deep ripping.	Asseng <i>et al.</i> , 1998
2	Soil type/RD/PAW	Historical daily weather data (T, rain and radiation)	Applied N (Kg/ha)/irrigation/sowing date/plant density	Asseng <i>et al.</i> , 2002
2	Not specified	Not specified	Not specified	Asseng <i>et al.</i> , 2004
4	Not specified	Not specified	Not specified	Wang <i>et al.</i> , 2003b
1	Soil type/PAWC/Root depth/maximum soil electrical conductivity	Historical daily weather data (T, rain and radiation)	Crop sequences/cultivars/sowing date/density/applied N (Kg/ha)	Wong & Asseng, 2006

these essential parameters: plant available water capacity (PAWC) which indicates the maximum amount of water that can be used by a plant, at the lower limit (LL) and the drained upper limit (DUL) of soil water availability.

These two categories of soil data are included in 100 percent of datasets. The final category of soil data included other parameters such as bulk density, organic matter, pH, soil Nitrogen (e.g., NO₃, NH₄) and soil's electrical conductivity. These data are used less often by the modelers, which indicates they are less important data for calibration.

Agricultural management data

The final major group of model parameters concerns crop management. Data for these parameters includes information about crop growth such as tillage, irrigation and nutrient supply (Wolday & Hruy, 2015). These data have an important impact on some critical model outputs such as the yield variations. For management practices, in all datasets we noticed that the major inputs are cultivated crops, the Nitrogen fertilization (rate and time of application) and the sowing date. Other data, such as cultivars, row spacing, and sowing depth, are mentioned less.

Statistical Metrics for Model Performance Assessment

The statistical evaluation of the model performance is an important part of the calibration protocol (Yang *et al.*, 2014). This evaluation involves the quantitative checking of the model by comparing simulated and observed values through the calculation of different statistical scores (Seidel *et al.*, 2018). It is a vital step in the calibration process as it guarantees that

the simulation results align with the observed values (Bellocchi *et al.*, 2011). Statistical scores utilized in the present review are indicated in Table 3. The indicators identified are the regression function; Spearman's non-parametric correlation test with bootstrapping; cumulative distribution function, the root-mean-squared error (RMSE), the root-mean-square deviation (RMSD) and R². Among the six indicators identified, we noticed that in 90 percent of the calibration protocols (26 datasets) (Table 3) modellers used the Root Mean Square (RMS) to calculate the magnitude of errors in simulation between estimates or predicted values, and measurements or observed values.

Accordingly, statistical assessment of the outputs reliability is recognized as an essential and fundamental step in the calibration process of any simulator including APSIM (Wallach *et al.*, 2022). However, there is no consensus on the exact number and the type of metrics that should be implemented. Yang *et al.* (2014) highlighted that quantitative analysis of data is an integral part of the tuning procedure, but there is no standard guide on how many, and which, statistics should be used. In the case of the application of the APSIM-Wheat, our review shows that the RMS is preferred by the modellers and it can be applied in association with other parameters, such as R². These findings are in line with previous research, since they used the APSIM-wheat model to simulate different wheat variables (e.g. phenology, Nitrogen Uptake, yield) and they evaluated the model performance using the RMS in addition to other metrics such as R². Moreover, it has been proven that this metric is applicable when evaluating the performance of the model to deliver reliable simulation outcomes in very specific topics such as the impact of the environment on the wheat Kernel Weight (Wang *et al.*, 2023b).

Table 3: Summary of statistical indices used for the validation of the calibration process

References	Number of datasets	Statistic metrics	Appreciation of model performance
Asseng et al., 2001	3	Regression function	APSIM-Wheat is able to markedly predict potential yields
Bryan et al., 2014	1	Spearman's non-parametric correlation test with bootstrapping	Not informed
Bell et al., 2009	1	RMSD	APSIM-Wheat simulated wheat biomass and grain yield well
Dolling et al., 2006	3	RMSD	Not informed
Lawes et al., 2009	2	RMSE, R ²	Generally, the model performed well across multiple years and soil types
Oliver & Robertson, 2013	1	RMSE	Not informed
Robertson et al., 2005	5	Cumulative distribution function	Increased confidence has been gained in the use of simulation models such as APSIM-Wheat as a means to evaluate effects on cropping system performance.
Monjardino et al., 2015	1	RMSE	The model explained 65% of the variation in yield, RMSE=0.6 t/ha
Oliver et al., 2006	1	RMSD	RMSD=0.5 t/ha
Asseng et al., 1998	4	RMSD/R ²	The overall performance of the APSIM-Wheat model was good
Asseng et al., 2002	2	RMSD	The improved model is robust enough to be used for specific simulation experiments to study grain protein interactions with management, soil types and environments in different climatic zones.
Asseng et al., 2004	2	RMSD/R ²	APSIM-Wheat reproduced observed phenology, biomass growth and yield adequately.
Wang et al., 2003a	4	RMSD	APSIM-Wheat is able to explain >65% of the biomass and yield variation, and it is able to explain >75% of variation in total N uptake
Wong & Asseng, 2006	1	RMSE	APSIM model adequately simulates yield variability across the field

Based on the results of the statistical analysis from all calibration protocols reviewed (Table 3), all simulations of different variables were performed with a high level of accuracy. In other words, the reliability of model outcomes was proven in all studies (Table 3), regardless of the objective of the use and application of APSIM-Wheat. Given its demonstrated performance in WA, our review highlights that the APSIM-Wheat model is recognized as a robust model which can be applied and adapted confidently in other regions that are characterized by similar climatic conditions, particularly Mediterranean areas (Asseng et al., 2002). In the literature, numerous publications that covered various studies conducted in regions outside Western Australia indicate RMS as a statistical tool for evaluating the goodness of the APSIM model (Briak & Kebede, 2021; Tahir et al., 2021). In line with this, in a study conducted in Pakistan addressing the impact of cropping systems on the yield gaps of the rice-wheat system, (Khaliq et al., 2019) used RMSE to validate the model applied.

CONCLUSION

The extent to which agricultural models contribute to the increase and improvement of scientific knowledge, as well as the degree to which their outcomes can be considered reliable and accepted by users, essentially depends on the calibration and validation step. Although the APSIM model has been widely used to advance knowledge on agricultural and environmental issues, similar to other crop models, its performance depends on the quality of the calibration validation process, the dataset incorporated into the model, and the statistical assessment adopted to validate the model. This review provides a case study

focussing on the APSIM-Wheat model in Western Australia. It analyses 31 protocols of calibration, highlighting the minimum required data and the most used statistical metrics to verify the goodness of APSIM-Wheat. In addition, the study shows that meteorological data (daily maximum and minimum air temperatures, rainfall (mm), and solar radiation), soil data (information about the texture and hydraulic characteristics) and agricultural management data (cultivated crops and Nitrogen fertilization) are reported in all datasets. For the statistical evaluation, it was observed that among the six indicators identified, 90 percent of studies analyzed in this review revealed the use of RMSE as a statistical metric to evaluate to which degree observed results fit the simulated ones, therefore the modelers validate the performance of the model and use it confidentially to analyse and study different scenarios. These findings are in line with other studies conducted around the world, not only in Western Australia which reported the use of RMSE for testing and validating the performance of the APSIM model. The results of this synthesis can serve as a guide for future users of the APSIM-Wheat model, especially in areas characterised by the same climate and soil conditions as WA to ensure the success of the calibration validation step.

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