

Bayesian Model Averaging for Estimating Evapotranspiration and Water Footprint in Wheat Cultivation

Arezoo Kazemi¹, Zahra Aghashariatmadari^{1*}

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Abstract

Water resource management is of utmost importance in arid and semi-arid regions. The incorporation of the water footprint (WF) concept, which connects various water-consuming sectors in crop production, serves as a practical tool for water sector policies. The accuracy of three crop models (CropSyst, DSSAT, and SSM-Wheat) in estimating evapotranspiration (ET) was compared with the FAO Penman-Monteith (FAO56) reference model. Subsequently, the Bayesian model averaging (BMA) approach was employed to integrate the models. The application of the BMA approach resulted in a reduction of the Normalized Root Mean Square Error (NRMSE) in comparison to the individual models. Moreover, the coefficient of determination (R^2), Nash-Sutcliffe efficiency (EF), and Kling-Gupta efficiency (KGE) achieved values of 99%, 0.99, and 0.96, respectively. In the subsequent step, the WF was calculated based on the yield and evapotranspiration values. The findings revealed that the green WF exceeded the blue WF in most fields, primarily due to sufficient rainfall in the area during the growth period, which allowed the plants to utilize soil moisture. Consequently, the pressure on soil moisture (effective rainfall) surpassed that on blue water. The objective of this study was to calculate the WF of wheat in Gorgan, Iran and the results highlight the requirement of effective crop management strategies to achieve a balance in water consumption, thereby minimizing the blue WF and maximizing yield. For instance, modifying the planting date to align with rainfall during the growth period can significantly reduce the blue WF.

Keywords: Crop modelling, Virtual water, Water policy, Water demand

Introduction

Access to water is a fundamental consideration in the establishment of advanced civilizations and plays a critical role in global development. The increasing depletion of

freshwater resources, driven by population growth, economic advancement, and climate change, necessitates a heightened focus on water harvesting in the upcoming decade.

¹Irrigation and Reclamation Engineering Department, University College of Agriculture and Natural Resources, University of Tehran, Karaj, Iran

*Corresponding author email address: zagha@ut.ac.ir

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To ensure effective water resource management, thorough studies of water resources are essential. Notably, the agricultural sector consumes over 85% of global freshwater resources (D'Odorico et al. 2020), underscoring the need for a comprehensive evaluation of water availability. While access to water is recognized as a fundamental human right, the rising demand for this vital resource calls for the application of concepts such as the water footprint (WF), introduced by Hoekstra (2002), to assess freshwater utilization in terms of quantity, timing, and location.

The WF of a crop represents the volume of freshwater used in its production, encompassing the entire supply chain (Hoekstra et al. 2009). Virtual water trade and footprint studies have been conducted across different geographical scales, ranging from local to global. The WF serves as an appropriate method for estimating the international flow of water through the trade of goods. Water trade plays a vital role in national policy and food security matters. Importing crops that have high water requirements instead of relying solely on domestic production helps conserve water resources within a region.

Arunrat et al. (2022) assessed the implications of climate change on the yield and water footprint (WF) of key crops in Thailand's drought- and flood-prone areas, utilizing climate projections from the Coupled Model Intercomparison Project Phase 6 (CMIP6). Their study revealed an expected increase in precipitation, as well as maximum and minimum temperatures, highlighting that substituting rice with crops like corn, soybeans, or mung beans could mitigate climate-related impacts. Moreover, implementing

twice-yearly corn cultivation and cassava planting could enhance agricultural viability in rainfed areas. Notably, the WFs of these alternatives were approximately half that of rice, designating them as viable options in the region.

The research conducted by Wang et al. (2022) revealed significant findings regarding the impact of plastic mulch on the agricultural water footprint within various crop systems. By analyzing data from 394 published studies on corn, wheat, and potatoes, the study determined that the implementation of plastic mulch resulted in notable reductions in volume of available water (VWA), global water footprint weighted by stress per unit of energy output (WFO), and water footprint per unit of net economic efficiency in crop production (WFE). Specifically, VWA decreased by 15.3% for corn, 14.1% for wheat, and 16.3% for potatoes, with corresponding reductions in WFO and WFE. Similarly, Deihimfard et al. (2022) assessed future climate implications on water footprint metrics for rainfed and irrigated wheat in Iran, predicting a decrease in total water footprint alongside an increase in the gray water footprint under future scenarios. Both studies underscore the potential for enhanced water resource management through strategic agricultural practices.

Iran, characterized by mean annual rainfall of approximately 250 mm—less than one-third of the global average—faces significant water resource challenges due to its classification as a dry and semi-arid region (Dehaghani et al., 2023). The distribution of rainfall varies significantly across the country, exacerbated by a rising population and

increasing demand for water across multiple sectors. Consequently, effective management of water resources is imperative, tailored to the existing water potential. The Water Footprint (WF) index provides insight into actual water consumption relative to regional climatic conditions, enabling a nuanced study of virtual water trade within the agricultural sector. By analyzing the interplay between climate, crop production, water consumption, and WF, stakeholders can enhance their understanding of policies and foster more efficient planning for sustainable water resource management in Iran. In the current study, an investigation was conducted to assess the individual capabilities of the DSSAT, CropSyst, and SSM-Wheat models in calculating evapotranspiration. Subsequently, the collective abilities of the models obtained through the BMA method in estimating evapotranspiration (ET) were analyzed. Furthermore, the blue and green water footprints (WFs) were calculated for the studied fields based on the output of both the individual crop models and the BMA models.

Material and methods

This study was conducted in Golestan

province, which is located in the northeast of Iran. The geographical location of Golestan province, including the meteorological station and the selected farms is illustrated in Figure 1.

Data source

Wheat yield simulation using the CropSyst, DSSAT, and SSM-wheat models requires accurate data. Given the limited availability of field study data, we have utilized data from field experiments carried out at Gorgan University of Agricultural Sciences and Natural Resources for the Koohdasht, Tajan, and Zagros wheat varieties during the years 2007-08 and 2008-09 (Table 1).

The daily meteorological data for the Hashem Abad synoptic station was obtained from Iran's National Meteorological Organization. This data includes information on maximum and minimum air temperature, relative humidity, rainfall, wind speed, and sunshine hours. The station experiences an annual minimum temperature of -10°C and a maximum temperature of 45°C . Based on a 30-year average, the station receives an average annual precipitation of 527.4 mm. According to the Köppen climate classification, the station has a moderate and humid



Fig. 1. Location of study farms and research stations

climate (Salarieh et al., 2021). The fields under study have a soil texture of silty clay loam, and the experiments were conducted under normal water and nitrogen conditions. Additionally, effective management of pests, diseases, and weeds was carried out during the experiments.

WF (Water Footprint)

The WF_{total} in the crop growing process (WF_{proc}) includes the sum of blue, green, and gray components (Hoekstra et al. 2009).

$$WF = WF_{green} + WF_{blue} + WF_{gray} \quad [1]$$

Where WF_{Blue} is blue water footprint, WF_{green} is green water footprint and WF_{gray} is gray water footprint which determines the volume of water employed to eliminate pollution created by plant cultivation and crop production in the environment. The WF during the growth process is expressed in terms of production units, i.e. water volume per mass (m^3/ton , which equals Lit/kg).

In this study, by entering the required data in selected crop models (DSSAT, SSM-wheat and CropSyst), wheat evapotranspiration and yield during the growing season were

calculated. A summary of the research process is shown in Figure 2. Finally, The WF is calculated in the form of Equations (2-4) (Ventrella et al. 2015).

$$WF_{green} = \frac{GW}{Y_{irr}} \quad [2]$$

$$WF_{blue} = \frac{BW}{Y_{irr}} \quad [3]$$

$$WF_{total} = WF_{irr} = WF_{green} + WF_{blue} = \frac{GW+BW}{Y_{irr}} \quad [4]$$

Where GW includes the volume of effective rainfall stored as moisture in the soil to be used by plants for crop production (m^3/ha), BW is considered as the water applied from surface and underground sources (m^3/ha) and Y_{irr} (ton/ha) represents the overall yield of the plant in irrigated condition (irrigation is applied in addition to rainfall).

BMA (Bayesian model averaging)

The BMA method combines the probability density function (pdf) of the predictions of different models and creates a weighted prediction distribution from them. Neuman (2003) proposed a maximum likelihood version (MLBMA) of BMA to render it computationally feasible and to allow dealing with cases where reliable prior information

Table 1. Properties of the surveyed farms

Field ID	Cultivar	planting density		References
		(grains per square meter)	Planting date	
1	Koohdasht	350	2008/1/30	(Dastmalchi et al. 2012)
2	Koohdasht	350	2007/12/29	
3	Koohdasht	350	2008/2/27	
4	Koohdasht	300	2008/12/20	(Ghadiryman
5	Tajan	300	2008/12/20	2011)
6	Tajan	350	2008/1/30	(Dastmalchi et
7	Zagros	350	2008/2/27	al. 2012)

is lacking. Here, BMA method was applied to combine crop models to increase accuracy in estimating wheat yield and WF. BMA is considered as an approach to combine the densities predicted by different models and generate a new prediction of their PDF. BMA method works on a dependent variable y , the training data y_t , and the sum of all predictions for members $X\{x_1, x_2, x_3, \dots, x_k\}$, where y is related to crop models and K represents the number of models. Based on the probability rule of sum, the PDF can display as equation [5] (Chen et al. 2015; kazemi et al. 2021).

$$p(y|x_1, x_2, \dots, x_k) = \sum_{k=1}^k g(y|\theta_k) \cdot w_k \quad [5]$$

Where g refers to the Gaussian distribution, $\theta_k = \{\mu_k, \sigma_k, k=1, \dots, k\}$ is the parameter vector, and W_k is statistical weight. W_k Shows the amount of correspondence between X_k and Y_T and the sum of weights of all models is 1 ($\sum_{k=1}^k w_k = 1$).

In equation (6) the Bayesian model to calcu-

late yield from selected crop models in Golestan province is represented (Kazemi and Aghashriatmadari 2022).

$$BMA_{Best} = 0.627 Y_{DSSAT} + 0.373 Y_{SSM} \quad [6]$$

Where Y_{DSSAT} and Y_{SSM} are wheat yields calculated from DSSAT and SSM-Wheat crop models.

Evaluation: verification and validation

To evaluate the accuracy of the models in estimating the evapotranspiration, R^2 , RMSE, NRMSE, EF, and KGE indicates were employed.

$$R^2 = \left(\frac{n(\sum O_i S_i) - (\sum O_i)(\sum S_i)}{\sqrt{[n \sum O_i^2 - (\sum O_i)^2][n \sum S_i^2 - (\sum S_i)^2]}} \right)^2 * 100 \quad [7]$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (S_i - O_i)^2} \quad [8]$$

$$NRMSE = \frac{RMSE}{\bar{O}_i} * 100 \quad [9]$$

$$EF = 1 - \frac{\sum_{i=1}^n (S_i - O_i)^2}{\sum_{i=1}^n (O_i - \bar{O}_i)^2} \quad [10]$$

Where O_i, \bar{O}_i, n , and S_i indicate the observed

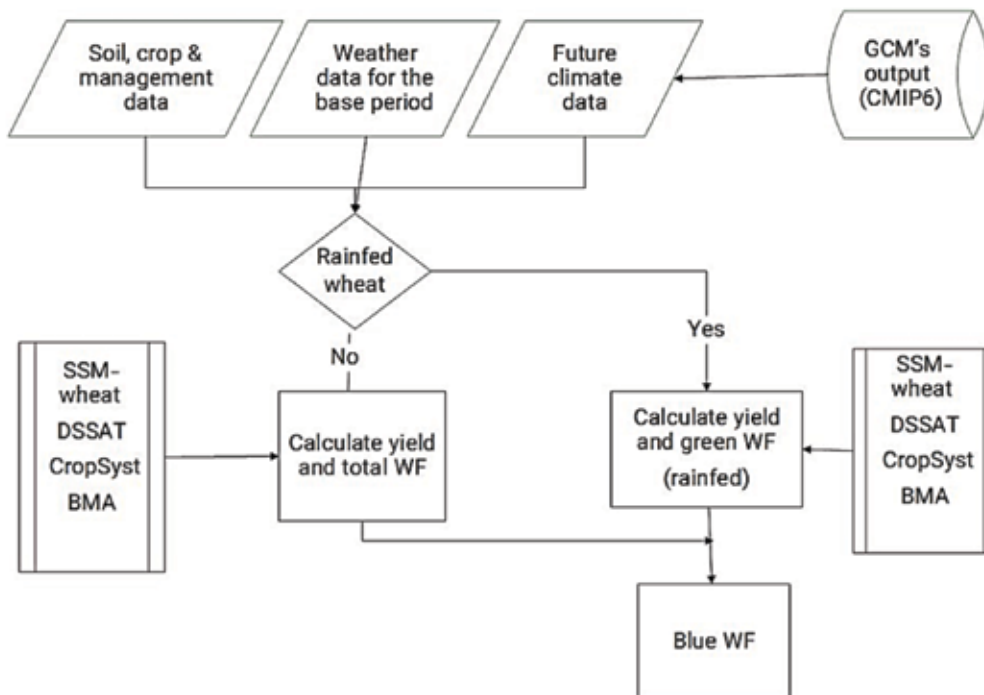


Fig. 2. Water footprint calculation flowchart (Kazemi., 2022)

values, average of the observed values, number of observations, and simulated values, respectively.

The Kling–Gupta efficiency (KGE) is a goodness-of-fit indicator that was used to comprehensively evaluate the efficiency of the models, which is calculated based on Equations (11-14) (Knoben et al. 2019).

$$KGE=1-ED \tag{11}$$

$$ED=\sqrt{(r-1)^2+(\alpha-1)^2+(\beta-1)^2} \tag{12}$$

$$\alpha=\frac{\sigma_s}{\sigma_o} \tag{13}$$

$$\beta=\frac{\mu_s}{\mu_o} \tag{14}$$

Where ED is Euclidean distance from the ideal point, and r is correlation coefficient between simulations and observations. In addition, μ_o and σ_o represent the mean and standard deviation (SD) of the observations, while μ_s and σ_s indicate the mean and SD of the simulations. The KGE ranges between -infinity and 1, where a value of 1 indicates perfect agreement between the model predictions and the observed data. The KGE

measures not only the accuracy of the model predictions but also its ability to reproduce the variability and timing of the observed data.

Results

ET calculating

The evapotranspiration (ET) calculated by the crop models and BMA-Best for rainfed conditions in the studied fields (Table 2). Previous studies have shown that the FAO-Penman-Monteith (FAO56) method is more accurate in estimating ET and its results are closer to lysimeter values. The International Commission on Irrigation and Drainage (ICID) and the Food and Agriculture Organization of the United Nations (FAO) have also recommended the FAO56 as the standard for comparing other models (Allen et al., 1998; Hargreaves, 1994). Therefore, the ET was calculated using the FAO56 model and used as a benchmark to compare the results of other models. The SSM-wheat and DSSAT models utilize the Priestley-Taylor (PT) method, while the

Table 2. ET values calculated by crop models for rainfed wheat (mm in the entire growth period)

ID	CropSyst	DSSAT	SSM	BMA-Best	FAO56
1	216	185	198	190	190
2	243	212	224	216	212
3	182	168	177	171	170
4	303	307	267	292	288
5	301	304	270	291	285
6	218	182	204	190	186
7	182	175	183	178	178

CropSyst model uses the Penman-Monteith (PM) method to calculate ET. The Table 2 presents the evapotranspiration values calculated by the crop models for rainfed wheat (mm) throughout the entire growth period. Furthermore, in Figure 3, the evapotranspiration estimated by the studied models is illustrated.

As indicated in Table 3, the SSM-Wheat model yields more accurate estimates of ET among the crop models, as evidenced by the NRMSE (6.18) and EF (0.92) indices. The DSSAT model achieves a higher R^2 value of 99.8 compared to the other models. However, its corresponding EF and NRMSE values are not considered satisfactory. The CropSyst model achieves a maximum KGE value of 0.91. Taking into account all evaluation indices, these models estimate ET with comparable accuracy, without a clear advantage over one another. Nevertheless, the BMA model outperforms the others, as indicated by all evaluation indices. In the BMA-Best model, the maximum R^2 value is 99.9, with an RMSE value of 3.5 mm throughout the entire growth period of wheat. This indicates a mere 3.5 mm error in ET calculation.

The optimal EF value is 1, while the BMA-Best model achieves an EF value of 0.99, highlighting its high efficiency. Overall, the BMA-Best model provides the most accurate ET simulation based on all evaluation indices. In a study conducted by Attarod et al. (2015) comparing radiation and temperature-based methods of ET estimation to the FAO56 method in Gorgan, the turk method was suggested as the best model with an R^2 value of 98%. However, by employing the BMA approach, the R^2 value increased to 99.9%.

Water footprint (WF)

The values of WF_{blue} and WF_{green} derived from crop models and BMA (Table 4). As mentioned previously, the BMA-Best method demonstrates the highest level of accuracy in estimating ET. Kazemi and Shariatmadari (2022), state that the BMA model outperforms individual models in accurately estimating wheat yield. Consequently, utilizing the BMA approach to calculate the water footprint, taking into account the precise amount of wheat yield and evapotranspiration, yields more accurate results.

Total water footprint (WF_{total}) calculated by

Table 3. Comparison of statistical indices for the evaluation of crop models and BMA model performance in estimating evapotranspiration

statistical index	CropSyst	DSSAT	SSM-Wheat	BMA-Best
R^2	95.79	99.83	97.02	99.91
RMSE (mm/plant season)	21.64	50.60	13.32	3.56
EF	0.78	-0.19	0.92	0.99
NRMSE	10.04	23.47	6.18	1.65
KGE	0.91	0.79	0.76	0.96

crop models and the BMA model, which is the sum of the blue water footprint and the green water footprint, is shown in Figure 4 (in this study the grey water footprint is neglected).

The WF_{blue} values for the studied models are presented side by side in Figure 5. According to the BMA-Best model, the WF_{blue} in the fields ranges from 96 to 561 millimeters. The Koohdasht variety was planted in fields 2 and 3. However, in field 2, which was planted on 29/12/2007 during a period of heavy rainfall and the potential for more rainfall usage, the WF_{blue} is approximately 100 millimeters lower compared to field 3, which was planted on 27/2/2008. Fields 1

and 6 were both planted on 30/01/2008 and managed similarly in terms of agronomics. Nevertheless, field 1 was planted with the Koohdasht variety, while field 6 was planted with the Tajan variety. This difference in varieties has resulted in variations in the water footprint for these fields. It can be concluded that the water footprint of the Tajan variety is higher compared to that of the Koohdasht variety. The calculated water footprint for fields 4 and 5 also supports this finding.

The quantity of WF_{green} for each assessed model is presented in Figure 6. According to the BMA-Best model, the amount of WF_{green} on farms ranges from 455 to 553 m^3 per ton. The highest value of WF_{green} , 553 m^3 per

Table 4. Blue and green WF values for irrigated conditions (m^3/ton)

Field ID	CropSyst		DSSAT		SSM-wheat		BMA-Best	
	WF_{green}	WF_{blue}	WF_{green}	WF_{blue}	WF_{green}	WF_{blue}	WF_{green}	WF_{blue}
1	506	286	457	427	451	455	455	437
2	558	285	441	371	492	163	460	296
3	470	284	495	482	422	289	464	400
4	468	170	472	115	497	58	480	96
5	519	169	524	122	579	249	541	163
6	553	289	557	498	548	521	553	507
7	446	331	456	559	480	564	465	561

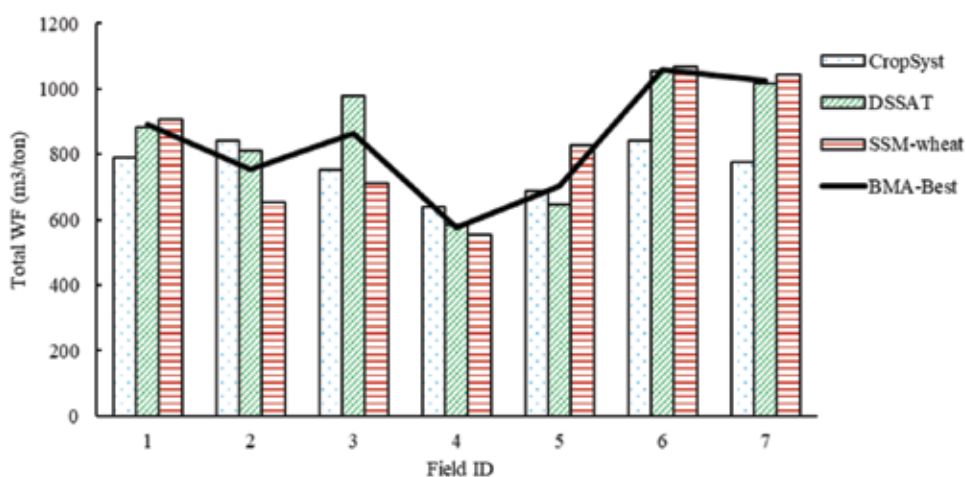


Fig. 4. Comparison of total WF calculated by individual crop models and BMA

ton, is associated with farm 6, which was cultivated on January 30, 2008, using the Tajan variety. Conversely, the lowest value is observed in farm 1, also cultivated on the same date but with the Koohdasht variety. Farms 4 and 5 have identical planting dates. However, farm 5, where the Tajan variety is planted, exhibits a higher amount of WF_{green} . Both farms 2 and 3 are cultivated using the Koohdasht variety. Nevertheless, farm 2, which was cultivated earlier on December 29, 2007, has a lower WF_{green} value. A comparison of the amounts of WF_{blue} , WF_{green} , and WF_{total} in the farms analyzed

using the BMA-Best model is illustrated in Figure 7. The highest WF_{total} , which accounts for the sum of WF_{blue} and WF_{green} , is observed in farm 6. This is attributed to the relatively later cultivation date (January 30, 2008) and the usage of the Tajan variety. On the other hand, farm 4 exhibits the lowest WF, primarily due to the cultivation of the Koohdasht variety and an earlier planting date (December 20, 2008) compared to the other farms. These findings indicate that the differences in WF among the farms can be related to variations in planting dates and wheat varieties.

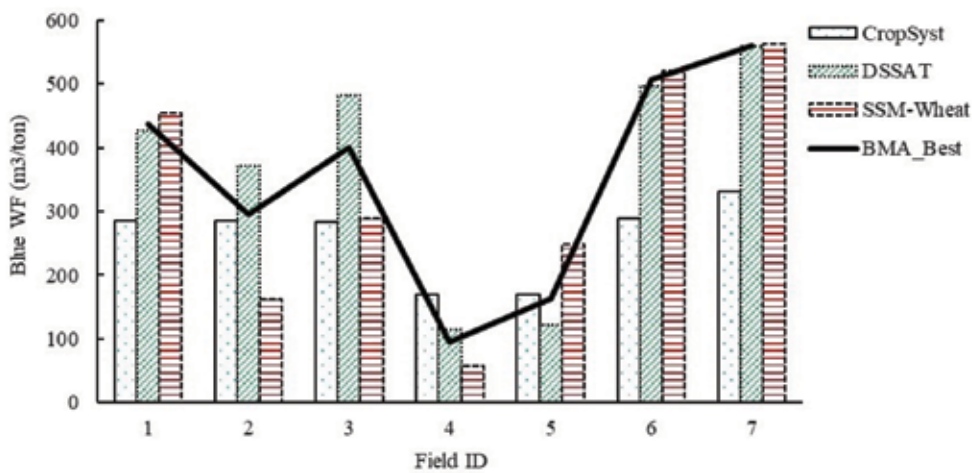


Fig. 5. Comparison of blue WF calculated by individual crop models and BMA

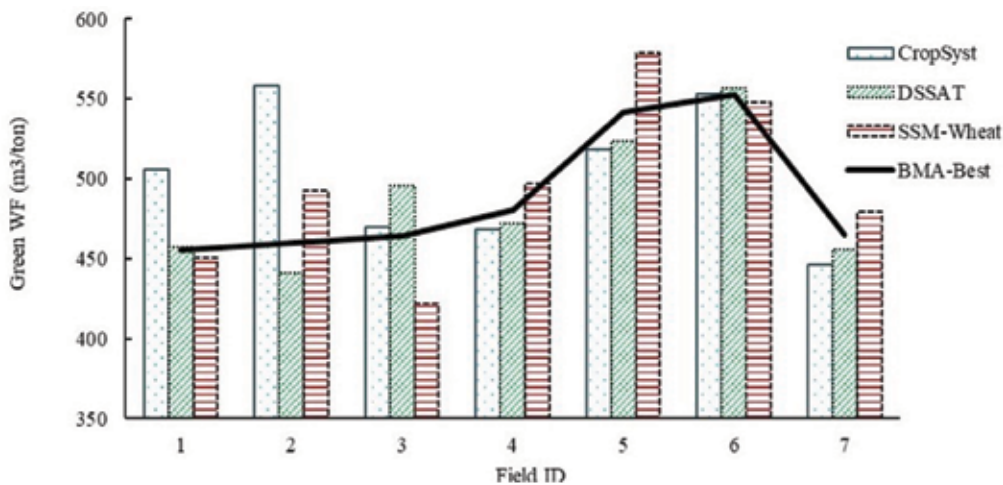


Fig 6. Comparison of green WF calculated by individual crop models and BMA

Based on the results, the WF_{green} is higher than the WF_{blue} in all farms except Farm 7, indicating that the pressure on soil moisture (effective rainfall) is greater than irrigation water for wheat production. In Farm 7, the late cultivation prevents the use of effective rainfall during the growth period, resulting in the need to compensate for the water requirement using blue water. These findings are consistent with previous studies in this field, highlighting the significant role of green water in wheat production. According to Anafajeh et al. (2020), the WF_{green} for wheat production is higher than the WF_{blue} in Khuzestan province. Additionally, Aligholinia et al. (2020) suggest that the highest

WF_{green} for wheat can be found in the northern and western parts of the country due to abundant rainfall in these areas.

As mentioned before, the main water requirement for wheat production in the farms is met through green water. However, the lack of blue water utilization leads to a decrease in yield. Therefore, careful planning is necessary to balance the use of blue water through supplementary irrigation in order to minimize the WF_{blue} and maximize yield.

The WF_{total} for wheat cultivation under WF_{irr} and $WF_{rainfed}$ conditions is presented in Figure 8. It can be observed that the WF for wheat cultivation under rainfed condition is higher than that under irrigated condition in

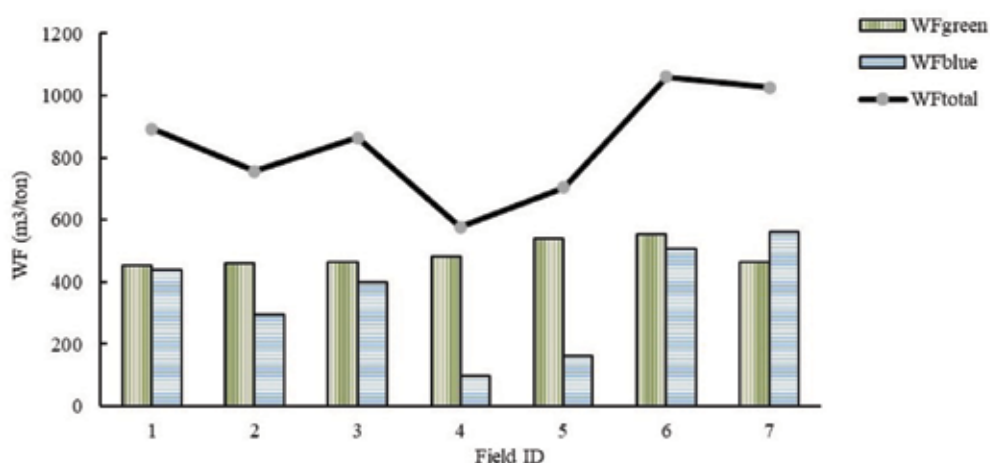


Fig. 7. Comparison of blue, green and total WF calculated by BMA-Best

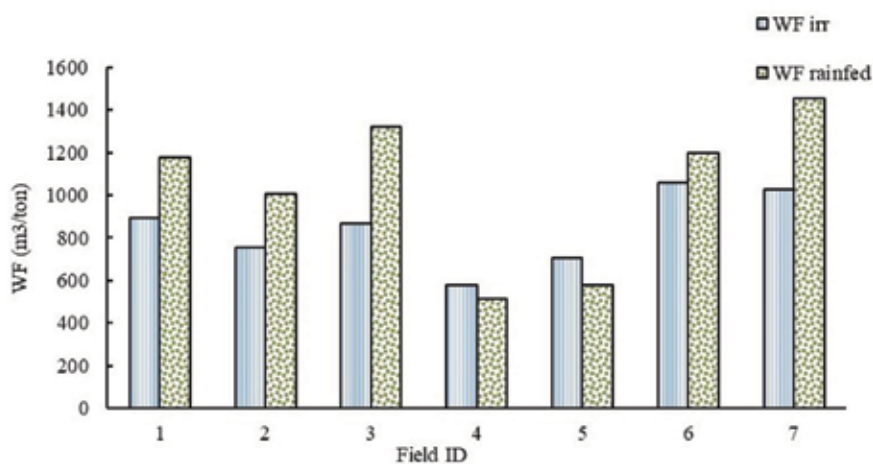


Fig. 8. Comparison of irrigated and rainfed wheat WF calculated by BMA-Best

all farms except Farms 4 and 5. The presence of irrigation increases yield compared to the rainfed condition in all mentioned farms, resulting in a decrease in the WF for wheat cultivation under irrigated condition compared to that under rainfed condition. Furthermore, Ababaei and Ramezani (2016) have argued that the WF_{total} of rainfed wheat is higher than that of irrigated wheat in Golestan province. Farms 4 and 5 have earlier planting dates, allowing for the use of rainfall. Irrigating these farms increases water consumption and the WF for irrigated wheat without increasing yield compared to the rainfed condition. In other words, their early planting, which allows for synchronization of the rainy season with the growing season, resulting in the plants' water needs being met through precipitation. In essence, irrigation does not contribute to an increase in wheat yield compared to rainfed conditions. Therefore, determining the appropriate planting date can be instrumental in conserving surface and underground water consumption.

Discussion

The present study assessed the accuracy of the crop models DSSAT, CropSyst, and SSM-Wheat, along with the BMA approach, in estimating ET (evapotranspiration). The evaluation was based on the NRMSE, R^2 , KGE, and EF indices, and the results were compared with those of FAO56, a standard method proposed by FAO (Allen et al. 1998; Hargreaves 1994). The findings indicate that all three investigated crop models estimate ET with similar accuracy, without any clear advantage of one model over the others.

However, the application of the BMA approach significantly enhances the accuracy of ET estimation. In the BMA-Best model, the values of NRMSE, R^2 , KGE, and EF were found to be 1.65, 99.9, 0.96, and 0.99%, respectively.

Moreover, the amount of WF (water footprint), including WF_{blue} and WF_{green} , for the studied farms was determined by utilizing the values of ET and yield calculated by the individual models under study and the BMA-Best. According to the outputs of the BMA-Best model, the farm cultivating the Tajan variety and planting it later than other farms had the highest WF. On the other hand, the farm cultivating the Koohdasht variety and planting it earlier than other farms had the lowest WF. Furthermore, WF_{green} was found to be higher than WF_{blue} in most farms. The cultivation date was identified as a crucial factor influencing the WF of the crop. For future studies, it is recommended to focus on comparing the ET estimated by the models to the lysimeter-based measurements.

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